Likelihood-free Model Choice for Simulator-based Models with the Jensen–Shannon Divergence

Jukka Corander  
Department of Mathematics and Statistics and Helsinki Institute of Information Technology (HIIT)  
University of Helsinki  
Pietari Kalmin katu 5, 00014 Helsinki Yliopisto, Finland  
Department of Biostatistics, Institute of Basic Medical Sciences  
University of Oslo  
Sognsvannsveien 9, 0372 Oslo, Norway  
Parasites and Microbes, Wellcome Sanger Institute  
Cambridge, CB10 1SA, UK

Ulpu Remes  
Department of Biostatistics, Institute of Basic Medical Sciences  
University in Oslo  
Sognsvannsveien 9, 0372 Oslo, Norway

Timo Koski  
Department of Mathematics and Statistics and Helsinki Institute of Information Technology (HIIT)  
University of Helsinki  
Pietari Kalmin katu 5, 00014 Helsinki Yliopisto, Finland  
KTH Royal Institute of Technology  
Lindstedtsvägen 25, 100 44 Stockholm, Sweden

Editor: NN

Abstract

Choice of appropriate structure and parametric dimension of a model in the light of data has a rich history in statistical research, where the first seminal approaches were developed in 1970s, such as the Akaike’s and Schwarz’s model scoring criteria that were inspired by information theory and embodied the rationale called Occam’s razor. After those pioneering works, model choice was quickly established as its own field of research, gaining considerable attention in both computer science and statistics. However, to date, there have been limited attempts to derive scoring criteria for simulator-based models lacking a likelihood expression. Bayes factors have been considered for such models, but arguments have been put both for and against use of them and around issues related to their consistency. Here we use the asymptotic properties of Jensen–Shannon divergence (JSD) to derive a consistent model scoring criterion for the likelihood-free setting called JSD-Razor. Relationships of JSD-Razor with established scoring criteria for the likelihood-based approach are analyzed and we demonstrate the favorable properties of our criterion using both synthetic and real modeling examples.
1. Introduction

A research field of increasing popularity deals with simulator-based models that lack an expression for the likelihood of data and consequently require likelihood-free inference approaches to be used for model fitting; for a recent comprehensive overview see Cranmer et al. (2020). In one of the pioneering works dealing with likelihood-free inference, such a model and its likelihood function were called *implicit* Diggle and Gratton (1984). In contrast, a model with explicit likelihood is a *prescribed* statistical model. The different simulator-based models share the basic idea to adjust the parameters by finding values which yield outputs that resemble the observed data, which raises the issue of the assessment of the discrepancy between the observed and simulated data. Considerable advances have been made in how such discrepancy can be converted into approximate likelihood or used to obtain samples from the corresponding posterior distribution of model parameters, however, the question of how to appropriately adjust the discrepancy for changes in model complexity/dimension have been given much less attention in likelihood-free inference research. Largely only the use of Bayes factors in the context of Approximate Bayesian Computation (ABC) have obtained a serious consideration, see Beaumont (2019), Didelot et al. (2011), Leuenberger and Wegmann (2010), Marin et al. (2018) and Robert et al. (2007).

In related work Corander et al. (2021), we studied the discrepancy between the observed and simulated data as measured by the (symmetric) Jensen–Shannon divergence (JSD). It was shown that the asymptotic properties of JSD can be succinctly used to derive estimators, confidence intervals and hypothesis tests for implicit models with categorical output distributions. Here we develop the theory further to obtain an information-theoretically inspired model scoring criterion for such implicit models that can be used for solving the model choice problem in a consistent manner. We restrict to simulator-based models that emit categorical data, as such data has been the main field of application of the method, see (Corander et al., 2017).

Our method of model choice is a modification of Occam’s Razor as developed by Balasubramanian and co-workers in Balasubramanian (2005), Balasubramanian (1996) and Myung et al. (2000). Occam’s Razor is based on an intuitive geometric interpretation of the meaning of complexity in model selection. To cite Balasubramanian (1996), complexity measures the ratio of the volume occupied by distinguishable distributions in a model that come close to the truth relative to the volume of the model as a whole. Briefly stated, our modification is to replace the Kullback Leibler divergence in Occam’s Razor with the Jensen–Shannon divergence and correspondingly call the result a JSD-Razor. Minimization of \(-\frac{1}{2} \log \text{JSD-Razor}\) leads to a criterion that can be used to ranking simulator-based models with respect to the fidelity of their simulation outputs, such that the complexity of the model is accounted for. Asymptotic analysis of the logarithm of JSD-Razor leads to two criteria for model choice, where the observed fit of a model is in terms of minimized JSD additively penalized. There are two expressions of penalty, the more subtle one is accounting for the complexity of the models in the sense of the geometric interpretation, but is not readily computable.

Model choice between prescribed models has been extensively studied by a number different approaches, see, e.g., Atkinson (1970), Massart (2000), or the survey in Rao and Wu (2001). A choice between models based on a measure that indicates the relative flexibility
of the models examining the extent to which the candidate models can mimic each other is studied in Wagenmakers et al. (2004). This mimicry is based on bootstrapping both observed and simulated data from prescribed models. Such a bootstrapping strategy could have been an option for this work, too.

The minimum description length, see Roos (2016), and Bayesian approaches, see Cavanaugh and Neath (1999), to model choice are broadly speaking dealing with the observed fit of a model additively penalized by terms accounting for the complexity of the models. The model choice by stochastic complexity incorporated in the normalized maximum likelihood estimate was developed in Rissanen (2007). The computational techniques of the normalization, when dealing with nonparametric models for categorical data are found in Kontkanen and Myllymäki (2007) and Mononen and Myllymäki (2008). When the observed fit is measured in terms of the maximized likelihood function, this is not feasible in simulator-based modeling.

JSD is an instance of a $\phi$-divergence, see, e.g., Österreicher (2002) for a survey. The work in Alba-Fernández et al. (2020) deals with model choice on misspecified prescribed models for categorical data using a general $\phi$-divergence for fit and an additive penalty for empty cells and is fundamentally different from the piece of work here.

2. Simulator-based Models for Categorical Data

In this section a set of definitions and notation is recapitulated for probability distributions for categorical data. This involves naturally the probability simplexes in Euclidean spaces. The notion of implicit statistical models for categorical data is defined formally. This introduces parameters $\theta$ in the formalism. Thereafter one can discuss the various settings for model choice: separate, overlapping and nested parameter spaces. Finally we present the so called Birch conditions for categorical probability distributions with parameter dependencies. These conditions lead to the existence of the maximum likelihood estimate in the implicit model.

2.1 Categorical Distributions

Let $\mathcal{A} = \{a_1, \ldots, a_k\}$ be a finite set, $k \geq 2$. We are concerned with a situation where $k$ and all categories $a_j$ are known. This excludes the issues of very large alphabets discussed in Kelly et al. (2012). $\mathbb{R}^\mathcal{A}$ denotes the set of real valued functions on $\mathcal{A}$. We introduce the set of categorical (probability) distributions as

$$\mathbb{P} = \{\text{all probability distributions on } \mathcal{A}\} \subset \mathbb{R}^\mathcal{A}. \quad (1)$$

The Iverson bracket $I_i(x) = [x = a_i] \in \mathbb{R}^\mathcal{A}$ is defined for each $a_i \in \mathcal{A}$ by

$$I_i(x) = [x = a_i] := \begin{cases} 1 & x = a_i \\ 0 & x \neq a_i \end{cases} \quad (2)$$

Any $P \in \mathbb{P}$ can be written as

$$P(x) = \prod_{i=1}^{k} p_i^{[x=a_i]}, x \in \mathcal{A}, \quad (3)$$
where \((0^0 = 1, 0^1 = 0)\), and \(p_i \geq 0, \sum_{i=1}^{k} p_i = 1\). The support of \(P \in \Phi\) is \(\text{supp}(P) = \{a_i \in A | p_i = P(a_i) > 0\}\). If \(X\) is a random variable (r.v.) assuming values on \(A\), \(X \sim P \in \Phi\) means that \(P(X = x) = P(x)\) for all \(x \in A\).

Any \(P \in \Phi\) is also identified as a probability vector \(p\), an element of the probability simplex \(\Delta_{k-1}\) defined by

\[
\Delta_{k-1} := \left\{ p = (p_1, \ldots, p_k) \mid p_i \geq 0, i = 1, \ldots, k; \sum_{i=1}^{k} p_i = 1 \right\} \subset \mathbb{R}^k.
\]

We write this one-to-one correspondence between \(\Phi\) and \(\Delta_{k-1}\) as

\[
\triangle(P) = p.
\]

The \(i\)-th face of \(\Delta_{k-1}\) is defined as \(\partial_i \Delta_{k-1} = \{p \in \Delta_{k-1} | p_i = 0\}\). Any face is in fact a probability simplex in \(\mathbb{R}^{k-1}\). The simplicial or topological interior of \(\Delta_{k-1}\) is \(\overset{\circ}{\Delta}_{k-1} = \{p \in \Delta_{k-1} | p_i > 0, i = 1, \ldots, k; \sum_{i=1}^{k} p_i = 1\}\).

We note that \(\text{supp}(P) = A \iff \triangle(P) \in \overset{\circ}{\Delta}_{k-1}\).

The assumption

\[
\triangle(P) \in \overset{\circ}{\Delta}_{k-1}
\]

is made for all models in the sequel.

Let us set \(z_i^* = \ln \frac{p_i}{p_k}\), and \(k^*(z^*) = -\ln p_k\). Then any categorical distribution in \(\Phi\) in Equation (3) can be written as

\[
P_{z^*}(x) = e^{\sum_{i=1}^{k} z_i^* [x=a_i] - k^*(z^*)}, \quad x \in A,
\]

which is an exponential family of distributions. It is shown in Amari and Cichocki (2010, p. 186) that \(p\) and \(z^*\) are, respectively, the primal and dual variables in the entropy geometry of \(\Phi\). In this \(\Phi\) is a Riemann manifold, where the squared local distance is determined by the Hessian of \(G(p) = \sum_{i=1}^{k} (p_i \ln p_i - p_i)\). Amari and Cichocki (2010) as well as Pistone (2018) deal with the information geometry of the non-parametric probability simplex, not the parameterized ones of Section 2.2. An argument for indexing probability simplices with parameters in terms of statistical precision is found in Altham (1984).

### 2.2 Simulator Modeling Represented as an Implicit Statistical Model

Consider \(P_o \in \Phi\) as the so-called true distribution. \(P_o\) is otherwise unknown, except the observed data \(D = (D_1, \ldots, D_{n_o})\), are assumed to be an i.i.d. \(n_o\)-sample from a data source under \(P_o\), \(D \sim P_o\). In likelihood-free inference one as a rule reduces the observed data \(D\) to some features, or summary statistics, before performing inference. The role of the
are implicit functions of \( \theta \). We are going to use the customary notation \( X \) for the category probabilities, i.e., \( p_i = \frac{n_i}{n} \), \( i = 1, \ldots, k \), where \( n_i \) is the number of samples \( Z_j \) in \( D \) such that \( Z_j = a_i \), and following Equation (3)

\[
\hat{P}_D(x) = \prod_{i=1}^{k} \hat{P}_i^{[x=a_i]}, \quad x \in \mathcal{A}.
\]  

(9)

The sufficiency of this summary statistics has been established in Corander et al. (submitted).

Let us consider simulator models \( M_C \) is a simulator model for the data source. Citing Lintusaari et al. (2017), simulator models can be understood in our case as computer programs that take as input random numbers \( V \) and the parameter \( \theta \in \Theta \subset \mathbb{R}^d \), \( d = \dim(\Theta) < k = |\mathcal{A}| \) and produce as output \( X = (X_1, \ldots, X_n) \), \( n \) i.i.d. samples of categories in \( \mathcal{A} \). The platform in Lintusaari et al. (2017) is not limited to categorical data. We write the corresponding function as \( M_C(\theta) \). By this designation, \( p_i(\theta) = P(X = a_i) = P(M_C(\theta) = a_i) \) for any \( \theta \in \Theta \) induces the category probabilities, i.e., \( k \) functions that have no (fully) explicit expression, i.e., they are implicit functions of \( \theta \) in the sense of Diggle and Gratton (1984) satisfying \( p_i(\theta) \geq 0 \), \( \sum_{i=1}^{k} p_i(\theta) = 1 \) for all \( \theta \in \Theta \). There is the distribution \( P_\theta \in \mathbb{P} \) given by

\[
P_\theta(x) := \prod_{i=1}^{k} p_i(\theta)^{[x=a_i]}, \quad x \in \mathcal{A}, \theta \in \Theta.
\]  

(10)

The implicit model representation of \( M_C \) in \( \mathbb{P} \) is denoted by \( M_p = \{ P_\theta \mid \theta \in \Theta \} \),

\[
M_C = \{ M_C(\theta) \mid \theta \in \Theta \} = M_p = \{ P_\theta \mid \theta \in \Theta \} \subset \mathbb{P}.
\]

We are going to use the customary notation \( X \sim P_\theta \) which is to be understood in the above sense of generative simulator-based sampling, not as sampling from a known categorical distribution. \( \hat{P}_X \in M_{n}(\theta) \) is a shorthand for the statement that \( \hat{P}_\theta \) is the summary statistics for \( X \sim P_\theta \). By Equation (5) there corresponds to the representation \( M_p \) a submanifold of \( \Delta_{k-1} \) by

\[
\Delta(M_p) = \{ p \in \Delta_{k-1} \mid \exists P_\theta \in M_p \text{ such that } p = \Delta(P_\theta) \}.
\]  

(11)

Let us consider simulator models \( M_p^{(l)} \), \( l = 1, \ldots, L \) with corresponding \( \Theta^{(l)} \subset \mathbb{R}^k \). There are three different situations for \( M_p^{(l_1)} \) and \( M_p^{(l_2)} \) to be related to each other. We assume the (weak) identifiability of the models, \( \theta \neq \theta' \Rightarrow P_\theta \neq P_{\theta'} \), see Section 2.3.

1. \( \Theta^{(l_1)} \) and \( \Theta^{(l_2)} \) are separate, i.e., \( \Theta^{(l_1)} \cap \Theta^{(l_2)} = \emptyset \). This can also mean that \( \Theta^{(l_1)} \) and \( \Theta^{(l_2)} \) have no relations between each other, this is the problem of model choice in Atkinson (1970).

2. \( \Theta^{(l_1)} \) and \( \Theta^{(l_2)} \) are overlapping, i.e. \( \Theta^{(l_1)} \) and \( \Theta^{(l_2)} \) have a nonempty intersection, but are not subsets of each other.
3. $\Theta^{(l_1)}$ and $\Theta^{(l_2)}$ are nested, e.g., $\Theta^{(l_1)} \subset \Theta^{(l_2)}$,

see, e.g., Vuong (1989, p. 317, p. 320, p. 323), where the submanifolds $M_p^{(l_i)}$ are for prescribed models.

**Example 1** Suppose that each category $a_i$ is associated with a predictor $\alpha^{(i)}$ with $d$ state variables $\alpha^{(i)}_s$, which may be real-valued, binary-valued, categorical-valued, etc., fixed characteristics of the category $a_i$. We consider a special case of Example 1 with $d = 2$. Let us write

$$a_i \leftrightarrow \alpha^{(i)} = (\alpha^{(i)}_1, \ldots, \alpha^{(i)}_d), \quad i = 1, \ldots, k - 1$$

$$a_k \leftrightarrow \alpha^{(k)} = \theta_0 := (0, \ldots, 0)$$

with the arbitrary choice of $a_k$ as a base of $d$ zero states. $\theta = (\theta_1, \ldots, \theta_d)$ is parameter vector in some $\Theta$. We set $\langle \alpha^{(i)}, \theta \rangle := \sum_{s=1}^{d} \alpha^{(i)}_s \theta_s$. Furthermore we set $M(\theta) := \ln \left(1 + \sum_{i=1}^{k-1} e^{\langle \alpha^{(i)}, \theta \rangle}\right)$ and the (prescribed) category probabilities in Equation (10) are defined by

$$p_i(\theta) := e^{\langle \alpha^{(i)}, \theta \rangle - M(\theta)}, \quad i = 1, \ldots, k,$$  \quad (12)

where the convention on $\alpha^{(k)}$ gives $p_k(\theta) = 1/ \left(1 + \sum_{i=1}^{k-1} e^{\langle \alpha^{(i)}, \theta \rangle}\right)$. Here we can obviously define nested models with different dimensions by identifying $\theta^{l_1} = (\theta_1, \ldots, \theta_{l_1}) \in \Theta^{(l_1)}$ as $\theta^{l_2} = (\theta_1, \ldots, \theta_{l_1}, 0, \ldots, 0) \in \Theta^{(l_2)}$, where $l_1 < l_2 < k$. The parameter vector $\theta = \theta_l$ with appropriate number of zeros lies thus in every $\Theta^{(l)}$, and Equation (12) becomes the discrete uniform distribution $P_U$ on $A$, i.e.,

$$P_U(x) = \prod_{i=1}^{d} \left(\frac{1}{k}\right)^{[x=a_i]}, \quad x \in A.$$

Hence $P_U$ can be regarded as a model with dimension zero, as $k$ is known in advance. $\triangle \left(P_U\right)$ is known as the barycenter of $\triangle_{k-1}$.

**Example 2** We consider a special case of Example 1 with $k = 3$ and $d = 0, 1, 2$. Suppose that each category $a_i$ is associated with a two-bit string as follows

$$a_1 \leftrightarrow \alpha^{(1)} = (1, 0), \quad a_2 \leftrightarrow \alpha^{(2)} = (0, 1), a_3 \leftrightarrow \alpha^{(3)} = (0, 0).$$

The nested models are given in terms of $\theta \in \mathbb{R}^2$.

(i) $\theta = (\theta_1, \theta_2)$ Substitution in Equation (12) gives $M_2(\theta) = \ln \left(1 + e^{\theta_1} + e^{\theta_2}\right)$ and

$$p_1(\theta) = e^{\theta_1 - M_2(\theta)}, \quad p_2(\theta) = e^{\theta_2 - M_2(\theta)}, \quad p_3(\theta) = \frac{1}{1 + e^{\theta_1} + e^{\theta_2}}.$$  \quad (14)

(ii) $\theta = (\theta_1, 0)$ Here $M_1(\theta) = \ln \left(2 + e^{\theta_1}\right)$ and Equation (12) gives

$$p_1(\theta) = e^{\theta_1 - M_1(\theta)}, \quad p_2(\theta) = \frac{1}{2 + e^{\theta_1}}, \quad p_3(\theta) = \frac{1}{2 + e^{\theta_1}}.$$  \quad (15)

(iii) $\theta = (0, 0)$ And $M_0(\theta) = \ln (3)$, Equation (12) gives

$$p_1(\theta) = \frac{1}{3}, p_2(\theta) = \frac{1}{3}, p_3(\theta) = \frac{1}{3}.$$  \quad (16)
2.3 Assumptions and Existence of Maximum Likelihood Estimate for Simulator Modeling

For the further analysis a set of notations and assumptions on the flexibility of the simulator model are required. This is analogous to the KOH theory of the smoothness of the functions in $M_C$ (Kennedy and O’Hagan, 2000, p. 2). We need some notational conventions. In the sequel $x \in \mathbb{R}^k$ is a $1 \times k$, a row vector, and $\theta \in \Theta \subset \mathbb{R}^d$ is a $1 \times d$ row vector. Hence $xx^T = \sum_{i=1}^k x_i^2$ is a scalar product. $||x||_{2,\mathbb{R}^k} = \sqrt{xx^T}$ is the Euclidean norm on $\mathbb{R}^k$ and similarly for $||\theta||_{2,\mathbb{R}^d}$.

**Assumption 1** For every $\theta_o$ in the interior of $\Theta$ and every $j = 1, \ldots, k$ we have

$$p_j(\theta) = p_j(\theta_o) + (\theta - \theta_o) p_j'(\theta_o)^T + o\left(||\theta - \theta_o||_{2,\mathbb{R}^d}\right).$$

where we have the $1 \times d$ total differential

$$p_j'(\theta) := \left(\frac{\partial}{\partial \theta_1} p_j(\theta), \ldots, \frac{\partial}{\partial \theta_d} p_j(\theta)\right).$$

Let us define for $i \in \{1, \ldots, d\}$ and $j \in \{1, \ldots, d\}$ and $X \sim P_\theta$ the expectation

$$I_{ij}(\theta) := E \left[\frac{\partial}{\partial \theta_i} \ln P_\theta(X) \frac{\partial}{\partial \theta_j} \ln P_\theta(X)\right].$$

The $d \times d$ matrix

$$I(\theta) := [I_{ij}(\theta)]_{i=1,j=1}^{d,d}$$

is the Fisher information matrix of $M_p$ at $\theta$.

**Assumption 2** For $\theta_o$ such that $p_j(\theta_o) > 0$ for each $j = 1, \ldots, k$ and for all $\theta$ in the interior of $\Theta$

$$p_j(\theta) = p_j(\theta_o) + (\theta - \theta_o) p_j'(\theta_o)^T + \frac{1}{2}(\theta - \theta_o)H(\theta_o)(\theta - \theta_o)^T + o\left(||\theta - \theta_o||_{2,\mathbb{R}^d}\right)$$

where $H(\theta_o)$ is the Hessian with the elements

$$H_{ij}(\theta_o) = -E \left[\frac{\partial^2}{\partial \theta_i \partial \theta_j} \ln P_{\theta_o}(X)\right].$$

Under further regularity assumptions we have $H(\theta_o) = -I(\theta_o)$.

The Jacobian $J(\theta)$ is the $k \times d$ matrix

$$J(\theta) := \begin{pmatrix} p_1'(\theta) \\ \vdots \\ p_k'(\theta) \end{pmatrix}$$

which has the vectors $p_j'(\theta)$ defined in Equation (21) as its rows. Furthermore we consider the $k \times k$ diagonal matrix

$$\Lambda(\theta) := \text{diag} \left(\frac{1}{\sqrt{p_1(\theta)}}, \ldots, \frac{1}{\sqrt{p_k(\theta)}}\right).$$
Let us define
\[ A(\theta) := \Lambda(\theta)J(\theta), \]  
which is a \( k \times d \)-matrix and assume

**Assumption 3** The rank of \( A(\theta) \) is \( d \).

The following assumption is the strong identifiability condition of Birch (1964, (B), p. 817).

**Assumption 4** For any \( \epsilon > 0 \) there exists \( \delta > 0 \) such that,
\[ \text{if } ||p(\theta) - p(\theta_0)||_{2,R^k} > \epsilon, \text{ then } ||\theta - \theta_0||_{2,R^d} > \delta. \]  

Clearly this implies the weak identifiability assumption

**Assumption 5**
\[ \theta \neq \theta' \Rightarrow P_\theta \neq P_{\theta'}. \]  

Under this assumption \( p = \Delta(P_\theta) \) is a one-to-one map between \( \Delta(\mathbb{M}_p) \) and \( \mathbb{M}_p \).

Birch (1964) proved under these assumptions that the MLE, maximum (prescribed) likelihood estimate of a true distribution \( P_{\theta_0} \) in a \( \mathbb{M}_p \) exists and is almost surely consistent. For simulator-modeling we re-formulate this by the next proposition.

**Proposition 6** MLE exists and is consistent for the simulator model \( \mathbb{M}_C = \{\mathbb{M}_C(\theta)\} \), in the sense that MLE exists and is consistent for \( \mathbb{M}_p = \{P_\theta \mid \theta \in \Theta\} \) for compact \( \Theta \) under Assumptions 1–4, where \( \mathbb{M}_C = \{\mathbb{M}_C(\theta) \mid \theta \in \Theta\} \models \mathbb{M}_p = \{P_\theta \mid \theta \in \Theta\} \).

The claim about existence is established in Birch (1964, p. 818) also for general \( \Theta \) by various considerations of how MLE can be introduced. It has been shown in Corander et al. (2021) for categorical data that the minimum JSD estimate, to be defined in Equation (49), and MLE are asymptotically equal, when \( n_o \to +\infty \). It is shown in Corander et al. (submitted) that the minimum JSD estimate exists and is measurable for compact \( \Theta \).

### 3. The Symmetric Jensen–Shannon Divergence

In this section we introduce the (symmetric) Jensen–Shannon divergence (JSD) as the measure of discrepancy between the observed and simulated data summaries. We note an interpretation of JSD as redundancy of the optimal source coding for a mixture source. We establish the JSD as a \( \phi \)-divergence, which makes it possible to use certain general properties of \( \phi \)-divergences for JSD.

#### 3.1 Definition of Symmetric JSD

Consider two generic categorical probability distributions \( P \in \mathbb{P}: P(x) = \prod_{i=1}^k p_i^{[x=a_i]} \) and \( Q \in \mathbb{P}: Q(x) = \prod_{i=1}^k q_i^{[x=a_i]} \). Then
\[ D_{\text{KL}}(P, Q) := \sum_{x \in \mathcal{A}} P(x) \ln \left( \frac{P(x)}{Q(x)} \right) = \sum_{i=1}^k p_i \ln \left( \frac{p_i}{q_i} \right) \]  

(28)
is known as the Kullback–Leibler divergence (KLD). In general \( D_{KL}(P, Q) \neq D_{KL}(Q, P) \), if \( P \neq Q \). We use \( 0 \ln 0 = 0 \) and if \( \text{supp}(Q) \subset \text{supp}(P) \), we take \( D_{KL}(P, Q) = +\infty \). Next, the symmetric Jensen–Shannon divergence is denoted by \( D_{JS}(P, Q) \), and is defined with \( M := \frac{1}{2}P + \frac{1}{2}Q \), i.e., \( M(x) = \prod_{i=1}^{k} \left( \frac{1}{2}p_i + \frac{1}{2}q_i \right)^{[x=0]} \), as

\[
D_{JS}(P, Q) := \frac{1}{2}D_{KL}(P, M) + \frac{1}{2}D_{KL}(Q, M). \tag{29}
\]

\( D_{JS}(P, Q) \) is a symmetrized version of KLD, as \( D_{JS}(P, Q) = D_{JS}(Q, P) \) and a smoothed version, since \( D_{JS}(P, Q) \) is uniformly bounded even if \( \text{supp}(Q) \subset \text{supp}(P) \) or \( \text{supp}(P) \subset \text{supp}(Q) \), as found in Equation (33).

The important result in the following proposition is provided for visibility and ease of reference.

**Proposition 7** \( \sqrt{D_{JS}(P, Q)} \) is a metric on \( \mathbb{P} \times \mathbb{P} \).

This is established in Endres and Schindelin (2003), see also Vajda (2009). We shall also use \( D_{JS}^{1/2}(P, Q) \) for \( \sqrt{D_{JS}(P, Q)} \).

The symmetric JSD is often used in machine learning, see e.g., Corander et al. (2017) and Corander et al. (2021) for references. There are reasons for that: \( D_{JS}(P, Q) \) is bounded, nonnegative and has an operational meaning pointed out next.

### 3.2 Interpretation as Redundancy of Source Code for \( X \sim \left( \frac{1}{2}P + \frac{1}{2}Q \right) \)

We recapitulate the idea from Topsøe (1979), see also Endres and Schindelin (2003, p. 1858). As above, consider drawing an i.i.d. sample \( X = (X_1, \ldots, X_n) \sim \left( \frac{1}{2}P + \frac{1}{2}Q \right) \), where \( P \) and \( Q \) are known distributions. For any \( X_i \) we do not know which of \( P \) or \( Q \) was drawn from. Next we seek the source coding that gives the shortest average code length for the compression of \( X \), see Cover and Thomas (2012, Ch. 5.3). Let \( R \in \mathbb{P} \) and \( l_i \) be the code length \( l_i = -\ln r_i \). Let us call this code \( \kappa \). Then the expected code length of \( \kappa \) is

\[
\frac{1}{2} \sum_{i=1}^{k} l_ip_i + \frac{1}{2} \sum_{i=1}^{k} l_iq_i.
\]

The minimal code length is obtained by selecting \( R = M \) and the minimum is the Shannon entropy of \( M \) in natural logarithm,

\[
H(M) = H \left( \frac{1}{2}P + \frac{1}{2}Q \right) := -\sum_{i=1}^{k} \left( \frac{1}{2}p_i + \frac{1}{2}q_i \right) \ln \left( \frac{1}{2}p_i + \frac{1}{2}q_i \right),
\]

see Cover and Thomas (2012, Ch. 5.3). On the other hand, a genie, who knows which of the two distributions was chosen to generate the individual \( X_i \), can by the same argument device a data compression code with a shorter expected minimum code length that is equal to \( \frac{1}{2}H(P) + \frac{1}{2}H(Q) \). Then \( D_{JS}(P, Q) \) is the redundancy of the code \( \kappa \), because

\[
D_{JS}(P, Q) = H(M) - \frac{1}{2}H(P) - \frac{1}{2}H(Q). \tag{30}
\]
This is a special case of an identity in Topsøe (1979, Lemma 4). The right hand side of Equation (30) is the Shannon-Jensen divergence $D_{JS}(P, Q)$ as defined in Lin (1991).

As is well-known, see Cover and Thomas (2012, p. 19), $D_{KL}(P, M)$ can be understood as the inefficiency of assuming that the true distribution is $M$ when it actually is $P$. Therefore then $D_{JS}(P, Q)$ could be seen as a minimum inefficiency distance, as formulated in Endres and Schindelin (2003, p. 1859).

3.3 JSD and φ-divergences

Consider $\phi_{JS}(u) = \frac{1}{2}u \ln u - \frac{1}{2}(u + 1) \ln \left(\frac{1}{2}u + \frac{1}{2}\right), 0 < u < +\infty$. (31)

One can check that $\phi_{JS}$ is a convex function on $(0, +\infty)$ and has the properties $0\phi_{JS}(\frac{1}{2}) = 0$ and $0\phi_{JS}(x/0) = \lim_{\epsilon \to 0} \epsilon\phi_{JS}(x/\epsilon)$, $\phi(1) = 0$. It holds also that

$$D_{JS}(P, Q) = \sum_{x \in A} Q(x)\phi_{JS} \left( \frac{P(x)}{Q(x)} \right).$$ (32)

Hence $D_{JS}(P, Q)$ is a special case of a φ-divergence, see Vajda (1989, Ch. 8 and 9) for the general theory and Österreicher (2002) for a concise summary. In addition the φ*-conjugate $\phi^*$ of any divergence function $\phi$ is defined by $\phi^*(u) := u\phi(1/u)$ for $0 \leq u < +\infty$. Then it turns out that

$$0 = \phi_{JS}(1) \leq D_{JS}(P, Q) \leq \phi_{JS}(0) + \phi^*_{JS}(0) = \ln(2).$$ (33)

The left equality implies the so-called identity of of indiscernibles, i.e., $D_{JS}(P, Q) = 0$ only if $P = Q$. The inequalities in Equation (33) are an instance of the range property due to Liese and Vajda in Liese and Vajda (2006, Thm 5) valid for all φ-divergences. The study Topsøe (2000) contains several additional explicit expressions and bounds, valid especially for $D_{JS}(P, Q)$.

The following inequality seems not be available in the literature, but is useful for our purposes.

**Lemma 8** $P \in \mathbb{P}$, $Q \in \mathbb{P}$. Then

$$D_{JS}(P, Q) \leq \frac{1}{2}D_{KL}(P, Q).$$ (34)

**Proof** If $\frac{1}{2}D_{KL}(P, Q) \geq \ln 2$, the lemma holds by Equation (33). Otherwise, a small piece of algebra applied on Equations (31) and (32) reveals that

$$D_{JS}(P, Q) = \frac{1}{2}D_{KL}(P, Q) - D_{KL}(M, Q).$$ (35)

Since $D_{KL}(M, Q) \geq 0$, the assertion follows.

The analysis of the asymptotics of JSD and model choice in the sequel requires additionally the introduction of the φ-divergence with $\phi(x) = |\sqrt{x} - 1|$. We obtain

$$V(P, Q) := \sum_{x \in A} Q(x)\left| \frac{P(x)}{Q(x)} - 1 \right| = \sum_{i=1}^{k} |p_i - q_i|. \quad (36)$$
V( P, Q) is called the variation distance. This is frequently discussed as the acceptance
criterion in ABC.

3.4 Information Radius and Model Evidence
Let \( p(\theta) \) be a prior density on \( \Theta \) and
\[
P( D \mid \mathbb{M}_p) := \int_{\Theta} P_\theta( D) p(\theta)d\theta. \tag{37}
\]
is the marginal data likelihood, also known as the model evidence. Here \( d\theta \) is the Lebesgue
measure induced on \( \Theta \).

In information theory \( \hat{P}_D \) is called the type of \( D \) on \( A \), see Csiszár and Körner (2011, Part I Ch. 2) and Cover and Thomas (2012, Ch. 11.1). Let \( n = n_o \). The type class of \( \hat{P}_D \) is defined, see Cover and Thomas (2012, Ch. 11.1-11.3), by
\[
T_n \left( \hat{P}_D \right) := \{ \mathbf{X} = (X_1, \ldots, X_n) \in A^n \mid \hat{P}_X = \hat{P}_D \} \tag{38}
\]
The set of all types on \( A \) for \( n \) samples
\[
P_n := \{ P \in \mathbb{P} \mid T_n (P) \neq \emptyset \}. \tag{39}
\]
Let
\[
A_\epsilon := \left\{ \mathbf{X} \in A^n \mid D_{\text{JS}}^{1/2} \left( \hat{P}_D, \hat{P}_X \right) \leq \epsilon \right\}. \tag{40}
\]
Let \( p(\theta) \) be a prior density on \( \Theta \).

**Proposition 9** Let \( n = n_o \). Then
\[
\lim_{\epsilon \downarrow 0} \int_{\Theta} P^{(n)}_\theta (A_\epsilon) p(\theta)d\theta = \frac{n_o!}{\prod_{j=1}^{K} n_{o,j}!} P( D \mid \mathbb{M}_p). \tag{41}
\]

**Proof** With the use of Equation (38) and Equation (39) we have
\[
P^{(n)}_\theta (A_\epsilon) = \sum_{\mathbf{X} \in A_\epsilon} P_\theta (\mathbf{X}) = \sum_{P \in P_n} \sum_{D_{\text{JS}}^{1/2} \left( \hat{P}_D, \hat{P}_X \right) \leq \epsilon} P_\theta (\mathbf{X})
\]
From Cover and Thomas (2012, Theorem 11.1.2) we have the identity
\[
P_\theta (D) = e^{-n_o H(\hat{P}_D) - n_o D_{\text{KL}}(\hat{P}_D, P_\theta)}, \tag{42}
\]
where \( H(\hat{P}_D) \) is the Shannon entropy of \( \hat{P}_D \) and thus
\[
\sum_{\mathbf{X} \in T_n (P)} P_\theta (\mathbf{X}) = \sum_{\mathbf{X} \in T_n (P)} e^{-n H(\hat{P}_X) - n D_{\text{KL}}(\hat{P}_X, P_\theta)}.
\]
However since \( \mathbf{X} \in T_n (P), \hat{P}_X = P \) by Equation (38) and, with the cardinality \( |T_n (P)| \),
\[
\sum_{\mathbf{X} \in T_n (P)} P_\theta (\mathbf{X}) = \frac{1}{|T_n (P)|} e^{-n H(P) - n D_{\text{KL}}(P, P_\theta)} |T_n (P)|
\]
and
\[ P_{\theta}^{(n)}(A_\epsilon) = \sum_{P \in \mathcal{P}_n|D^{1/2}_{JS}(\hat{P}_D,P) \leq \epsilon} e^{-nH(P) - nD_{KL}(P,P_\theta)} |T_n(P)|. \]

The sum has a finite number of terms and hence the change of order between summation and integration is permitted, and we have
\[ \int_{\Theta} P_{\theta}^{(n)}(A_\epsilon) p(\theta) d\theta = \sum_{P \in \mathcal{P}_n|D^{1/2}_{JS}(\hat{P}_D,P) \leq \epsilon} |T_n(P)| \int_{\Theta} e^{-nH(P) - nD_{KL}(P,P_\theta)} d\theta. \]

As \( \epsilon \downarrow 0 \), the set of types \( \{P \in \mathcal{P}_n|D^{1/2}_{JS}(\hat{P}_D,P) \leq \epsilon\} \) decreases to \( \{P \in \mathcal{P}_n|D^{1/2}_{JS}(\hat{P}_D,P) = 0\} \). Since \( D^{1/2}_{JS}(\hat{P}_D,P) = 0 \) if and only if \( \hat{P}_D = P \), and since \( \hat{P}_D \in \mathcal{P}_n \), as \( n = n_o \), the limit set is the singleton set \( \{\hat{P}_D\} \). Hence the sum reduces in the limit to a single term, or, to
\[ \lim_{\epsilon \downarrow 0} \int_{\Theta} P_{\theta}^{(n)}(A_\epsilon) p(\theta) d\theta = |T_n(\hat{P}_D)| \int_{\Theta} e^{-nH(\hat{P}_D) - nD_{KL}(\hat{P}_D,P_\theta)} p(\theta) d\theta \]
\[ = |T_n(\hat{P}_D)| \int_{\Theta} P_{\theta}(D) p(\theta) d\theta, \]
where Equation (42) was used again. Now, by combinatorics \( |T_n(\hat{P}_D)| = n_o! / \prod_{j=1}^{k} n_{o,j}! \). By Equation (37) we have found the assertion in Equation (41).

The proof above contains the following special case, which shows a scaled \( P_{\theta}^{(n)}(A_\epsilon) \) as an asymptotically correct estimate of the implicit likelihood function.

**Corollary 10**
\[ \frac{\Pi_{j=1}^{k} n_{o,j}!}{n_o!} \lim_{\epsilon \downarrow 0} P_{\theta}^{(n)}(A_\epsilon) = P_{\theta}(D). \] (43)

The integral \( \int_{\Theta} P_{\theta}^{(n)}(A_\epsilon) p(\theta) d\theta \) is known in the literature as the acceptance rate of certain ABC algorithms Leuenberger and Wegmann (2010, p. 247). Section 4 discusses a criterion of model choice that in view of Proposition 9 will also maximize the acceptance rate at small \( \epsilon \).

### 3.5 Use in Parameter Estimation

The present work uses symmetric JSD as a model fit measure. We assume an observed data set \( D \) summarized as \( \hat{P}_D \) and a simulator-based model that produces categorical observation data. Assuming that we can calculate category probabilities \( P_\theta \) based on the model parameters \( \theta \), we can find the parameters that maximize the model fit to observed data as
\[ \hat{\theta}_{JSD} = \arg \min_{\theta} D_{JS}(\hat{P}_D,P_\theta). \] (44)

This is a special case of the minimum \( \phi \)-divergence estimate see, e.g., Pardo (2018, Ch. 5.1–5.3). For the minimum \( \phi \)-divergence estimate for discrete (incl. categorical) distributions,
see Morales et al. (1995). The parameter estimate $\hat{\theta}_{\text{JSD}}$ is equivalent to the maximum likelihood estimate $\hat{\theta}_{\text{ML}}$, when the observation count $n_0 \to \infty$ (Corander et al., 2021).

Simulator-based or likelihood-free estimation methods are needed when the mapping between model parameters and category probabilities is complicated or unknown so that a direct comparison between the observed data and model parameters is not possible. The idea is that while we cannot calculate $D_{\text{JS}}(\hat{P}_D, P_\theta)$, we can simulate data with the model parameters $\theta$ and evaluate model fit based on comparison between the observed and simulated data. In practice, the individual simulations are used to calculate $D_{\text{JS}}(\hat{P}_D, \hat{P}_{X_\theta})$ and the optimization task is to find the model parameters that minimize the expected discrepancy $E[D_{\text{JS}}(\hat{P}_D, \hat{P}_{X_\theta})]$.

To summarize, when the mapping between model parameters and category probabilities is unknown, we substitute $D_{\text{JS}}(\hat{P}_D, P_\theta)$ with $E[D_{\text{JS}}(\hat{P}_D, \hat{P}_{X_\theta})]$. However, minimization of $E[D_{\text{JS}}(\hat{P}_D, \hat{P}_{X_\theta})]$ is more difficult than minimizing $D_{\text{JS}}(\hat{P}_D, P_\theta)$ (which can be quite difficult, too). We can show that in certain conditions $D_{\text{JS}}(\hat{P}_D, \hat{P}_{X_\theta}) \to D_{\text{JS}}(\hat{P}_D, P_\theta)$ when the simulation count $n \to \infty$ (Corander et al., submitted), but otherwise the discrepancies calculated based on individual simulation results $D_{\text{JS}}(\hat{P}_D, \hat{P}_{X_\theta})$ are best understood as $E[D_{\text{JS}}(\hat{P}_D, \hat{P}_{X_\theta})]$ observed with additive noise. This makes optimization difficult. Since running simulations can be expensive, we want to limit the total simulation count, and we need an optimization method that can balance between running simulations with the same parameter values to improve the expected JSD estimates locally and running simulations with new parameter values to find the expected JSD minimum globally. The experiments carried out in this work use Bayesian optimization. For a tutorial and review, see Frazier (2018).

4. Likelihood-free Model Choice based on JSD Razor

As outlined in the Introduction, Section 1, the purpose of statistical model selection is to select from a set of alternative explanations or models, the one that best explains the data, here categorical $\mathbf{D}$. The task is not elementary, as there are two conflicting requirements of a good model, namely that of generalizability and that of goodness of fit. Here goodness of fit measures how well a model fits the observed $\mathbf{D}$. By generalizability we refer to the capability of the model to fit well novel data sets.

Occam’s Razor is known as the dictum that the simpler model, for example a model with fewer parameters, is to be preferred (a.k.a. the principle of parsimony). In terms of information theory the Occam Razor proposes that the shortest description of the data is the best model.

In this section we start from the interpretation of Occam’s Razor in Balasubramanian (1996). JSD is related to this Razor by bounds for the model evidence. We derive an expression for the JSD Razor by finding the total differential and Hessian of JSD w.r.t. the parameters. Then the multivariable Laplace approximation is applied to get an approximate expression of the JSD Razor to be minimized by choice of model family.
4.1 Bounds for the Model Evidence

For a finite number $L$ of alternative models $M^{(l)}_p$ for $D$, the Bayesian rule of selecting among them is to pick the model that maximizes the posterior probability given $D$. If the models have equal prior probabilities, this means selecting the model that maximizes the model evidence as defined in Equation (37).

Next we drop for convenience of writing the superscript in $M^{(l)}_p$. It has been shown in Corander et al. (submitted) that $\hat{P}_D$ is Bayes sufficient summary statistic of the data $D$. This follows effectively by the multinomial probability

$$P_{\theta}(\hat{P}_D) = \frac{n_o!}{\prod_{j=1}^k n_{o,j}!} P_{\theta}(D).$$

Thus we define the model evidence based on the sufficient summary of $D$, $P(\hat{P}_D|M_p)$, by modification of Equation (37) as

$$P(\hat{P}_D|M_p) := \frac{n_o!}{\prod_{j=1}^k n_{o,j}!} P(D|M_p) = \int_\Theta P_{\theta}(\hat{P}_D)p(\theta)d\theta,$$

cf., Equation (41). In view of Equation (45) and Equation (42) and evaluation of $e^{-n_oH(\hat{P}_D)}$ by definition of the Shannon entropy we obtain

$$\int_\Theta P_{\theta}(\hat{P}_D)p(\theta)d\theta = \frac{n_o!}{\prod_{j=1}^k n_{o,j}!} \prod_{j=1}^k \left( \frac{n_{o,j}}{n_o} \right)^{n_{o,j}} \int_\Theta e^{-n_oD_{KL}(\hat{P}_D,P_{\theta})}p(\theta)d\theta.$$  

The multiplicative factor in front of the integral in the right hand side is $<1$ since it is the probability of the event $\xi = (n_1, \ldots, n_k)$ w.r.t. to the multinomial distribution with parameters $n_o$ and $\left(\frac{n_1}{n_o}, \ldots, \frac{n_k}{n_o}\right)$. By Lemma 8 we have found

$$\int_\Theta P_{\theta}(\hat{P}_D)p(\theta)d\theta \leq \int_\Theta e^{-n_oD_{KL}(\hat{P}_D,P_{\theta})}p(\theta)d\theta \leq \int_\Theta e^{-2n_oD_{JS}(\hat{P}_D,P_{\theta})}p(\theta)d\theta.$$  

The idea is to use the integral in the right hand side of the second inequality to find an implementable criterion for likelihood-free simulator-based models choice. For a special prior density $p(\theta)$ the integral will below be called the JSD-Razor.

4.2 Definition of the JSD Razor and Outline

Let $I(\theta)$ be the Fisher information matrix (see Section 2.3). Consider the prior

$$p(\theta) = \frac{\sqrt{\det I(\theta)}}{V(\Theta)},$$

where $V(\Theta) := \int_\Theta \sqrt{\det I(\theta)}d\theta$ is assumed to exist. Hence $p(\theta)$ is Jeffreys' prior, which is rigorously constructed in Balasubramanian (1996) by a convergence argument from a
discrete uniform prior on a finite number of $P_\theta$ indistinguishable (in a sense made precise in Balasubramanian (1996)) from $P_{\theta_o}$. Then we define the JSD-Razor $R_{n_o}(M_p)$ by

$$R_{n_o}(M_p) := \int_{\Theta} e^{-2n_o D_{JS}(\hat{P}_D, P_\theta)} \sqrt{\det I(\theta)} V(\Theta) d\theta.$$  \hspace{1cm} (47)

Occam’s Razor as introduced in Balasubramanian (1996, Equation (35), p. 20) becomes

$$\int_{\Theta} e^{-n_o D_{KL}(\hat{P}_D, P_\theta)} \sqrt{\det I(\theta)} V(\Theta) d\theta.$$  

We have seen above (Equation 46) that Occam’s Razor is bounded upwards by $R_{n_o}(M_p)$.

In the following Section 4.5 we argue for and derive from maximization of the JSD-Razor $R_{n_o}(M_p)$ two rules for model choice. The criterion $\text{SIC}_{JSD}(M_p)$ below is the cruder version of the asymptotics of the JSD-Razor $R_{n_o}(M_p)$. It chooses the model $M_p^{(l)}$ that minimizes

$$\text{SIC}_{JSD}(M_p^{(l)}) := 2n_o D_{JS}(\hat{P}_D, P_{\theta_JSD}^{(l)}) + \text{dim}(\Theta^{(l)}) \ln \sqrt{\frac{n_o}{8\pi}}$$  \hspace{1cm} (48)

among a finite number $L$ of alternative models $M_p^{(l)}$ for $D$, where it is understood that $n_o > 8\pi$, and where we define the minimum JSD estimate of $\theta \in \Theta^{(l)}$ by

$$\hat{\theta}_JSD^{(l)} = \hat{\theta}_JSD^{(l)}(D) = \text{argmin}_{\theta \in \Theta^{(l)}} D_{JS}(\hat{P}_D, P_\theta).$$  \hspace{1cm} (49)

It is shown in Corander et al. (submitted) that $\hat{\theta}_JSD^{(l)}$ exists for compact $\Theta^{(l)}$. Asymptotic (in $n_o$) properties of $\hat{\theta}_JSD^{(l)}$ can be extracted from the results on general minimum $\phi$-divergence estimates in Morales et al. (1995) for prescribed models. The criterion in Equation (48) contains, as it should, the trade-off between fit and model dimension: the JSD-fit will be smaller in a model with a larger parameter space. In Equation (48) we have a criterion which is computable for choice between simulator-based models in the sense that the computational minimization of $E_{P_\theta}[D_{JS}(\hat{P}_D, \hat{P}_X)]$ by the software function BOLFI should approximately find $\hat{\theta}_JSD$, as defined by Equation (49).

### 4.3 Step One for Derivation of $\text{SIC}_{JSD}$: Total Differential and Hessian of JSD w.r.t $\theta$

The following result is well-known, see, e.g., Morales et al. (1995, p. 355).

**Lemma 11**

$$I(\theta) = A(\theta)^T A(\theta).$$  \hspace{1cm} (50)

*Under Assumption 3, the matrix $I(\theta)$ is invertible.*

It is appropriate here to use the simplex map from Equation (5) for the distributions in $P$. In other words, we shall work with functions of vectors in $\Delta_{k-1}$. Then $p_\theta =
\((p_1(\theta), \ldots, p_k(\theta)) = \triangle (P_\theta), \hat{p} = \triangle (\hat{P}_D)\), and we obtain by means of Iverson bracket (Equation 2) and Equation (32) that
\[
D_{JS} (\hat{p}, p_\theta) = D_{JS} (\hat{P}_D, P_\theta).
\] (51)

Since we are going to at first deal with this quantity by partial derivatives w.r.t. \(\theta\) for fixed \(\hat{p}\), we introduce for ease of writing the function
\[
\Phi (\hat{p}, \theta) := D_{JS} (\hat{p}, p_\theta) \tag{52}
\]
defined on \(\triangle_{k-1} \times \Theta\). We compute with dropping the hat so that \(p \leftarrow \hat{p}\). We recall the generating \(\phi\) of symmetric JSD in Equation (31)
\[
\phi(u) = \frac{1}{2} u \ln u - \frac{1}{2} (u + 1) \ln \left(\frac{1}{2} u + \frac{1}{2}\right), 0 \leq u < +\infty.
\]
The first derivative is
\[
\phi' (u) = \frac{1}{2} \ln u - \frac{1}{2} \frac{u}{\left(\frac{1}{2} u + \frac{1}{2}\right)}, 0 < u < +\infty, \tag{53}
\]
We can rewrite
\[
\phi'(u) = \frac{1}{2} \ln \left(\frac{u}{(u/2 + 1)}\right), \tag{54}
\]
and this gives
\[
\phi(u) = u \phi'(u) - \frac{1}{2} \ln \left(\frac{u}{2} + \frac{1}{2}\right). \tag{55}
\]
Next we get
\[
\phi'' (u) = \frac{1}{2u(u + 1)}, 0 < u < +\infty. \tag{56}
\]

**Lemma 12** Assume \(p(\theta) \in \triangle_{k-1}^0\). Let us define the \(1 \times k\) vector
\[
\Phi (p, \theta) = \left(\phi' \left(\frac{p_1(\theta)}{p_1}\right), \ldots, \phi' \left(\frac{p_k(\theta)}{p_k}\right)\right). \tag{57}
\]
Then the \(1 \times d\) total differential \(\frac{\partial}{\partial \theta} \Phi (p, \theta)\) is given by
\[
\frac{\partial}{\partial \theta} \Phi (p, \theta) = \Phi (p, \theta) J(\theta), \tag{58}
\]
where \(J(\theta)\) is the Jacobian in Equation (23).

The straightforward computational proof is found in Appendix B.2

Let us define the \(k \times k\) diagonal matrix
\[
\Lambda(p, \theta) := \text{diag} \left(\frac{1}{\sqrt{p_1 + p_1(\theta)}}, \ldots, \frac{1}{\sqrt{p_k + p_k(\theta)}}\right), \tag{59}
\]
And let us define with the Jacobian \(J(\theta)\) in Equation (23)
\[
A(p, \theta) := \Lambda (p, \theta) J(\theta). \tag{60}
\]
Lemma 13 Assume \( p \in \triangle_{k-1} \) and \( p(\theta) \in \triangle_{k-1} \). The Hessian matrix of \( \Phi (p, \theta) \) is the \( d \times d \) matrix \( H(\Phi (p, \theta)) \) with elements given by

\[
\frac{\partial^2}{\partial \theta_i \partial \theta_j} \Phi (p, \theta) = \sum_{i=1}^{k} \phi'(p_i(\theta)) \frac{\partial^2}{\partial \theta_i \partial \theta_j} p_i(\theta) + \frac{1}{2} I_{lj}(\theta) - \frac{1}{2} \left[ A(p, \theta)^T A(p, \theta) \right]_{lj}.
\]

(61)

The proof is found in the Appendix B.2. We introduce the \( d \times d \) matrix

\[
H_{p_1, \ldots, p_k}(\theta) := \left[ \sum_{i=1}^{k} \phi'(p_i(\theta)) \frac{\partial^2}{\partial \theta_i \partial \theta_j} p_i(\theta) \right]_{d,d}.
\]

Then Equation (61) becomes the matrix equality.

Proposition 14 Assume \( p \in \triangle_{k-1} \) and \( p(\theta) \in \triangle_{k-1} \). The Hessian matrix w.r.t. \( \theta \) of \( \Phi (p, \theta) \) in Equation (52)

\[
H(\Phi (p, \theta)) = H_{p_1, \ldots, p_k}(\theta) + \frac{1}{2} I(\theta) - \frac{1}{2} A(p, \theta)^T A(p, \theta).
\]

(62)

4.4 Step Two for Derivation of SIC\(_{JSD} \): Laplace Approximation of the JSD-Razor

We adapt for the current setting some pertinent standard results of Breitung (2006, Ch. 5) or Wong (2001, Ch. XI) for Laplace approximation of multivariate integrals, in this case for \( R_{n_o}(M_p) \) in Equation (47). The work in Lapiński (2019) adds convergence rates of this approximation. We use the map \( \Phi (\hat{p}, \theta) \) in Equation (52). Hence by Equation (49) we write \( \hat{\theta}_{JSD} = \hat{\theta}_{JSD}(D) = \arg\min_{\theta \in \Theta} \Phi (\hat{p}, \theta) \).

Lemma 15 Assume Assumptions 1-4. Assume that \( \Theta \) is a compact subset of \( \mathbb{R}^d \) and that \( \Phi (\hat{p}, \theta) \) has a unique minimum at \( \hat{\theta}_{JSD} \) in the interior of \( \Theta \) and that the Hessian \( H(\Phi (\hat{p}, \hat{\theta}_{JSD})) \) is positive definite, and that the prior density \( p(\theta) \) is a continuous function of \( \theta \). Then it holds that

\[
R_{n_o}(M_p) \approx \left( \frac{2\pi}{n_o} \right)^{d/2} e^{-2n_o D_{JSD}(\hat{p}, \hat{\theta}_{JSD})} \sqrt{\det I(\hat{\theta}_{JSD})} \sqrt{\det H(\Phi (\hat{p}, \hat{\theta}_{JSD}))} \frac{1}{V(\Theta)}.
\]

(63)

Proof Due to the differentiability properties of \( \phi_{JSD}(u) \) in Equation (31) and the assumptions the map \( \Phi (\hat{p}, \theta) \) is a twice differentiable as a function of \( \theta \) in the interior of \( \Theta \), as has been checked in the preceding section. Then the equality Equation (63) is valid for \( R_{n_o}(M_p) \) in Equation (47), as follows by Breitung (2006, Thm 4.1, p. 56) or Wong (2001, Thm 3. pp. 494-495).
Lemma 16 Let the assumptions of Lemma 15 hold for any \( n_o \). Assume that there is \( P_{\theta_o} \in \mathbb{M} \) such that \( D \sim P_{\theta_o} \). Then with \( P_{\theta_o} \)-probability one,

\[
H_{\Phi} \left( \hat{p}, \hat{\theta}_{\text{JSD}} \right) \approx \frac{1}{4} I \left( \hat{\theta}_{\text{JSD}} \right).
\]

(64)

for all large \( n_o \), where \( I \left( \hat{\theta}_{\text{JSD}} \right) \) is the Fisher information matrix defined in Equation (19) evaluated at \( \hat{\theta}_{\text{JSD}} \).

Proof We know by Lemma A.1 that

\[
\frac{\sqrt{2}}{4} \left\| \hat{P}_D - P_{\theta_{\text{JSD}}} \right\|_2 \leq D_{JS}^{1/2} \left( \hat{P}_D, P_{\theta_{\text{JSD}}} \right).
\]

(65)

In force of Proposition 7, we can use the triangle inequality to the effect that

\[
D_{JS}^{1/2} \left( \hat{P}_D, P_{\theta_{\text{JSD}}} \right) \leq D_{JS}^{1/2} \left( \hat{P}_D, P_{\theta_o} \right) + D_{JS}^{1/2} \left( P_{\theta_o}, P_{\theta_{\text{JSD}}} \right).
\]

(66)

It has been shown in Corander et al. (2021, Lemma 5.1, Proposition 5.2) that \( D_{JS}^{1/2} \left( P_{\theta_o}, P_{\theta_{\text{JSD}}} \right) \to 0 \), \( P_{\theta_o} \) a.s., as \( n_o \to +\infty \), when \( P_{\theta_o} \in \mathbb{M} \) and \( D \sim P_{\theta_o} \). Let us recall the total variation distance \( V(P, Q) \) defined in (36). It holds that \( D_{JS}^{1/2} \left( \hat{P}_D, P_{\theta_o} \right) \to 0 \), if \( V \left( \hat{P}_D, P_{\theta_o} \right) \to 0 \), \( P_{\theta_o} \) a.s., as \( n_o \to +\infty \), which convergence is well known, for a proof see e.g., Appendix A of Corander et al. (submitted), as \( P_{\theta_o} \in \mathbb{M} \) and \( D \sim P_{\theta_o} \). Hence in Equation (65), the norm

\[
\left\| \hat{P}_D - P_{\theta_{\text{JSD}}} \right\|_2 = \sqrt{\sum_{i=1}^{k} (\hat{p}_i - p_i(\hat{\theta}_{\text{JSD}}))^2} \to 0,
\]

(67)

\( P_{\theta_o} \) a.s., as \( n_o \to +\infty \).

The Hessian \( H_{\Phi} \left( \hat{p}, \hat{\theta}_{\text{JSD}} \right) \) has by Proposition 14, Equation (62), by Equation (B.17) and Equation (B.18) the elements

\[
\frac{\partial^2}{\partial \theta_i \partial \theta_j} \Phi \left( \hat{p}, \hat{\theta}_{\text{JSD}} \right) = \sum_{i=1}^{k} \phi' \left( \frac{p_i(\hat{\theta}_{\text{JSD}})}{\hat{p}_i} \right) \frac{\partial^2}{\partial \theta_i \partial \theta_j} p_i(\hat{\theta}_{\text{JSD}})
\]

(68)

\[
+ \frac{1}{2} I_{ij}(\hat{\theta}_{\text{JSD}}) - \frac{1}{2} \sum_{i=1}^{k} \frac{\partial}{\partial \theta_i} p_i(\hat{\theta}_{\text{JSD}}) \frac{\partial}{\partial \theta_j} p_i(\hat{\theta}_{\text{JSD}}) \frac{\hat{p}_i + p_i(\hat{\theta}_{\text{JSD}})}{\hat{p}_i + p_i(\hat{\theta}_{\text{JSD}})}.
\]

Since \( (\hat{p}_i - p_i(\hat{\theta}_{\text{JSD}}))^2 \to 0 \), \( \phi' \left( \frac{p_i(\hat{\theta}_{\text{JSD}})}{\hat{p}_i} \right) \approx \phi'(1) = 0 \), where we used Equation (54). For the same reason

\[
\frac{\partial}{\partial \theta_i} p_i(\hat{\theta}_{\text{JSD}}) \frac{\partial}{\partial \theta_j} p_i(\hat{\theta}_{\text{JSD}}) \approx \frac{1}{2} \frac{\partial}{\partial \theta_i} p_i(\hat{\theta}_{\text{JSD}}) \frac{\partial}{\partial \theta_j} p_i(\hat{\theta}_{\text{JSD}}).
\]

18
Now Lemma 11, or the expression Equation (B.2) in its proof, gives
\[
\frac{1}{2} \sum_{i=1}^{k} \frac{\partial}{\partial \theta_j} p_i \left( \hat{\theta}_{JSD} \right) \frac{\partial}{\partial \theta_j} p_i \left( \hat{\theta}_{JSD} \right) \approx \frac{1}{4} H_{ij} \left( \hat{\theta}_{JSD} \right).
\]

When the approximate expressions above have been applied in Equation (68), the right hand side of Equation (64) is obtained.

4.5 Step Three for Derivation of SIC\(_{JSD}\) : Two Versions

Next we produce the rule in Equation (48). We want to find the model \(M_p^{(l)}\), which minimizes
\[-\ln R_{n_o} \left( M_p^{(l)} \right).\]
Following Balasubramanian (1996, (35), p. 20) we define
\[V_c(\Theta) := \left( \frac{2\pi}{n_o} \right)^{d/2} \frac{\sqrt{\det I \left( \hat{\theta}_{JSD} \right)}}{\sqrt{\det H_{\hat{p}, \hat{\theta}_{JSD}}}}.\] (69)

Here \(\ln \frac{V(\Theta)}{V_c(\Theta)}\) acts as a penalty for model complexity in the geometric sense of model volume, see Balasubramanian (1996) and Balasubramanian (2005) and Myung et al. (2000).

By Lemma 15,
\[-\ln R_{n_o} \left( M_p^{(l)} \right) \approx 2n_o D_{JS} \left( \hat{p}_D, P_{\hat{\theta}_{JSD}} \right) + \ln \frac{V(\Theta)}{V_c(\Theta)},\] (70)

By an expansion we get
\[
\ln \frac{V(\Theta)}{V_c(\Theta)} = \frac{d}{2} \ln \frac{n_o}{2\pi} + \ln \int_{\Theta} \sqrt{\det I(\theta)} d\theta + \frac{1}{2} \ln \frac{\det H_{\hat{p}, \hat{\theta}_{JSD}}}{\det I \left( \hat{\theta}_{JSD} \right)}.
\]

By Lemma 16, Equation (64), and the rules for determinants we have
\[
\det H_{\hat{p}, \hat{\theta}_{JSD}} \approx \frac{1}{4^d} \det I \left( \hat{\theta}_{JSD} \right),
\]
and
\[
\ln \frac{V(\Theta)}{V_c(\Theta)} \approx \frac{d}{2} \ln \frac{n_o}{2\pi} + \ln \int_{\Theta} \sqrt{\det I(\theta)} d\theta - d \ln 2,
\] (71)

whereby Equation (48) is obtained by dropping \(\ln \int_{\Theta} \sqrt{\det I(\theta)} d\theta\). An example of explicit computation of \(\det I(\theta)\) is presented in Appendix B (Example B.1).
5. Properties of $\text{SIC}_{\text{JS}}$

In this section we study the properties of $\text{SIC}_{\text{JS}}\left(\mathbb{M}_p^{(l)}\right)$ as approximately obtained from JSD Razor in the preceding section and stated in Equation (48). We make a comparison of $\text{SIC}_{\text{JS}}$ with the well known Schwarz’s information criterion (SIC) for model determination. This criterion is also known as Bayesian information criterion (BIC). Then we prove the consistency of $\text{SIC}_{\text{JS}}\left(\mathbb{M}_p^{(l)}\right)$ for nested models both when the true data source has a model included in one of the models and when it is not.

5.1 An Upper Bound by Two-Part MDL

Let $\hat{\theta}_{\text{ML}}^{(l)}$ denote the maximum likelihood estimate of $\theta$. The minimization of

$$\text{SIC}\left(\mathbb{M}_p^{(l)}\right) := -\ln P_{\hat{\theta}_{\text{ML}}^{(l)}}(\mathcal{D}) + \frac{\dim(\Theta^{(l)})}{2} \ln n_o$$

(72)

as a function on the set of models $\mathbb{M}_p^{(l)}$, $l = 1, \ldots, L$, is known as Schwarz’s information criterion for model determination, see Cavanaugh and Neath (1999) for the derivation, Neath and Cavanaugh (2012) for a recent survey of applications, and Rissanen (2007, pp. 5–6) and Robert (2007, section 7.2.3, pp. 352–353) for critical remarks. It is needless to point out that minimization of $\text{SIC}\left(\mathbb{M}_p^{(l)}\right)$ is not available for implicit models and likelihood-free inference.

Rissanen proved that the model achieving the minimum of $\text{SIC}\left(\mathbb{M}_p^{(l)}\right)$ gives the least redundant coding possible of $\mathcal{D}$ amongst all universal codes, where optimal quantization of $\Theta$ is achieved by using accuracy of order $1/\sqrt{n_o}$, see Roos (2016, p. 2) for the result and further references.

By Section 3.2 above, the term $2n_o D_{\text{JS}}\left(\hat{P}_\mathcal{D}, P_{\hat{\theta}_{\text{JS}}^{(l)}}\right)$ in Equation (48) can be regarded as redundancy in a different sense. In other words, $\text{SIC}_{\text{JS}}\left(\mathbb{M}_p^{(l)}\right)$ is a sum of redundancy and a penalty term of basically same form as in the two part redundancy code length in Equation (72). The next proposition is suggested by Section 4.1.

Proposition 17: With $\text{SIC}$ as defined in Equation (72) and $\text{SIC}_{\text{JS}}$ from Equation (48) it holds that

$$\text{SIC}_{\text{JS}}\left(\mathbb{M}_p^{(l)}\right) < \text{SIC}\left(\mathbb{M}_p^{(l)}\right).$$

(73)

Proof: By definition of $\hat{\theta}_{\text{JS}}$ in Equation (49) we have for $\hat{\theta}_{\text{ML}}$, the maximum likelihood estimate of $\theta$ based on $\mathcal{D}$,

$$2n_o D_{\text{JS}}\left(\hat{P}_\mathcal{D}, P_{\hat{\theta}_{\text{JS}}^{(l)}}\right) \leq 2n_o D_{\text{JS}}\left(\hat{P}_\mathcal{D}, P_{\hat{\theta}_{\text{ML}}}\right)$$

(74)
and by Lemma 8 and definition of $D_{KL}$ (Equation 28)

\[
2n_o D_{JS} \left( \hat{P}_D, P_{\hat{\theta}} \right) \leq n_o D_{KL} \left( \hat{P}_D, P_{\hat{\theta}_{ML}} \right) \\
= \sum_{j=1}^{k} n_{o,j} \ln \left( \frac{n_{o,j}}{n_o} \right) - \sum_{j=1}^{k} n_{o,j} \ln \left( p_j \left( \hat{\theta}_{ML} \right) \right) \\
< - \sum_{j=1}^{k} n_{o,j} \ln \left( p_j \left( \hat{\theta}_{ML} \right) \right),
\]

since $\sum_{j=1}^{k} n_{o,j} \ln \left( \frac{n_{o,j}}{n_o} \right) < 0$. Hence we have established that

\[
2n_o D_{JS} \left( \hat{P}_D, P_{\hat{\theta}_{JSD}} \right) < - \ln P_{\hat{\theta}_{ML}} (D).
\]

Since $\frac{\text{dim}(\Theta(l))}{8\pi} \ln \frac{n_o}{8\pi} < \frac{\text{dim}(\Theta(l))}{2} \ln n_o$, the inequality in the proposition holds by the definitions in Equations (48) and (72).

The criteria in Equations (48) and (72) are also inherently connected via the already cited fact that $\hat{\theta}_{JSD}$ and $\hat{\theta}_{ML}$ are asymptotically equal, when $n_o \to +\infty$, as shown in Corander et al. (2021).

The inequality Equation (73) tells that if for the optimal model $M_{p}^{(l_o)}$ w.r.t SIC the minimum value of SIC $\left( M_{p}^{(l_o)} \right)$ is very small, then $M_{p}^{(l_o)}$ is likely to be the minimizer of SIC$_{JSD}$, too.

### 5.2 Consistency of the JSD-Razor Rule

We show next a consistency property of the JSD-Razor model selection criterion for nested models. Consistency means that the criterion will asymptotically select, with probability one, amongst candidate models $M_{p}^{(l)}$, $l = 1, \ldots, L$, the the most parsimonious $\Theta^{(l)}$ model containing the true generating distribution. From a theoretical point of view such consistency is a very strong optimality property of the JSD-Razor model choice.

**Proposition 18** The models $M_{p}^{(l)}$, $l = 1, \ldots, L$ are nested

\[
\Theta^{(1)} \subseteq \Theta^{(2)} \subseteq \ldots \subseteq \Theta^{(L)}
\]

and $\dim \left( \Theta^{(1)} \right) \leq \dim \left( \Theta^{(2)} \right) \leq \ldots \leq \dim \left( \Theta^{(L)} \right) (< k)$. Suppose that $l_o$ is the smallest integer in $\{1, \ldots, L\}$ such that the true probability $P_{\theta_o} \in M_{p}^{(l_o)}$. Then for large $n_o$

\[
\text{SIC}_{JSD} \left( M_{p}^{(l_o)} \right) \leq \text{SIC}_{JSD} \left( M_{p}^{(l)} \right) \text{ for every } l \neq l_o \quad (74)
\]

with $P_{\theta_o}$-probability one.

**Proof** For economy of space let us set $C \left( l, n_o \right) := \text{dim}(\Theta(l)) \ln \frac{n_o}{8\pi}$. There are two cases with distinct arguments.
l > l_o$: When \( P_{\theta_o} \in \mathcal{M}^{(l_o)} \), then \( P_{\theta_o} \in \mathcal{M}^{(l)} \) by the nesting property. It holds thus that \( \theta_o \in \Theta^{(l_o)} \) implies \( \theta_o \in \Theta^{(l)} \) for every \( l \) such that \( l > l_o \), too. Let now \( \hat{\theta}^{(l)}_{\text{JSD}} = \hat{\theta}^{(l)}_{\text{JSD}}(D) \) be given in (49). As already stated above, Corander et al. (2021, Lemma 5.1, Proposition 5.2) shows that when \( P_{\theta_o} \in \mathcal{M}^{(l)} \), then

\[
D_{\text{JS}} \left( P_{\theta_o}, P^{(l)}_{\hat{\theta}_{\text{JSD}}} \right) \to 0
\]

\( P_{\theta_o} \) a.s., as \( n_o \to +\infty \) for all \( l > l_o \) and also for \( l = l_o \). This means that there is some \( n_\epsilon \) such that for \( n_o > n_\epsilon \)

\[
\text{SIC}_{\text{JSD}} \left( \mathcal{M}^{(l_o)}_p \right) = 2n_o \epsilon + C (l_o, n_o) \leq 2n_o \epsilon + C (l, n_o). \tag{75}
\]

since \( C (l_o, n_o) \leq C (l, n_o) \) for every \( l > l_o \), when \( n_o > 8\pi \).

\( l < l_o \): Since \( P_{\theta_o} \notin \mathcal{M}^{(l)} \) for \( l < l_o \), then it holds for every \( l < l_o \) and for a \( \delta > 0 \) defined by the inefficiency of \( \mathcal{M}^{(l)} \) w.r.t. \( P_{\theta_o} \) that

\[
\delta := \min_{\theta \in \Theta^{(l)}} D_{\text{JS}}^{1/2} \left( P_{\theta_o}, P_{\theta} \right) \leq D_{\text{JS}}^{1/2} \left( P_{\theta_o}, P^{(l)}_{\hat{\theta}_{\text{JSD}}(D)} \right)
\]

with \( \hat{\theta}^{(l)}_{\text{JSD}}(D) \) defined as in Equation (49) for any \( l < l_o \). In view of Proposition 7 we can apply the triangle inequality in the right-hand side to the effect that

\[
D_{\text{JS}}^{1/2} \left( P_{\theta_o}, P^{(l)}_{\hat{\theta}_{\text{JSD}}(D)} \right) \leq D_{\text{JS}}^{1/2} \left( P_{\theta_o}, \hat{P}_D \right) + D_{\text{JS}}^{1/2} \left( \hat{P}_D, P^{(l)}_{\hat{\theta}_{\text{JSD}}(D)} \right) .
\]

Hence

\[
D_{\text{JS}} \left( P_{\theta_o}, P^{(l)}_{\hat{\theta}_{\text{JSD}}(D)} \right) \leq 2D_{\text{JS}} \left( P_{\theta_o}, \hat{P}_D \right) + 2D_{\text{JS}} \left( \hat{P}_D, P^{(l)}_{\hat{\theta}_{\text{JSD}}(D)} \right) .
\]

As \( D \sim P_{\theta_o}, D_{\text{JS}}^{1/2} \left( P_{\theta_o}, \hat{P}_D \right) \to 0 \), as \( n_o \) increases to \( +\infty \), as shown in Corander et al. (2021, Lemma 5.1, Proposition 5.2). It follows that

\[
\delta^2 < \liminf_{n_o \to +\infty} 2D_{\text{JS}} \left( \hat{P}_D, P^{(l)}_{\hat{\theta}_{\text{JSD}}(D)} \right) .
\]

Hence for \( l < l_o \)

\[
\text{SIC}_{\text{JSD}} \left( \mathcal{M}^{(l)}_p \right) = 2n_o D_{\text{JS}} \left( \hat{P}_D, P^{(l)}_{\hat{\theta}_{\text{JSD}}(D)} \right) + C (l, n_o) \tag{76}
\]

is a function of \( n_o \) that will ultimately with \( P_{\theta_o} \) -probability one exceed \( \text{SIC}_{\text{JSD}} \left( \mathcal{M}^{(l_o)}_p \right) = 2n_o \epsilon + C (l_o, n_o) \) established in the first case of this proof. In more detail, suppose that \( \epsilon < \delta^2 \) and that \( n_o \) satisfies

\[
2n_o \left[ D_{\text{JS}} \left( \hat{P}_D, P^{(l)}_{\hat{\theta}_{\text{JSD}}(D)} \right) - \epsilon \right] > \frac{n_o}{8\pi} \Delta, \tag{77}
\]

where \( \Delta := (\dim(\Theta^{(l_o)}) - \dim(\Theta^{(l)})) > 0 \). As \( 2n_o \) grows faster than \( \ln \frac{n_o}{8\pi} \) when \( n_o \) grows, and by Equation (33) the positive factor multiplying \( 2n_o \) is bounded, there is an integer \( N \) such that Equation (77) holds for all \( n_o > N \) with \( P_{\theta_o} \) probability one. The inequality in Equation (77) is equivalent to

\[
\text{SIC}_{\text{JSD}} \left( \mathcal{M}^{(l)}_p \right) - \text{SIC}_{\text{JSD}} \left( \mathcal{M}^{(l_o)}_p \right) > 0
\]

22
Hence we have proved the required consistency property.

5.3 JSD-Razor Rule, when the True Distribution is not Covered by the Models

We shall apply the following result, which is valid for any $P_o$, inside or outside the models.

**Proposition 19** Assume that Equation (8) holds for $P_o \in \mathbb{P}$ and for any $P_{\theta} \in \mathcal{M}_p$. Let $D = (D_1, \ldots, D_{n_o})$ be an i.i.d. $n_o$-sample $\sim P_o$. Then it holds that

$$\lim_{n_o \to +\infty} D_{\text{JS}}\left(\hat{P}_D, P_{\theta}\right) = D_{\text{JS}}(P_o, P_{\theta}).$$

$p_o$-a.s..

The proof is found in Corander et al. (submitted). Proposition 19 is next applied to study of model choice by minimization of $\text{SIC}_{\text{JS}}(\mathcal{M}_p(l))$ when there are $L$ nested models $\mathcal{M}_p(l)$ such that $P_o$ is outside of $\mathcal{M}_p(l)$ for every $l$. Of course, Lemma 16 used in derivation of $\text{SIC}_{\text{JS}}$ requires that $P_o \in \mathcal{M}_p$. The result below is perhaps in spite of this a natural extension. Here $D_{\text{JS}}(P_o, P_{\theta(l)}) > 0$ for every $P_{\theta(l)} \in \mathcal{M}_p(l)$ for every $l$.

**Lemma 20** The models $\mathcal{M}_p(l)$, $l = 1, \ldots, L$ are nested

$$\Theta^{(1)} \subseteq \Theta^{(2)} \subseteq \ldots \subseteq \Theta^{(L)}$$

and $\dim(\Theta^{(1)}) \leq \dim(\Theta^{(2)}) \leq \ldots \leq \dim(\Theta^{(L)}) (< k)$. Suppose $P_o \notin \mathcal{M}_p(l)$ for every $l$. Let $D = (D_1, \ldots, D_{n_o})$ be an i.i.d. $n_o$-sample $\sim P_o$. The assumption in Equation (8) holds for $P_o \in \mathbb{P}$. Let us assume that there is $P_{\theta(l^*)} \in \mathcal{M}_p(l^*)$ such that

$$0 < \delta^* := D_{\text{JS}}^{1/2}(P_o, P_{\theta(l^*)}) = \min_{1 \leq l \leq L} \min_{\theta(l) \in \Theta(l)} D_{\text{JS}}^{1/2}(P_o, P_{\theta(l)})$$

(79)

Then, for every $l \geq l^*$, as $n_o \to +\infty$,

$$D_{\text{JS}}\left(\hat{P}_D, P_{\hat{\theta}^{(l^*)}_{\text{JS}}(D)}\right) \to (\delta^*)^2$$

(80)

with $P_o$-probability one, where $\hat{\theta}^{(l)}_{\text{JS}}$ is computed in Equation (49).

**Proof** It holds by Equation (79) for every $l \geq l^*$ that

$$0 < \delta^* \leq D_{\text{JS}}^{1/2}(P_o, P_{\hat{\theta}^{(l^*)}_{\text{JS}}(D)})$$

(81)

By the triangle inequality justified by Proposition 7 we have

$$D_{\text{JS}}^{1/2}(P_o, P_{\hat{\theta}^{(l)}_{\text{JS}}(D)}) \leq D_{\text{JS}}^{1/2}(P_o, \hat{P}_D) + D_{\text{JS}}^{1/2}(\hat{P}_D, P_{\hat{\theta}^{(l^*)}_{\text{JS}}(D)}).$$

(82)
By definition of $\hat{\theta}^{(l)}_{\text{JSD}}$ and since the models are nested and $l \geq l^*$, we bound the right hand side upwards by
\begin{equation}
\leq D_{\text{JS}}^{1/2}(P_o, \widehat{P}_D) + D_{\text{JS}}^{1/2}(\widehat{P}_D, P_{\hat{\theta}^{(l^*)}}) .
\end{equation}
(83)
The proof of Theorem 17 in Corander et al. (submitted) can be used ad verbatim to show that
\begin{equation}
D_{\text{JS}}^{1/2}(P_o, \widehat{P}_D) \to 0, \text{ as } n_o \to +\infty
\end{equation}
(84)
P$_o$-a.s.. In addition, Proposition 19 entails that
\begin{equation}
D_{\text{JS}}^{1/2}(\widehat{P}_D, P_{\hat{\theta}^{(l^*)}}) \to 0, \text{ as } n_o \to +\infty.
\end{equation}
(85)
P$_o$-a.s.. In view of Equations (81)–(85), we have
\begin{equation}
0 < \delta^* \leq \min_{\theta \in \Theta^{(l)}} D_{\text{JS}}^{1/2}(P_o, P_{\theta}) \leq \min_{\theta \in \Theta^{(l)}} D_{\text{JS}}^{1/2}(\widehat{P}_D, P_{\hat{\theta}^{(l^*)}}) JSD(D).
\end{equation}
(86)
Hence the claim in Equation (80) is established.

**Proposition 21** Under the assumptions of Lemma 20, it holds for large $n_o$ and every $l$
\begin{equation}
\text{SIC}_{\text{JSD}} \left( M_p^{(l^*)} \right) \leq \text{SIC}_{\text{JSD}} \left( M_p^{(l)} \right) \text{ for every } l \neq l_o
\end{equation}
with $P_o$- probability one.

**Proof**

$l > l^*$: By Lemma 20 and replacement of $P_{\hat{\theta}}$ with $P_o$, the proof of Proposition 18 can be modified to entail the statement in Equation (75) in the form that there is some $n_\epsilon$ such that for $n_o > n_\epsilon$
\begin{equation}
\text{SIC}_{\text{JSD}} \left( M_p^{(l_o)} \right) = 2n_o(\delta^*)^2 + C(l^*, n_o) \leq 2n_o(\delta^*)^2 + C(l, n_o).
\end{equation}
(87)
since $C(l^*, n_o) \leq C(l, n_o)$ for every $l > l^*$, when $n_o > 8\pi$.

$l < l^*$: Since $P_o \notin M^{(l)}$ for $l < l^*$, then it holds for every $l < l_o$ and for $\delta^* > 0$ in Equation (79) that
\begin{equation}
0 < \delta^* \leq \min_{\theta \in \Theta^{(l)}} D_{\text{JS}}^{1/2}(P_o, P_{\theta}) \leq D_{\text{JS}}^{1/2}(P_o, P_{\hat{\theta}^{(l_o)}}) JSD(D).
\end{equation}

It follows modifying the second case proof of Proposition 18 that
\begin{equation}
(\delta^*)^2 < \lim_{n_o \to +\infty} \inf 2D_{\text{JS}} \left( \widehat{P}_D, P_{\hat{\theta}^{(l_o)}} \right).
\end{equation}
Hence for \( l < l^* \)

\[
\text{SIC}_{\text{JSD}} \left( M^{(l)}_p \right) = 2n_o D_{\text{JS}} \left( \hat{P}_D, P_{\hat{\theta}^{(l)}} \right) + C \left( l, n_o \right).
\] (88)

is a function of \( n_o \) that will ultimately with \( P_o \)-probability one exceed \( \text{SIC}_{\text{JSD}} \left( M^{(l^*)}_p \right) = 2n_o(\delta^*)^2 + C \left( l^*, n_o \right) \) established in the first case of this proof. The rest of the proof is as in Proposition 18.

6. Simulation Experiments

The experiments carried out in this work are aimed to evaluate the proposed SIC-JSD rule and its simulator-based approximation SIC-BOLFI. We evaluate the model selection rules using simulation experiments where the true model is known, and test simulator-based model selection in a real task studied in previous work (Corander et al., 2017). Section 6.1 reviews the model selection rules used in the experiments while Sections 6.2–6.4 present the experiments and results in more detail.

6.1 Methods

The model selection experiments considered in this work compare candidate models \( M^{(l)}_p \) fitted to observed data. We run experiments with simulated observations to evaluate how the proposed model selection rule and its simulator-based approximation behave in different test conditions and when we increase the observed data set size \( n_o \). While the present work focuses on parameter estimation and model selection in simulator-based models with intractable likelihoods, the simulation experiments in Section 6.2–6.3 were carried out with models where the mapping between model parameters \( \theta \) and observation probabilities \( P_{\theta} \) is available. These experiments allowed us to evaluate model selection based on SIC (Equation 72) and SIC-JSD (Equation 48).

When the mapping between model parameters and observation probabilities is complicated or unknown, parameter estimation and model selection are carried out based on comparison between observed and simulated data. The present experiments use BOLFI (Gutmann and Corander, 2016) to find parameter values that minimize the expected JSD between observed and simulated data. The experiments were carried out with the implementation available in ELFI (Lintusaari et al., 2018). Gaussian process regression with a normal likelihood and squared exponential kernel was used to model the dependencies between simulator parameters and expected JSD between observed and simulated data in BOLFI, and the parameter values used in the simulations were selected based on the lower confidence bound acquisition rule (Section 6.2–6.3) or the maximum variance acquisition rule (Section 6.4). The candidate models studied in Section 6.2 were fitted using 1000 iterations and the candidate models Section 6.3 and 6.4 using 2000 iterations.
6.2 Experiment 1

This experiment studies model selection using the nested model introduced in Example 2. We simulate 100 observation sets with \( n_o = 100 \) and \( n_o = 1000 \) samples using model \( M_p^{(0)} \) which corresponds to \( \theta = (0, 0) \), model \( M_p^{(1)} \) with \( \theta = (0.2, 0) \) and \( \theta = (0.7, 0) \), and model \( M_p^{(2)} \) with \( \theta = (0.2, 0.2) \), \( \theta = (0.7, 0.2) \), \( \theta = (0.2, 0.7) \), and \( \theta = (0.7, 0.7) \). The corresponding category probabilities are visualized in Figure 1.

The candidate models \( M_p^{(0)} \), \( M_p^{(1)} \), and \( M_p^{(2)} \) are each fitted to the simulated observation sets and model selection is carried out based on SIC, SIC-JSD, and SIC-BOLFI. The model selection results calculated based on observation sets with \( n_o = 100 \) observations are presented in Figure 2 and the results calculated based on observation sets with \( n_o = 1000 \) observations in Figure 3. We observe that when \( n_o = 100 \), all model selection rules favor \( M_p^{(0)} \) in test conditions where the true model parameters have low values, and \( M_p^{(1)} \) in test conditions where the second parameter alone has a low value. However the model selection rules do not agree in all experiments. SIC chooses \( M_p^{(0)} \) or \( M_p^{(1)} \) over the true model in more experiments than SIC-JSD or SIC-BOLFI, while SIC-JSD and SIC-BOLFI choose \( M_p^{(2)} \) over
Figure 2: Model selection results calculated based on 100 observation sets with $n_o = 100$ observations simulated with the models in Figure 1. Model selection rules used in the experiment are (a) SIC, (b) SIC-JSD, and (c) SIC-BOLFI.

the true model in more experiments than SIC. This difference disappears when $n_o = 1000$, and all model selection rules also choose the true model in more experiments.

6.3 Experiment 2

The second experiment studies model selection between log-linear models that describe the association and interaction patterns between two categorical random variables. The counts in a two-way table are modeled as a sample from a multinomial distribution with $k = 4$ categories and expected observation counts $\mu_i$ modeled as

$$\log(\mu_i) = \lambda + X_i\lambda^X + Y_i\lambda^Y + X_iY_i\lambda^{XY}, \quad i = 1, 2, 3, 4,$$

(89)

where $i$ indexes the categories and $X_i$ and $Y_i$ are effect-coded variables that take values 1 or -1 as indicated in Table 1. The model parameters $\lambda^X$ and $\lambda^Y$ then encode expected difference in the proportion between 1 and -1 values in variables $X$ and $Y$, and the parameter $\lambda^{XY}$ encodes possible association between the two variable values. Finally the constant $\lambda$ is calculated based on the other parameter values and sample size $n$ so that the sum over expected counts equals $n$.

We run experiments with a two-parameter model $M_p^{(2)}$ where $\lambda^{XY} = 0$ and the model parameters $\theta = (\lambda^X, \lambda^Y)$ and a saturated or three-parameter model $M_p^{(3)}$ where the model parameters $\theta = (\lambda^X, \lambda^Y, \lambda^{XY})$. The observation sets used in the experiments are simulated with parameter values selected as follows. The model parameters $\lambda^X$ and $\lambda^Y$ are first associated with 100 values selected at random within $[-1, 1] \times [-1, 1]$ while the interaction
Figure 3: Model selection results calculated based on 100 observation sets with \( n_o = 1000 \) observations simulated with the models in Figure 1. Model selection rules used in the experiment are (a) SIC, (b) SIC-JSD, and (c) SIC-BOLFI.

| \( i \) | 1 | 2 | 3 | 4 |
|---|---|---|---|---|
| \( X_i \) | 1 | 1 | -1 | -1 |
| \( Y_i \) | 1 | -1 | 1 | -1 |

Table 1: Effect coding in the log-linear example.
Likelihood-free Model Choice with the Jensen–Shannon Divergence

\[
\begin{array}{cccccccccccc}
\lambda^{XY} & -0.5 & -0.4 & -0.3 & -0.2 & -0.1 & 0.0 & 0.1 & 0.2 & 0.3 & 0.4 & 0.5 \\
SIC & 0.94 & 0.75 & 0.53 & 0.33 & 0.11 & 0.01 & 0.00 & 0.42 & 0.59 & 0.77 & 0.93 \\
SIC-JSD & 0.99 & 0.87 & 0.67 & 0.44 & 0.20 & 0.10 & 0.17 & 0.55 & 0.76 & 0.92 & 0.96 \\
SIC-BOLFI & 0.99 & 0.89 & 0.68 & 0.46 & 0.24 & 0.16 & 0.22 & 0.58 & 0.77 & 0.94 & 0.96 \\
\end{array}
\]

\[
\begin{array}{cccccccccccc}
\lambda^{XY} & -0.5 & -0.4 & -0.3 & -0.2 & -0.1 & 0.0 & 0.1 & 0.2 & 0.3 & 0.4 & 0.5 \\
SIC & 1.00 & 1.00 & 1.00 & 0.96 & 0.41 & 0.00 & 0.43 & 0.95 & 1.00 & 1.00 & 1.00 \\
SIC-JSD & 1.00 & 1.00 & 1.00 & 0.95 & 0.39 & 0.00 & 0.41 & 0.95 & 1.00 & 1.00 & 1.00 \\
SIC-BOLFI & 1.00 & 1.00 & 1.00 & 0.95 & 0.39 & 0.00 & 0.39 & 0.95 & 1.00 & 1.00 & 1.00 \\
\end{array}
\]

Table 2: \( M_p^{(3)} \) selection rate calculated based on 100 observation sets with (a) \( n_o = 100 \) or (b) \( n_o = 1000 \) observations simulated with the log-linear model.

parameter is associated with 11 values selected at interval 0.1 between −0.5 and 0.5. We then combine each \( \lambda^{XY} \) value with the \( \lambda^X \) and \( \lambda^Y \) values to create \( 11 \times 100 \) parameter combinations and use each combination to simulate observation sets with \( n_o = 100 \) and \( n_o = 1000 \) samples.

Model selection results between \( M_p^{(2)} \) and \( M_p^{(3)} \) are presented in Table 2. We observe that SIC-JSD and SIC-BOLFI choose \( M_p^{(3)} \) over \( M_p^{(2)} \) in more experiments than SIC when \( n_o = 100 \), but the differences disappear when \( n_o = 1000 \). Comparison between the model selection rates in experiments with \( n_o = 100 \) and \( n_o = 1000 \) also indicates that all model selection rules choose the true model in more experiments when \( n_o = 1000 \).

6.4 Experiment 3

The last experiment is carried out with the simulator models and data used in previous work (Corander et al., 2017). Corander et al. (2017) studied negative frequency-dependent selection (NFDS) in genotype frequencies in post-vaccine pneumococcal populations. We replicate a comparison between three simulators that model the evolution in genotype frequencies as a discrete-time process where the population at time \( t \) is sampled with replacement from population at time \( t - 1 \) using reproduction probabilities calculated based on simulator parameters \( \theta \). The candidate models are nested and include the neutral model, the homogeneous-rate multilocus NFDS model, and the heterogeneous-rate multilocus NFDS model.

The models considered in this experiment calculate the reproduction probabilities based on 2–5 parameters as follows. The neutral model \( M_p^{(2)} \) takes into account the migration rate \( m \) and the vaccine selection strength \( v \). These capture the negative pressure due to migration into population and the negative selection pressure on vaccine-type isolates. The other model variants extend the neutral model to take into account how isolates with rare variations in their accessory genome could experience positive selection pressure under NFDS. The difference between the two models is how variations that occur in different loci contribute in the selection pressure. The homogeneous-rate multilocus NFDS model \( M_p^{(3)} \)
associates all variations with the maximal selection pressure $\sigma_f$ while the heterogeneous-rate multilocus NFDS model $M_p^{(5)}$ associates variations in some loci with a weaker selection pressure $\sigma_w$. The proportion of loci under stronger NFDS is captured with the model parameter $p_f$.

The candidate models are fitted to data that was collected to follow how vaccination affected the pneumococcal population in Massachusetts (Croucher et al., 2013). The data set used in this experiment includes a pre-vaccination ($t = 0$) sample with 133 isolates and two post-vaccination samples with 203 isolates collected at $t = 36$ and 280 isolates collected at $t = 72$. The isolates have been divided into 41 sequence clusters and typed as vaccine or non-vaccine type as discussed in previous work (Corander et al., 2017). The data set is visualized in Figure 4. The negative selection pressure on vaccine-type isolates is observed as a reduction in the vaccine-type isolates over time. In addition we observe a change in the relative frequencies between sequence clusters represented in the population that is non-vaccine type. This could indicate that the vaccine resulted in a positive selection pressure on isolates in certain sequence clusters.

Parameter estimation is carried out as proposed in the previous work. We sample the pre-vaccine ($t = 0$) data to initialize the simulated population in each candidate model and use BOLFI to find the parameter estimates that minimize the expected JSD between observed and simulated data sets at $t = 36$ and $t = 72$. Hence the sample size used in parameter estimation and model selection $n_o = 483$. Parameter estimation is carried out over $\ln(m) \in [-7, -1.6]$, $\ln(n) \in [-7, -0.7]$, $\ln(\sigma_f) \in [-7, -1.6]$, $\ln(\sigma_w) \in [-7, -1.9]$, and
Likelihood-free Model Choice with the Jensen–Shannon Divergence

| Model  | Selection rate | JSD   | $\hat{m}$ | $\hat{v}$ | $\hat{\sigma}_f$ | $\hat{\sigma}_w$ | $\hat{\rho}_f$ |
|--------|----------------|-------|-----------|-----------|-------------------|-------------------|---------------|
| $M_p^{(2)}$ | 0.00          | 0.23  | 0.007     | 0.037     |                   |                   |               |
| $M_p^{(3)}$ | 0.00          | 0.20  | 0.006     | 0.073     | 0.008             |                   |               |
| $M_p^{(5)}$ | 1.00          | 0.14  | 0.005     | 0.088     | 0.114             | 0.002             | 0.372         |

Table 3: Model selection rate and median parameter estimation results calculated based on 100 BOLFI experiments with the pneumococcal population models and data.

| Model | Selection rate | JSD   |
|-------|----------------|-------|
| $M_p^{(2)}$ | 0.84          | 0.11  |
| $M_p^{(3)}$ | 0.10          | 0.11  |
| $M_p^{(5)}$ | 0.06          | 0.11  |

Table 4: Model selection rate and median minimum expected JSD calculated based on 100 observation sets simulated with the pneumococcal population models (a) $M_p^{(2)}$ and (b) $M_p^{(3)}$.

$p_f \in [0, 1]$ with the constraint $\sigma_f > \sigma_w$, and the model selection criterion is evaluated based on the average over the expected JSD at $t = 36$ and $t = 72$. The parameter estimation and model selection are replicated 100 times to capture possible random variation between parameter estimates and model fit evaluated with BOLFI.

The model selection results reported in Table 3 indicate that SIC-BOLFI chooses the heterogeneous multilocus NFDS model $M_p^{(5)}$ over the neutral model $M_p^{(2)}$ or the homogeneous multilocus NFDS model $M_p^{(3)}$. The outcome seems reasonable since $M_p^{(5)}$ introduces a notable improvement in the model fit. However we also check that the model selection rule is not biased towards $M_p^{(5)}$ by running an additional simulation experiment. We simulate 100 observation sets with 250 isolates sampled at $t = 36$ and $t = 72$ ($n_o = 500$) using $M_p^{(2)}$ with $m = 0.007$ and $v = 0.050$ and $M_p^{(3)}$ with $m = 0.007$, $v = 0.050$, and $\sigma_f = 0.007$. The model selection results reported in Table 4 show that the true model is selected in most experiments.

7. Discussion and Conclusions

Model choice as a statistical problem has a rich history in computer science, inspired in particular by information theory, and in statistics, where the major innovations have been
founded on Bayesian thinking, which provides an intrinsic solution to the need to penalize more complex models by the prior distribution of the model parameters. However, literature on model choice for the likelihood-free inference setting is scarce, which is understandable since the vast majority of existing model scoring criteria use the likelihood in one way or another to measure the fidelity of a model as a data representation.

The approach introduced here (JSD-Razor) was inspired by the Occam’s Razor as developed by Balasubramanian and co-workers in Balasubramanian (2005), Balasubramanian (1996) and Myung et al. (2000), as well as by our previous work on the asymptotics of likelihood-free parameter inference under JSD (Corander et al. 2021). To the best of our knowledge, this is the first information-theoretic model scoring criterion introduced for simulator-based likelihood-free modeling setting. We anticipate that there are multiple opportunities for future developments in this area that can broaden the applicability of JSD-Razor to several other classes of models and spawn even more refined scoring criteria. For example, in model classes with continuous output, it would be possible to consider quantization to make JSD-Razor applicable, which raises several interesting questions related to the relative loss of information as a function quantization scheme and the sample size.

Acknowledgments

The authors wish to acknowledge CSC – IT Center for Science, Finland, for computational resources. J.C. and U.R. are supported by ERC grant 742158 and T.K. is supported by FCAI (=Finnish Center for Artificial Intelligence).
Appendix A. Expressions and Bounds for JSD

Let us next define the metric $||.||_2$ on $\mathbb{P} \times \mathbb{P}$ by means of the norm on $\mathbb{R}^k$ as

$$||P - Q||_2 := \sqrt{\sum_{x \in A} (P(x) - Q(x))^2} = ||\Delta(P) - \Delta(Q)||_{2, \mathbb{R}^k}. \quad (A.1)$$

**Lemma A.1** For any $(P, Q) \in \mathbb{P} \times \mathbb{P}$

$$D_{JS}^{1/2}(P, Q) \geq \frac{\sqrt{2}}{\sqrt{4}} \cdot ||P - Q||_2. \quad (A.2)$$

**Proof** Since the square root is a concave function on $[0, +\infty)$, we have by Equation (29)

$$D_{JS}^{1/2}(P, Q) \geq \frac{1}{2} D_{KL}(P, M) + \frac{1}{2} D_{KL}(Q, M). \quad (A.3)$$

It is shown in Birch (1964, Lemma 1 p. 819) that for any $(P, Q) \in \mathbb{P} \times \mathbb{P}$

$$D_{KL}(P, Q) \geq \frac{1}{2} ||P - Q||_2^2. \quad (A.4)$$

Hence we bound downwards in the right hand side of Equation (A.3) by

$$\geq \frac{1}{2\sqrt{2}} (||P - M||_2 + ||Q - M||_2). \quad (A.5)$$

Here by Equation (A.1)

$$||P - M||_2 = \sqrt{\sum_{i=1}^{k} \left( p_i - \frac{1}{2} (p_i + q_i) \right)^2} = \frac{1}{2} ||P - Q||_2,$$

and

$$||Q - M||_2 = \frac{1}{2} ||Q - P||_2 = \frac{1}{2} ||P - Q||_2.$$ 

When we insert the last two equalities in Equation (A.5), the assertion in the lemma follows.

The inequality above gives a minor observation with

$$\int_{\Theta} e^{-2n_0 D_{JS}(\hat{P}_D, P_0)} p(\theta) d\theta \leq \int_{\Theta} e^{-\frac{n_0}{4} ||\hat{P}_D - P_0||_2^2} p(\theta) d\theta.$$ 

The right-hand integral contains formally the non-normalized multivariate normal density with the $d \times d$ unit matrix multiplied by $\frac{n_0}{2}$ as covariance matrix, thus a kind of likelihood function for $\theta$. 

33
Appendix B. Differential Calculus for the Fisher Information Matrix of $\mathcal{M}_p$ and the Hessian of JSD

B.1 Information Matrix

Next we check Lemma 11.

**Proof** By definition $I_{ij}(\theta)$ is

$$I_{ij}(\theta) = \sum_{x \in \mathcal{A}} \left( \frac{\partial}{\partial \theta_i} \ln P_\theta(x) \frac{\partial}{\partial \theta_j} \ln P_\theta(x) \right) P_\theta(x) \quad \text{(B.1)}$$

By properties of the Iverson bracket and Equation (10) it follows readily that

$$I_{ij}(\theta) = \sum_{s=1}^k \frac{\frac{\partial}{\partial \theta_i} p_s(\theta) \frac{\partial}{\partial \theta_j} p_s(\theta)}{p_s(\theta)} \quad \text{(B.2)}$$

We have by rules of matrix multiplication and the Jacobian given in Equation (25) that

$$A(\theta)^T A(\theta) = \sum_{s=1}^k \frac{p_s'(\theta)^T p_s'(\theta)}{p_s(\theta)} \quad \text{(B.3)}$$

where $^T$ is the vector transpose and each $p_s'(\theta)^T p_s'(\theta)$ is a $d \times d$-matrix. The array at position $(i, j)$ in this matrix is by Equation (18)

$$\left( p_s'(\theta)^T p_s'(\theta) \right)_{i,j} = \frac{\frac{\partial}{\partial \theta_i} p_s(\theta) \frac{\partial}{\partial \theta_j} p_s(\theta)}{p_s(\theta)} \quad \text{(B.4)}$$

Hence the array at position $(i, j)$ in $A(\theta)^T A(\theta)$ is

$$(A(\theta)^T A(\theta))_{i,j} = \sum_{s=1}^k \frac{\frac{\partial}{\partial \theta_i} p_s(\theta) \frac{\partial}{\partial \theta_j} p_s(\theta)}{p_s(\theta)} \quad \text{(B.5)}$$

But a comparison with Equation (B.2) and Equation (20) yields the asserted formula. \[\square\]

**Example B.1** Explicit expressions for the Fisher information are established for the nested families in Example 2.

(i) $\theta = (\theta_1, \theta_2)$ The $2 \times 2$ Fisher information matrix $I(\theta)$ is computed for Equation (14) by the formula in Equation (B.5) and is found elementwise as

$$I_{1,1}(\theta) = e^{-3M_2(\theta)} e^{\theta_1} \left[ e^{\theta_1} + \left( 1 + e^{\theta_2} \right)^2 + e^{\theta_1+\theta_2} \right], \quad \text{(B.6)}$$

$$I_{1,2}(\theta) = -e^{-3M_2(\theta)} e^{\theta_1+\theta_2} \left[ 1 + e^{\theta_1} + e^{\theta_2} \right] = I_{2,1}(\theta),$$

$$I_{2,2}(\theta) = e^{-3M_2(\theta)} e^{\theta_2} \left[ e^{\theta_2} + \left( 1 + e^{\theta_1} \right)^2 + e^{\theta_1+\theta_2} \right].$$

The expression $\sqrt{\det I(\theta)}$ is readily evaluated and the integral $V(\Theta) := \int_\Theta \sqrt{\det I(\theta)} d\theta$ in Equation (71) can be computed, at least numerically, for $\Theta$ such that the integral exists.
(ii) $\theta = (\theta_1, 0)$ The scalar Fisher information $I(\theta)$ is computed for Equation (15) by the formula in Equation (B.5).

\[ I(\theta) = 2e^{-3M_1(\theta)}e^{\theta_1} \left[ 2 + e^{\theta_1} \right]. \]  

(B.7)

This agrees with $I_{1,1}(\theta)$ by setting $\theta_2 = 0$ in Equation (B.6). Since $M_1(\theta) = \ln \left( 2 + e^{\theta_1} \right)$, $I(\theta)$ in Equation (B.7) simplifies to $I(\theta) = 2e^{\theta_1} / (2 + e^{\theta_1})^2$. Thereby the integral in Equation (71) becomes

\[ V(\Theta) = \sqrt{2} \int_{\Theta} e^{\theta_1/2} (2 + e^{\theta_1})^2 d\theta_1. \]  

(B.8)

When $\Theta = [a, b]$ we get by some changes of the variable of integration that

\[ V([a, b]) = \frac{2}{\pi} \left[ \arctan \left( \frac{e^{b/2}}{\sqrt{2}} \right) - \arctan \left( \frac{e^{a/2}}{\sqrt{2}} \right) \right]. \]  

(B.9)

Hence $0 < V([a, b]) < 2\pi$ for $-\infty < a < b < +\infty$.

(iii) $\theta = (0, 0)$ The rule in Equation (B.5) is not defined. However, from (ii), $2e^0 / (2 + e^0)^2 = 2/9$.

B.2 Hessian

First we prove Lemma 12.

**Proof** This is most conveniently done by differentiating the generic expression

\[ \Phi(p, \theta) = \sum_{i=1}^{k} p_i(\theta) \phi \left( \frac{p_i}{p_i(\theta)} \right), \]  

(B.10)

where $\phi$ is given in Equation (31). For $j = 1, \ldots, d$

\[ \frac{\partial}{\partial \theta_j} \Phi(p, \theta) = \sum_{i=1}^{k} \left[ \phi \left( \frac{p_i}{p_i(\theta)} \right) - \frac{p_i}{p_i(\theta)} \phi' \left( \frac{p_i}{p_i(\theta)} \right) \right] \frac{\partial}{\partial \theta_j} p_i(\theta). \]  

(B.11)

By Equation (55) we obtain

\[ \frac{\partial}{\partial \theta_j} \Phi(p, \theta) = -\frac{1}{2} \sum_{i=1}^{k} \ln \left( \frac{1}{2} \left( \frac{p_i + p_i(\theta)}{p_i(\theta)} \right) \right) \frac{\partial}{\partial \theta_j} p_i(\theta), \]

i.e.

\[ \frac{\partial}{\partial \theta_j} \Phi(p, \theta) = \frac{1}{2} \sum_{i=1}^{k} \ln \left( \frac{2p_i(\theta)}{p_i + p_i(\theta)} \right) \frac{\partial}{\partial \theta_j} p_i(\theta). \]  

(B.12)

By Equation (54), the definition of the the $k \times d$ Jacobian $J(\theta)$ in Equation (23) and rules of matrix multiplication the expression in Equation (58) is established. \qed

35
Next we prove Lemma 13.

**Proof** It is convenient to compute by means of Equation (B.11). For \( l = 1, \ldots, d \) we get by the chain rule

\[
\frac{\partial^2}{\partial \theta_i \partial \theta_j} \Phi(p, \theta) = \frac{\partial}{\partial \theta_i} \sum_{i=1}^{k} \left[ \phi \left( \frac{p_i}{p_i(\theta)} \right) - \frac{p_i}{p_i(\theta)} \phi' \left( \frac{p_i}{p_i(\theta)} \right) \right] \frac{\partial}{\partial \theta_j} p_i(\theta) \tag{B.13}
\]

\[
= \sum_{i=1}^{k} \left[ \phi \left( \frac{p_i}{p_i(\theta)} \right) - \frac{p_i}{p_i(\theta)} \phi' \left( \frac{p_i}{p_i(\theta)} \right) \right] \frac{\partial^2}{\partial \theta_i \partial \theta_j} p_i(\theta)
+ \sum_{i=1}^{k} \frac{\partial}{\partial \theta_i} \left[ \phi \left( \frac{p_i}{p_i(\theta)} \right) - \frac{p_i}{p_i(\theta)} \phi' \left( \frac{p_i}{p_i(\theta)} \right) \right] \frac{\partial}{\partial \theta_j} p_i(\theta).
\]

As observed in the proof of Lemma 12

\[
\sum_{i=1}^{k} \left[ \phi \left( \frac{p_i}{p_i(\theta)} \right) - \frac{p_i}{p_i(\theta)} \phi' \left( \frac{p_i}{p_i(\theta)} \right) \right] \frac{\partial^2}{\partial \theta_i \partial \theta_j} p_i(\theta) = \sum_{i=1}^{k} \phi' \left( \frac{p_i(\theta)}{p_i} \right) \frac{\partial^2}{\partial \theta_i \partial \theta_j} p_i(\theta). \tag{B.14}
\]

The second sum in the right hand side is computed termwise as

\[
\frac{\partial}{\partial \theta_i} \left[ \phi \left( \frac{p_i}{p_i(\theta)} \right) - \frac{p_i}{p_i(\theta)} \phi' \left( \frac{p_i}{p_i(\theta)} \right) \right] =
\]

\[
= -\phi' \left( \frac{p_i}{p_i(\theta)} \right) \frac{p_i}{p_i^2(\theta)} \frac{\partial}{\partial \theta_i} p_i(\theta) + \frac{p_i}{p_i(\theta)} \frac{\phi''}{\phi'} \left( \frac{p_i}{p_i(\theta)} \right) \frac{\partial}{\partial \theta_i} p_i(\theta) +
\]

\[
+ \frac{p_i^2}{p_i^3(\theta)} \phi'' \left( \frac{p_i}{p_i(\theta)} \right) \frac{\partial}{\partial \theta_i} p_i(\theta).
\tag{B.15}
\]

By Equation (56)

\[
\phi'' \left( \frac{p_i}{p_i(\theta)} \right) = \frac{p_i^2(\theta)}{2 p_i(p_i + p_i(\theta))}.
\]

Hence

\[
\frac{p_i^2}{p_i^3(\theta)} \phi'' \left( \frac{p_i}{p_i(\theta)} \right) = \frac{p_i}{2 p_i(p_i + p_i(\theta))}. \tag{B.16}
\]

After Equation (B.16) has been inserted in Equation (B.15), Equation (B.15) and Equation (B.14) are used in the rightmost expression in Equation (B.13) we obtain

\[
\frac{\partial^2}{\partial \theta_i \partial \theta_j} \Phi(p, \theta) = \sum_{i=1}^{k} \phi' \left( \frac{p_i(\theta)}{p_i} \right) \frac{\partial^2}{\partial \theta_i \partial \theta_j} p_i(\theta)
+ \sum_{i=1}^{k} \frac{p_i}{2 p_i(\theta) (p_i + p_i(\theta))} \frac{1}{\partial \theta_i} p_i(\theta) \frac{\partial}{\partial \theta_j} p_i(\theta). \tag{B.17}
\]
We re-organize the second term in the right-hand side of Equation (B.17) as

$$
\sum_{i=1}^{k} \frac{p_i}{2p_i(\theta) (p_i + p_i(\theta))} \frac{\partial p_i(\theta)}{\partial \theta_l} \frac{\partial p_i(\theta)}{\partial \theta_j} = \frac{1}{2} \sum_{i=1}^{k} \frac{\partial p_i(\theta)}{\partial \theta_l} \frac{\partial p_i(\theta)}{\partial \theta_j} \frac{p_i}{(p_i + p_i(\theta))}. 
$$

Next we use \( \frac{p_i}{(p_i + p_i(\theta))} = 1 - \frac{p_i(\theta)}{(p_i + p_i(\theta))} \) and by Equation (B.2) obtain

$$
= \frac{1}{2} I_{lj}(\theta) - \frac{1}{2} \sum_{i=1}^{k} \frac{\partial p_i(\theta)}{\partial \theta_l} \frac{\partial p_i(\theta)}{\partial \theta_j} \frac{p_i}{(p_i + p_i(\theta))}. 
$$

Then the argument in the proof of Lemma 11 and Equation (60) can be repeated to verify the elementwise equality

$$
\sum_{i=1}^{k} \frac{\partial p_i(\theta)}{\partial \theta_l} \frac{\partial p_i(\theta)}{\partial \theta_j} \frac{p_i}{(p_i + p_i(\theta))} = [A(p, \theta)^T A(p, \theta)]_{lj}. 
$$

Hence we have obtained the sum term in the right-hand side of Equation (B.17) as

$$
= \frac{1}{2} I_{lj}(\theta) - \frac{1}{2} [A(p, \theta)^T A(p, \theta)]_{lj}. 
$$

When we use Equation (B.20) in Equation (B.17), the asserted expression in Equation (13) of Lemma 61 is there. 

\[\blacksquare\]
References

M V Alba-Fernández, M D Jiménez-Gamero, and F Jiménez-Jiménez. Model selection based on penalized ϕ-divergences for multinomial data. *Journal of Computational and Applied Mathematics*, pages 113–18, 2020.

P M E Altham. Improving the precision of estimation by fitting a model. *Journal of the Royal Statistical Society: Series B (Methodological)*, 46(1):118–119, 1984.

S Amari and A Cichocki. Information geometry of divergence functions. *Bulletin of the Polish academy of sciences. Technical sciences*, 58(1):183–195, 2010.

A C Atkinson. A method for discriminating between models. *Journal of the Royal Statistical Society: Series B (Methodological)*, 32:323–345, 1970.

V Balasubramanian. A geometric formulation of Occam’s razor for inference of parametric distributions. *arXiv preprint adap-org/9601001*, 1996.

V Balasubramanian. MDL, Bayesian inference, and the geometry of the space of probability distributions. *Advances in minimum description length: Theory and applications*, pages 81–98, 2005.

M A Beaumont. Approximate Bayesian computation. *Annual Review of Statistics and Its Application*, 6:379–403, 2019.

M W Birch. A new proof of the Pearson-Fisher theorem. *The Annals of Mathematical Statistics*, 35(2):817–824, 1964.

K W Breitung. *Asymptotic Approximations for Probability Integrals*. Springer, 2006.

J E Cavanaugh and A A Neath. Generalizing the derivation of the Schwarz information criterion. *Communications in Statistics-Theory and Methods*, 28(1):49–66, 1999.

J Corander, C Fraser, M U Gutmann, B Arnold, W P Hanage, S D Bentley, M Lipsitch, and N J Croucher. Frequency-dependent selection in vaccine-associated pneumococcal population dynamics. *Nature Ecology & Evolution*, 1(12):1950–1960, 2017.

J Corander, U Remes, and T Koski. On the Jensen-Shannon divergence and the variation distance for categorical probability distributions. *Kybernetika*, 57(6):879–907, 2021.

J Corander, U Remes, I Holopainen, and T Koski. Non-parametric likelihood-free inference with Jensen-Shannon divergence for categorical simulator-based models. submitted.

T M Cover and J A Thomas. *Elements of Information Theory*. John Wiley & Sons, 2 edition, 2012.

K Cranmer, J Brehmer, and G Louppe. The frontier of simulation-based inference. *PNAS*, 117(48):30055–30062, 2020.

N J Croucher, J A Finkelstein, S I Pelton, P K Mitchell, G M Lee, J Parkhill, S D Bentley, W P Hanage, and M Lipsitch. Population genomics of post-vaccine changes in pneumococcal epidemiology. *Nature Genetics*, 45(6):656–663, 2013.
I Csiszár and J Körner. *Information Theory: Coding Theorems for Discrete Memoryless Systems*. Cambridge University Press, 2011.

X Didelot, R G Everitt, A M Johansen, and D J Lawson. Likelihood-free estimation of model evidence. *Bayesian Analysis*, 6(1):49–76, 2011.

P J Diggle and R J Gratton. Monte Carlo methods of inference for implicit statistical models. *Journal of the Royal Statistical Society: Series B (Methodological)*, 46(2):193–212, 1984.

D M Endres and J E Schindelin. A new metric for probability distributions. *IEEE Transactions on Information Theory*, 49(7):1858–1860, 2003.

P I Frazier. A tutorial on Bayesian optimization. *arXiv preprint arXiv:1807.02811*, 2018.

M U Gutmann and J Corander. Bayesian optimization for likelihood-free inference of simulator-based statistical models. *Journal of Machine Learning Research*, 17(125):1–47, 2016.

B G Kelly, A B Wagner, T Tularak, and P Viswanath. Classification of homogeneous data with large alphabets. *IEEE transactions on information theory*, 59(2):782–795, 2012.

M C Kennedy and A O’Hagan. Predicting the output from a complex computer code when fast approximations are available. *Biometrika*, 87(1):1–13, 2000.

P Kontkanen and P Myllymäki. A linear-time algorithm for computing the multinomial stochastic complexity. *Information Processing Letters*, 103:227–233, 2007.

T M Lapiński. Multivariate Laplace’s approximation with estimated error and application to limit theorems. *Journal of Approximation Theory*, 248:105305, 2019.

C Leuenberger and D Wegmann. Bayesian computation and model selection without likelihoods. *Genetics*, 184(1):243–252, 2010.

F Liese and I Vajda. On divergences and informations in statistics and information theory. *IEEE Transactions on Information Theory*, 52(10):4394–4412, 2006.

J Lin. Divergence measures based on the Shannon entropy. *IEEE Transactions on Information Theory*, 37(1):145–151, 1991.

J Lintusaari, M U Gutmann, R Dutta, S Kaski, and J Corander. Fundamentals and recent developments in approximate Bayesian computation. *Systematic Biology*, 66(1):e66–e82, 2017.

J Lintusaari, H Vuollekoski, A Kangasräätä, K Skytén, M Järvenpää, P Marttinen, M U Gutmann, A Vehtari, J Corander, and S Kaski. ELFI: Engine for likelihood-free inference. *Journal of Machine Learning Research*, 19(16):1–7, 2018.

J-M Marin, P Pudlo, A Estoup, and C Robert. Likelihood-free model choice. In *Handbook of Approximate Bayesian Computation*, pages 153–178. Chapman and Hall/CRC, 2018.
P Massart. Some applications of concentration inequalities to statistics. *Annales de la Faculté des sciences de Toulouse: Mathématiques*, 9(2):245–303, 2000.

T Mononen and P Myllymäki. Computing the multinomial stochastic complexity in sub-linear time. In *Proc. 4th European Workshop on Probabilistic Graphical Models*, pages 209–216, 2008.

D Morales, L Pardo, and I Vajda. Asymptotic divergence of estimates of discrete distributions. *Journal of Statistical Planning and Inference*, 48(3):347–369, 1995.

I J Myung, V Balasubramanian, and M A Pitt. Counting probability distributions: Differential geometry and model selection. *Proceedings of the National Academy of Sciences*, 97(21):11170–11175, 2000.

A A Neath and J E Cavanaugh. The Bayesian information criterion: background, derivation, and applications. *Wiley Interdisciplinary Reviews: Computational Statistics*, 4(2):199–203, 2012.

F Österreicher. Csiszár’s f-divergences - basic properties, 2002.

L Pardo. *Statistical inference based on divergence measures*. CRC press, 2018.

G Pistone. *Information Geometry of the Probability Simplex: A Short Course*. CRC press, 2018.

C R Rao and Y Wu. On model selection. *Lecture Notes-Monograph Series*, pages 1–64, 2001.

J Rissanen. *Information and complexity in statistical modeling*. Springer Science & Business Media, 2007.

C P Robert. *The Bayesian choice: from decision-theoretic foundations to computational implementation*. Springer, 2007.

C P Robert, J-M Cornuet, J-M Marin, and N S Pillai. Lack of confidence in ABC model choice. *Proceedings of the National Academy of Sciences*, 108(37):15112–15117, 2007.

T Roos. Minimum description length principle. In C Sammut and G I Webb, editors, *Encyclopedia of Machine Learning and Data Mining*. Springer Science+Business Media, 2016.

F Topsøe. Information-theoretical optimization techniques. *Kybernetika*, 15(1):8–27, 1979.

F Topsøe. Some inequalities for information divergence and related measures of discrimination. *IEEE Transactions on Information Theory*, 46(4):1602–1609, 2000.

I Vajda. *Theory of Statistical Inference and Information*. Kluwer Academic Pub., 1989.

I Vajda. On metric divergences of probability measures. *Kybernetika*, 45(6):885–900, 2009.

Q H Vuong. Likelihood ratio tests for model selection and non-nested hypotheses. *Econometrica: Journal of the Econometric Society*, pages 307–333, 1989.
E-J Wagenmakers, R Ratcliff, P Gomez, and G J Iverson. Assessing model mimicry using the parametric bootstrap. *Journal of Mathematical Psychology*, 48(1):28–50, 2004.

R Wong. *Asymptotic Approximations of Integrals*. SIAM, 2001.