Robust parametric inference for finite Markov chains

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Abstract
We consider the problem of statistical inference in a parametric finite Markov chain model and develop a robust estimator of the parameters defining the transition probabilities via minimization of a suitable (empirical) version of the popular density power divergence. Based on a long sequence of observations from a first-order stationary Markov chain, we have defined the minimum density power divergence estimator (MDPDE) of the underlying parameter and rigorously derived its asymptotic and robustness properties under appropriate conditions. Performance of the MDPDEs is illustrated theoretically as well as empirically for some common examples of finite Markov chain models. Its applications in robust testing of statistical hypotheses are also discussed along with (parametric) comparison of two Markov chain sequences. Several directions for extending the MDPDE and related inference are also briefly discussed for multiple sequences of Markov chains, higher order Markov chains and non-stationary Markov chains with time-dependent transition probabilities. Finally, our proposal is applied to analyze corporate credit rating migration data of three international markets.

Keywords Minimum density power divergence estimator · Finite Markov chain · Parametric inference · Robustness

Mathematics Subject Classification Primary 62F35 · 62M02; Secondary 60J20

1 Introduction

Finite Markov chain models and their probabilistic characteristics are widely used to explain the behavior of physical systems or phenomenons; such understanding of
physical mechanisms is further applied to answer important research questions in psychology, genetics, epidemiology and also several types of social studies (Iosifescu 2007). For these applications, it is important to estimate the probabilistic structure of the assumed Markov chain model based on the sample data from the underlying physical process(es).

Consider one long, unbroken sequence $X_T = \{X_0, X_1, \ldots, X_T\}$ of $(T + 1)$ observations from a stationary Markov chain with finite state-space $S = \{1, 2, \ldots, K\}$ and transition probability matrix $\Pi = (\pi_{ij})_{i,j=1,\ldots,K}$. Note that, for each $i = 1, \ldots, K$, the vector $\pi_i = (\pi_{i1}, \ldots, \pi_{iK})$ is a probability measure on $S$; let us denote all such probability vectors over $S$ by $\mathcal{P}_S$. By stationarity, the initial probability $\pi_{i0} = P(X_0 = i)$ is independent of $t$ for each $i = 1, \ldots, K$. We assume that the Markov chain is ergodic (irreducible and aperiodic) and consider the problem of making inference about these unknown probabilities $\pi_{ij}$s and $\pi_{i0}$s based on the observed sequence $X_T$. Assuming no further structure, their nonparametric (maximum likelihood) estimates are, respectively, given by

$$\hat{\pi}_{ij} = \frac{v_{ij}}{v_{i+}}, \quad \text{and} \quad \hat{\pi}_{i0} = \frac{v_{i+}}{T}, \quad i, j = 1, \ldots, K,$$

where $I(A)$ denotes the indicator function of the event $A$, $v_{ij} = \sum_{t=0}^{T-1} I(X_t = i, X_{t+1} = j)$ and $v_{i+} = \sum_{j=1}^{K} v_{ij}$ for $i, j = 1, \ldots, K$. The estimated transition probability matrix is then given by $\hat{\Pi} = (\hat{\pi}_{ij})_{i,j=1,\ldots,K}$. More details about these estimates and their asymptotic properties can be found in, e.g., Jones (2004), Rajarshi (2014) and the references therein. However, in several applications in epidemiology, biology, Genomics, reliability studies, etc., we often model the transition probability matrix $\Pi$ by a parametric model family of $K \times K$ transition matrices $\mathcal{F} = \{P(\theta) = (p_{ij}(\theta))_{i,j=1,\ldots,K} : \theta \in \Theta \subseteq \mathbb{R}^d\}$, where $p_{ij}(\theta)$ are known functions depending on some unknown $d$-dimensional parameter vector $\theta = (\theta_1, \ldots, \theta_d)' \in \Theta$, the parameter space, and $P_i(\theta) = (p_{i1}(\theta), \ldots, p_{iK}(\theta)) \in \mathcal{P}_S$ for every $\theta \in \Theta$, for each $i, j = 1, \ldots, K$. We assume, throughout this paper, that this model family $\mathcal{F}$ is identifiable in the sense $P(\theta_1) = P(\theta_2)$, for any two parameter values $\theta_1, \theta_2 \in \Theta$, must imply $\theta_1 = \theta_2$. Then, any inference has to be performed based upon an estimate of $\theta$ which is consistent and asymptotically normal under suitable regularity conditions. The maximum likelihood estimator (MLE) is an immediate (optimum) candidate for this purpose, which were studied by Billingsley (1961) and is still the mostly used method of inference in a finite Markov chain. Some modified likelihood-based approach (e.g., PL, QL) are also developed for computational feasibility; see Hjort and Varin (2008) and the references therein.

Although asymptotically optimal, a well-known drawback of all these likelihood-based inference is their non-robustness against outliers or data contamination leading to erroneous insights. Since outliers are not infrequent in several real life applications, a robust statistical procedure automatically taking care of the outliers is of great value to produce robust estimators and subsequent stable inference in such cases. An alternative to the MLE based on the minimum distance approach was discussed by Menendez et al. (1999) using disparity measures, but they did not discuss the issue
of robustness. In general the robustness concern in the present context of finite Markov chains is not well-studied, although several works are available in the literature that developed robust procedures under general Markov (chains) models or important time series models as its special case; see, among many others, Birge (1983), Kunsch (1984), Martin and Yohai (1986), Lee and Lee (2010), Lee and Song (2013), Kang and Lee (2014), Bertail et al. (2018).

Here, we will develop a robust methodology for parameter estimation and associated inference, particularly for the finite Markov chain models with a general parametric structure. As a way to solve the robustness issue, here, we consider the popular minimum distance approach based on the density power divergence (DPD) measure that was originally introduced by Basu et al. (1998) for IID data. The DPD measure is a one-parameter generalization of the Kullback-Leibler divergence (KLD); for any two densities $g$ and $f$, with respect to some common dominating measure $\mu$, the DPD measure is defined in terms of a tuning parameter $\alpha \geq 0$ as

$$\begin{align*}
d_\alpha(g, f) &= \int \left[ f^{1+\alpha} - \left(1 + \frac{1}{\alpha}\right) f^\alpha g + \frac{1}{\alpha} g^{1+\alpha} + \frac{1}{\alpha} g^\alpha \right] \, d\mu, \quad \alpha \geq 0, \\
d_0(g, f) &= \lim_{\alpha \to 0} d_\alpha(g, f) = \int g \log(g/f) \, d\mu.
\end{align*}$$

Note that, $d_0(g, f)$ is the KLD measure, and $d_1$ is the squared $L_2$ distance. Since the MLE can be thought of as a minimizer of the KLD measure between the data and the model, a generalized estimator can be obtained by minimizing the corresponding DPD measure for any given $\alpha > 0$. The resulting minimum DPD estimator (MDPDE) has recently become popular due to the simplicity in its construction and computation along with high robustness properties; it is also highly efficient with the tuning parameter $\alpha$ controlling the trade-offs between its efficiency and robustness , [see, e.g., Basu et al. (2011)]. This approach, based on the MDPDE, is applied successfully in several disciplines and contexts to produce robust insights against possible data contamination; see, e.g., Basu et al. (2006, 2018); Ghosh and Basu (2013, 2018); Ghosh et al. (2016, 2018), among many more. However, the MDPDE has not yet been developed for general set-ups of dependent observations except for a few special cases like time series and diffusion processes in scattered attempts (e.g., Lee and Lee 2010; Lee and Song 2013; Kang and Lee 2014), and related works). In particular, advantages of the MDPDEs are yet to be investigated for finite Markov chains and other general stochastic processes.

In this paper, we study the MDPDEs for the general class of finite Markov chain models as a robust generalization of the MLE and use it for further robust inference. Although the implementation of the MDPDE in this context is somewhat straightforward, due to the dependence between observations, derivation of its theoretical properties needs non-trivial extensions of the existing results. Such new asymptotic results for the MDPDE, defined under the finite Markov chain models, are major contributions of the present paper, along with several illustrative examples, their use in robust inference (both confidence interval and hypothesis testing) and several important extensions.
We start by defining the MDPDE as a minimizer of an appropriate (generalized) total
discrepancy measure in terms of the DPD between rows of the empirical estimate \( \hat{\Pi} \)
and the model transition matrix \( P(\theta) \), and then derive its asymptotic and robustness
properties. In particular, we prove the consistency and asymptotic normality of the
MDPDE as \( T \to \infty \) with suitable new arguments involving the Markov chain theory.
The performance of the MDPDEs is illustrated through several interesting examples
of finite Markov chains. The asymptotic relative efficiency (ARE) of the MDPDEs
(defined as the ratio of its asymptotic variance over that of the MLE) are used to study
the effect of tuning parameter and finite sample simulation studies are performed to
justify the robustness benefits of the MDPDEs. These illustrations indeed show, for
the first time, the usefulness of the robust MDPDE for finite Markov chain models.

Further, we describe the application of these MDPDEs in performing statistical
testing of general composite hypotheses. Besides the derivation of general asymptotic properties of the MDPDE based Wald-type tests, an example of testing for the Bernoulli-Laplace diffusion model against a suitable parametric family of alternatives is discussed. The MDPDE-based testing procedure is also developed for (parametrically) comparing two Markov chain sequences.

Finally, we discuss important extensions of the MDPDE for a few complex finite
Markov chain model set-ups. These include the case of multiple sequence of observations obtained from the same finite Markov chain model, where the asymptotics of the MDPDE are discussed for both the cases of diverging sequence length (with finite number of sequences) and diverging number of observed sequences (of finite length each). Definitions of the MDPDE are also extended for higher-order Markov chains and those with time-dependent (non-stationary) transition probabilities.

Due to page restrictions, all proofs and some illustrations are presented in the Online Supplement.

2 Robust estimation for a finite Markov chain

2.1 The minimum density power divergence estimator

Let us consider the set-up and notation of Sect. 1. The widely popular MLE of \( \theta \) is
defined as the maximizer of the likelihood function

\[
L_T(\theta) = p_{X_0X_1}(\theta) p_{X_1X_2}(\theta) \cdots p_{X_{T-1}X_T}(\theta) = \prod_{i,j=1}^K p_{ij}(\theta)^{\nu_{ij}}.
\]

Then, the log-likelihood function is given by (see Online Supplement, Section A.1, for derivation)

\[
\frac{1}{T} \log L_T(\theta) = - \sum_{i=1}^K \sum_{j=1}^K \hat{\pi}_{ij} \log \hat{p}_{ij} + \sum_{i=1}^K \sum_{j=1}^K \hat{\pi}_{ij} \log \hat{\pi}_{ij},
\]

(4)
where the first term is a weighted average of KLD measure between the estimated probability vector \( \hat{\pi}_i = (\hat{\pi}_{i1}, \ldots, \hat{\pi}_{iK}) \) and the model probability vector \( P_i(\theta) = (p_{i1}(\theta), \ldots, p_{iK}(\theta)) \) over different \( i = 1, \ldots, K \). Hence, the MLE can be obtained by minimizing such total KLD measure. Since DPD is a generalization of the KLD measure at \( \alpha > 0 \), in view of (4), we can define the MDPDE at any \( \alpha > 0 \) as the minimizer of a similarly defined total DPD measure given by

\[
\sum_{i=1}^{K} \sum_{j=1}^{K} \pi_{io} d_\alpha(\hat{\pi}_i, P_i(\theta)) = \sum_{i=1}^{K} \pi_{io} \sum_{j=1}^{K} \left\{ p_{ij}(\theta)^{1+\alpha} - \left( 1 + \frac{1}{\alpha} \right) p_{ij}(\theta)^\alpha \hat{\pi}_{ij} + \frac{1}{\alpha} \hat{\pi}_{ij}^{1+\alpha} \right\},
\]

with respect to \( \theta \in \Theta \). Since the last term within the bracket in the above equation does not depend on \( \theta \), the MDPDE can be obtained by minimizing, in \( \theta \in \Theta \), the simpler objective function

\[
H_{T,\alpha}(\theta) = (1 + \alpha)^{-1} 1_K^T \Delta(\hat{\Pi}) V_{\alpha}(\hat{\Pi},\theta) 1_K,
\]

where \( 1_K \) denotes a \( K \)-vector having each entry one, \( \Delta(\Pi) = \text{Diag}\{\pi_{io} : i = 1, \ldots, K\} \) and \( V_{\alpha}(\Pi,\theta) \) is a \( K \times K \) matrix having \( (i, j) \)th element as \( \{p_{ij}(\theta)^{1+\alpha} - (1 + \frac{1}{\alpha}) p_{ij}(\theta)^\alpha \pi_{ij}\} \). Under the assumption of differentiability of \( p_{ij}(\theta) \) in \( \theta \), we can obtain the estimating equations of the MDPDE at any \( \alpha > 0 \) as given by

\[
U_{T,\alpha}(\theta) := \sum_{i=1}^{K} \pi_{io} \sum_{j=1}^{K} \psi_{ij}(\theta) \left( p_{ij}(\theta) - \hat{\pi}_{ij} \right) p_{ij}(\theta)^\alpha = 0_d,
\]

where \( \psi_{ij}(\theta) = \frac{\partial}{\partial \theta} \log p_{ij}(\theta) \) and \( 0_d \) denotes a \( d \)-vector having all entries zero. Note that, at \( \alpha = 0 \), the MDPDE estimating equation (6) coincides with the score equation corresponding to the MLE. Thus, the MDPDE coincides with the MLE at \( \alpha = 0 \) and provides its robust generalization at \( \alpha > 0 \). We next show that the MDPDE estimating equations are indeed unbiased at the model.

In this regard, we define the statistical functional, say \( F_{\alpha}(\Pi) \), corresponding to the MDPDE with tuning parameter \( \alpha \geq 0 \), at any general (true) transition matrix \( \Pi \), as the minimizer of \( \sum_{i=1}^{K} \pi_{io} d_\alpha(\hat{\Pi}_i, P_i(\theta)) \) with respect to \( \theta \in \Theta \), where \( \hat{\Pi}_i \) denote the \( i \)th row of \( \Pi \) and \( \pi_{io} \)s are the true initial probabilities depending on \( \Pi \). In consistence with the MDPDE objective function in (5), we can write \( F_{\alpha}(\Pi) = \arg \min_{\theta} H_{\alpha}(\Pi,\theta) \), where \( H_{\alpha}(\Pi,\theta) = (1 + \alpha)^{-1} 1_K^T \Delta(\Pi) V_{\alpha}(\Pi,\theta) 1_K \). The corresponding estimating equation for the MDPDE functional \( F_{\alpha}(\Pi) \) has the form

\[
U_{\alpha}(\Pi, P(\theta)) := \sum_{i=1}^{K} \pi_{io} \sum_{j=1}^{K} \psi_{ij}(\theta) \left( p_{ij}(\theta) - \hat{\pi}_{ij} \right) p_{ij}(\theta)^\alpha = 0_d.
\]
Note that, clearly \( H_\alpha(\widehat{H}, \theta) = H_{T, \alpha}(\theta) \) and \( U_\alpha(\widehat{H}, P(\theta)) = U_{T, \alpha}(\theta) \) which implies \( F_\alpha(\widehat{H}) \) is indeed the proposed MDPDE. Further, if the model is correctly specified with the true transition matrix being \( P(\theta_0) \) for some \( \theta_0 \in \Theta \), then the estimating equation \( U_\alpha(P(\theta_0), P(\theta)) = 0_d \) has a solution at \( P(\theta) = P(\theta_0) \). Under the assumption of identifiability of our model family \( \mathcal{F} \), it further implies \( \theta = \theta_0 \) and hence \( F_\alpha(P(\theta_0)) = \theta_0 \), i.e., the MDPDE functional \( F_\alpha \) is Fisher consistent at the model family \( \mathcal{F} \) [see, e.g., Basu et al. (2011) for definition of Fisher Consistency]. When the true transition matrix \( \Pi \) does not belong to the model family \( \mathcal{F} \), we will denote the corresponding MDPDE functional \( \theta_\pi = F_\alpha(\Pi) \) as the ‘best fitting parameter’ value (in the DPD sense) and we will show that the corresponding MDPDE is also asymptotically consistent for this \( \theta_\pi \).

Some illustrative examples of the MDPDE under finite Markov chain models are provided in Sect. 3. Another interesting example, where the MDPDE equals to the MLE for every \( \alpha \geq 0 \), is presented in the Online Supplement (Section B).

2.2 Asymptotic properties

In order to derive the asymptotic properties of the proposed MDPDE under the finite Markov chain models, we first assume the following regularity conditions on the model transition probabilities.

(A1) For each \( \theta \in \Theta \), the model transition probability matrix \( P(\theta) \) has the same sets of zero elements, i.e., the set \( C = \{ (i, j) : p_{ij}(\theta) > 0 \} \) is independent of \( \theta \). Put \( c = |C| \). Additionally, \( C \) is regular in the sense that any Markov chain with transition probabilities \( \pi_{ij} \) satisfying “\( \pi_{ij} > 0 \) if and only if \( (i, j) \in C \)” is irreducible [see, e.g., Iosifescu (2007)].

(A2) For every \( (i, j) \in C \), the function \( p_{ij}(\theta) \) is twice continuously differentiable in \( \theta \in \Theta \).

(A3) The \( c \times d \) matrix \( J(\theta) = (J_{ij, u}(i, j) \in C, u = 1, \ldots, d) \) has rank \( d \), for all \( \theta \in \Theta \), where

\[
J_{ij, u} = \frac{\partial p_{ij}(\theta)}{\partial \theta_u}.
\]

Based on (A1), for any \( K \times K \) transition matrix \( \Pi \in \mathcal{P}_S^K \), we define the \( c \)-vector \( \Pi_C \) having elements \( \pi_{ij} \) only for \( (i, j) \in C \) (the elements are stacked row-wise in our convention) and denote the set of all such vectors as \( \Sigma_C = \{ \Pi_C : \Pi \in \mathcal{P}_S^K \} \). Then, in view of Theorem 3.1 of Billingsley (1961), for a stationary and ergodic finite Markov chain having true transition matrix \( \Pi \), we have

\[
\eta := \sqrt{T} \left( \widehat{\Pi}_C - \Pi_C \right) \xrightarrow{D} \mathcal{N}_c \left( \theta_C, \Lambda(\Pi) \right), \quad \text{as } T \to \infty,
\]

where \( \widehat{\Pi} = (\widehat{\pi}_{ij}) \) from (1) and \( \Lambda(\Pi) = (\lambda_{ij, kl}(i, j), (i, l) \in C) \) is a \( c \times c \) matrix having entries \( \lambda_{ij, kl} = \delta_{ik} \left( \delta_{jl} \pi_{ij} - \pi_{ij} \pi_{il} \right) / \pi_{io} \). The rate of convergence in (8) is uniform in a neighborhood of \( \Pi \) and also \( \widehat{\Pi}_C \to \Pi_C \) almost surely (a.s.) as \( T \to \infty \) (Lifshits 1979; Sirazhdinov and Formanov 1984).

We now define a few matrices which are required for our asymptotic derivations. For any \( \Pi \in \mathcal{P}_S^K \) satisfying (A1) and any \( \theta \in \Theta \), define the \( c \times c \)
matrix \( B_\alpha(\Pi, \theta) = \text{Diag}\left\{ \frac{p_{ij}(\theta)^{1-\alpha}}{\pi_{io}} : (i, j) \in C \right\} \). Also, let us define two \( d \times d \) matrices, which are non-singular by Assumption (A3), as given by \( \Omega_\alpha(\Pi, \theta) = J(\theta)^T B_\alpha(\Pi, \theta)^{-1} \Lambda(\Pi) B_\alpha(\Pi, \theta)^{-1} J(\theta) \) and

\[
\Psi_\alpha(\Pi, \theta) = J(\theta)^T B_\alpha(\Pi, \theta)^{-1} J(\theta) + \sum_{(i,j) \in C} \pi_{io} p_{ij}(\theta)^{1-\alpha} \left[ \alpha \psi_{ij}(\theta)^T \psi_{ij}(\theta) + \frac{\partial \psi_{ij}(\theta)}{\partial \theta} \right] \left( p_{ij}(\theta) - \pi_{ij} \right),
\]

(9)

Now, let us first restrict ourselves to the cases where the assumed parametric model family is correctly specified and hence the true transition probability matrix \( \Pi \) belongs to the model family, i.e., \( \Pi = P(\theta_0) \) for some \( \theta_0 \in \Theta \). For simplicity, we put \( P^o = P(\theta_0) \). Note that, in such cases we have, for any \( \theta \in \Theta \) (including \( \theta_0 \)), \( \Psi_\alpha(P(\theta), \theta) = J(\theta)^T B_\alpha(\Pi, \theta)^{-1} J(\theta) \). From now on, we will use the notation \( p_{io}(\theta) := \pi_{io} \), the initial probabilities, when \( \Pi = P(\theta) \) and assume that \( P_{io}(\theta) = (p_{io}(\theta), \ldots, p_{Ko}(\theta)) \in \mathcal{P}_S \) for all \( \theta \in \Theta \). Then, using the result (8) with \( \Pi = P^o \) and extending the arguments from Menendez et al. (1999), we prove the asymptotic consistency of the MDPDEs at the model which is presented in the following theorem.

**Theorem 2.1** Consider a finite Markov chain that is stationary and ergodic having true transition matrix \( P^o = P(\theta_0) \in \mathcal{P}_S^K \) for \( \theta_0 \in \Theta \). Fix \( \alpha \geq 0 \). Then, under Assumptions (A1)–(A3), we have the following results.

(i) There exists a solution \( \hat{\theta}_\alpha \) (MDPDE) to the estimating equation (6) which is unique a.s. in a neighborhood of \( \theta_0 \) and satisfies the relation

\[
\sqrt{T} \left( \hat{\theta}_\alpha - \theta_0 \right) = \Psi_\alpha(P^o, \theta_0)^{-1} J(\theta_0)^T B_\alpha(P^o, \theta_0)^{-1} \eta + o_P(1),
\]

as \( T \to \infty \).

(10)

(ii) The MDPDE \( \hat{\theta}_\alpha \) is consistent for \( \theta_0 \) and also asymptotically normal with

\[
\sqrt{T} \left( \hat{\theta}_\alpha - \theta_0 \right) \overset{\mathcal{D}}{\to} \mathcal{N}_d \left( 0_d, \Sigma_\alpha(P^o, \theta_0) \right), \quad \text{as} \ T \to \infty,
\]

(11)

where \( \Sigma_\alpha(\Pi, \theta) = \Psi_\alpha(\Pi, \theta)^{-1} \Omega_\alpha(\Pi, \theta) \Psi_\alpha(\Pi, \theta)^{-1} \).

Theorem 2.1 can also be extended under model misspecifications, where the true transition matrix, say \( \Pi^o \), does not belong to the assumed model family. In this case, we can talk about the consistency only at the “best fitting parameter value” \( \theta_\pi = F_\alpha(\Pi^o) \) defined in Sect. 2.1. Then, the conclusions of Theorem 2.1 still hold with slight modifications as given in the next theorem.

**Theorem 2.2** Consider a finite Markov chain that is stationary and ergodic having true transition matrix \( \Pi^o \), which does not necessarily belongs to the model family \( \mathcal{F} \), and fix an \( \alpha \geq 0 \). Let \( \theta_\pi = F_\alpha(\Pi^o) \) denote the “best fitting parameter value” in the DPD sense. Then, under Assumptions (A1)–(A3), we have the following results.
There exists a solution \( \hat{\theta}_{\alpha} \) (MDPDE) to the estimating equation (6) which is unique a.s. in a neighborhood of \( \theta_\pi \) and satisfies the relation

\[
\sqrt{T} \left( \hat{\theta}_{\alpha} - \theta_\pi \right) = \Psi_{\alpha}(\Pi^\circ, \theta_\pi)^{-1} J(\theta_\pi) B_{\alpha}(\Pi^\circ, \theta_\pi)^{-1} \eta + o_P(1),
\]

as \( T \to \infty \). (12)

(i) The MDPDE \( \hat{\theta}_{\alpha} \) is consistent for \( \theta_\pi \) and \( \sqrt{T} \left( \hat{\theta}_{\alpha} - \theta_\pi \right) \to^D N_d(0_d, \Sigma_{\alpha}(\Pi^\circ, \theta_\pi)) \) as \( T \to \infty \).

(ii) The MDPDE \( \hat{\theta}_{\alpha} \) is consistent for \( \theta_\pi \) and \( \sqrt{T} \left( \hat{\theta}_{\alpha} - \theta_\pi \right) \to^D N_d(0_d, \Sigma_{\alpha}(\Pi^\circ, \theta_\pi)) \) as \( T \to \infty \).

The proof of Theorem 2.2 is given in the Online Supplement (Section A.2). Then, Theorem 2.1 follows from Theorem 2.2 as a special case by substituting \( \Pi^\circ, \theta_\pi \) by \( P^0_0 \) and \( \theta_0 \), respectively.

Remark 2.1 (The special case \( \alpha = 0 \)) We have already argued that the MDPDE is a generalization of the classical MLE and, in fact, coincides with the MLE at \( \alpha = 0 \). We can also find out the asymptotic distribution of the MLE, at the model, as a special case of Theorem 2.1 at \( \alpha = 0 \). In particular, some algebra lead us to \( \Psi_0(P^\circ, \theta_0) = \Omega_0(P^\circ, \theta_0) \). Then the asymptotic variance of (\( \sqrt{T} \) times) MLE turns out to be \( \Psi_0(P^\circ, \theta_0)^{-1} \). This coincides with the usual maximum likelihood theory, since \( \Psi_0(P^\circ, \theta_0) \) is indeed the Fisher information matrix of our model. Further, interestingly, the minimum disparity estimators, discussed in Menendez et al. (1999), also have the same asymptotic distribution as that of the MDPDE at \( \alpha = 0 \). Further, putting \( \alpha = 0 \), Theorem 2.2 provides an additional result in this context, yielding the asymptotic distribution of the MLE under model misspecification.

2.3 Robustness of the MDPDE

Suppose that the data are observed from a stationary ergodic finite Markov chain having true transition matrix \( \Pi^\circ \), which does not necessarily belong to the model family \( \mathcal{F} \). Consider a contaminated transition matrix \( \Pi_\epsilon = (1 - \epsilon)\Pi^\circ + \epsilon D_t \) where \( \epsilon \in [0, 1] \) denote the contamination proportion, \( t = (t_1, \ldots, t_K) \in S^K \) is the contamination point and \( D_t \) has entry one at \( (i, t_i) \)th position for all \( i = 1, \ldots, K \) and zero in all other positions. These leads to contaminated probability vector for each row of the transition matrix. We then define the influence function (IF) of the MDPDE functional \( F_\alpha(\Pi) \) at a fixed \( \alpha \geq 0 \), under the present finite Markov model set-up, as

\[
IF(t; F_\alpha, \Pi^\circ) = \lim_{\epsilon \downarrow 0} \frac{F_\alpha(\Pi_\epsilon) - F_\alpha(\Pi^\circ)}{\epsilon} = \frac{\partial}{\partial \epsilon} F_\alpha(\Pi_\epsilon) \bigg|_{\epsilon = 0}.
\]

It is necessary to justify the above definition of IF in the present context with dependence data; this is important in the view of the existing literature discussing that the IF of Hampel et al. (1986) is not necessarily correct for some dependent situations, e.g., time series (Martin and Yohai 1986). Although the IF was initially defined for IID data in Hampel et al. (1986), it has latter been extended for several other scenarios of non-homogeneous data; see, e.g., Ghosh and Basu (2013); Ghosh et al. (2016). Although
we have dependent data following a Markov chain, in above, we have defined IF in terms of transition matrix of the whole data instead of the dependent distributions of the individual observations $X_i$s, which allows us to avoid the associated complications. Since a transition matrix uniquely characterizes the distribution of the whole sample together, our definition of the IF, in the line of Hampel et al. (1986), is perfectly justified. Additionally, our definition indeed measures the amount of (asymptotic) bias of the MDPDE functional $F_\alpha(\Pi)$ against infinitesimal contamination at $t$; this is also in the same spirit as that of the general concept of IF. However, the contamination here is characterized by transition matrices leading to possible misclassifications within the state-spaces (via $t$), rather than a distant outlying observation as the case was in its classical definition by Hampel et al. (1986).

Now, in order to derive this IF in the present context, we note that $F_\alpha(\Pi_{\epsilon})$ satisfies the estimating equation (7) with $\Pi$ replaced by $\Pi_{\epsilon}$, i.e., $U_\alpha(\Pi_{\epsilon}, P(F_\alpha(\Pi_{\epsilon}))) = 0_d$. Differentiating it with respect to $\epsilon$ and evaluating at $\epsilon = 0$, we can get the IF of the MDPDE functional as presented in the following theorem. The proof is given in the Online Supplement (Section A.3).

**Theorem 2.3** Consider a finite Markov chain that is stationary and ergodic having true transition matrix $\Pi^o$ and fix an $\alpha \geq 0$. Let $\theta_\pi = F_\alpha(\Pi^o)$ denote the “best fitting parameter value” in the DPD sense. Then, the influence function of the MDPDE functional $F_\alpha$ is given by

$$IF(t; F_\alpha, \Pi^o) = \psi_\alpha(\Pi^o, \theta_\pi)^{-1} \sum_{i=1}^{K} \pi_{i,o} \times \left[ \sum_{j=1}^{K} \psi_{ij}(\theta_\pi) p_{ij}(\theta_\pi)^{\alpha} \pi_{i,j} - \psi_{iti}(\theta_\pi) p_{iti}(\theta_\pi)^{\alpha} \right].$$

The above formula can be further simplified at the model where $\Pi^o = P(\theta_0)$ for some $\theta_0 \in \Theta$.

The only term of the IF that depends on the contamination point is $\psi_\alpha(t_i) = \psi_{iti}(\theta_\pi) p_{iti}(\theta_\pi)^{\alpha}$; but this term is bounded for each $i$ and every $\alpha \geq 0$ because of the finite state space. So, in this case, the boundedness of the IF is always evident and we cannot talk about the robustness by just looking at the bounded IF. Note that, the contamination considered here is not far away from the majority of the data, rather it covers the misclassification within the state-spaces arising from small-scale errors. So, using this IF, we can still talk about the robustness under such contaminations in relative terms (and not as an absolute measure), i.e., compare two estimators by looking at the maximum value of the IF (in an appropriate norm) over all possible $t$ (misclassification types); as this maximum becomes smaller the estimator becomes more robust. This measure of quantifying the extent of robustness, commonly known as the sensitivity measure, is formally defined as $\gamma_\alpha(\Pi^o) = \sup_{t \in S_K} ||IF(t; F_\alpha, \Pi^o)||$. For most common examples, this sensitivity indeed decreases with increasing $\alpha > 0$, indicating the gain in robustness by the MDPDEs at larger $\alpha > 0$. 

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An alternative (global) measure of robustness, that can provide further insights about the (absolute) robustness in the present case of finite state-spaces, is the maxbias curve of the functional defined as its maximum asymptotic bias under all possible contaminated (misspecified) distributions for a given contamination proportion. Although Theorem 2.2 provides some insights about the consistency of the MDPDE to the best fitting parameter (with respect to the DPD) even under such contaminated scenarios, derivation of the exact form of the maxbias curve is not straightforward. But, it would surely be interesting and important future work to study the maxbias curve for the MDPDE under different model set-ups including the present finite Markov chain models.

2.4 Estimating standard error and confidence interval

In any application, it is important to report the standard error of the estimator used. The same can also be done for the MDPDEs under the present set-up by using the asymptotic variance formulas given in Theorems 2.1 and 2.2. Firstly, based on Theorem 2.1, a consistent estimate of the asymptotic variance matrix of \((\sqrt{T} \times)\) the MDPDE can be obtained as \(\Sigma_\alpha(P(\hat{\theta}_\alpha), \hat{\theta}_\alpha)\); note that this estimator is model specific. Alternatively, based on Theorem 2.2, another model-robust estimator of the asymptotic variance matrix is given by \(\Sigma_\alpha(\hat{\Pi}, \hat{\theta}_\alpha)\); this can be shown to be a consistent variance estimator under standard regularity conditions. This second estimator works better compared to the previous model specific variance estimator \(\Sigma_\alpha(P(\hat{\theta}_\alpha), \hat{\theta}_\alpha)\) under model misspecification, but the first one works better against outliers with respect to a fixed model. Using either of these two variance estimators, and denoting it by \(\hat{\Sigma} = (\hat{\sigma}_{ij})_{i,j=1,\ldots,d}\), the standard error of the \(i\)th component of \(\theta\) is then obtained as \(\hat{s}_i = \sqrt{\hat{\sigma}_{ii}/T}\) for each \(i = 1, \ldots, d\).

Once we estimate the standard error of the parameter estimate, its immediate use is to construct the confidence intervals. Utilizing the asymptotic normality of the MDPDEs, we can actually construct the corresponding robust asymptotic confidence interval of the underlying parameters. In particular, a robust asymptotically 100\((1 - \xi)\)% confidence interval for the \(i\)th component \((\hat{\theta}_i)\) of the parameter vector \(\theta\) is given by \((\hat{\theta}_i - \hat{s}_i z_{\tau/2}, \hat{\theta}_i + \hat{s}_i z_{\tau/2})\), where \(\hat{s}_i\) is the estimated standard error of the MDPDE \(\hat{\theta}_i\) as defined above and \(z_{\tau}\) is the \((1 - \tau)\)th quantile of the standard normal distribution \((\tau = \xi/2\) here). These confidence intervals can be combined over all \(i\), along with the necessary Bonferroni correction, to obtain a robust and asymptotic simultaneous confidence set (rectangle) for the whole parameter vector \(\theta\). Alternatively, using the joint asymptotic distribution of the MDPDE of \(\theta\) and the variance matrix estimator \(\hat{\Sigma}\), one can also construct, in a straightforward way, robust asymptotic simultaneous confidence ellipsoid for the whole parameter vector. Such asymptotic confidence sets for any (differentiable) function of the parameters can also be constructed by inverting the MDPDE based Wald-type tests to be introduced in Sect. 4.
3 Examples and illustrations

3.1 Example 1: a random walk type model with binomial probabilities

Let us consider an example of finite Markov chain, over the state-space $S = \{1, 2, \ldots, K\}$, with reflecting barriers and Bin(2, $\theta$) distribution for moving from each internal position to its nearest (both sided) three positions. The corresponding transition matrix is then given by

$$
P(\theta) =
\begin{bmatrix}
0 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 \\
(1-\theta)^2 & 2\theta(1-\theta) & \theta^2 & 0 & \cdots & 0 & 0 & 0 \\
0 & (1-\theta)^2 & 2\theta(1-\theta) & \theta^2 & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & \cdots & (1-\theta)^2 & 2\theta(1-\theta) & \theta^2 \\
0 & 0 & 0 & 0 & \cdots & 0 & 1 & 0
\end{bmatrix}.
$$

(14)

Such a model often arise in real-life applications, e.g., in genetics, with different values of $K$. Here, the target parameter $\theta \in \Theta = [0, 1]$ is scalar and the Markov chain is stationary and ergodic with initial (stationary) probabilities $\{\pi_{io} = p_{io}(\theta) : i = 1, 2, \ldots, K\}$, where

$$
p_{1o}(\theta) = \frac{(1-\theta)^2(1-2\theta)}{2[(1-\theta)^2K-1 - \theta^2K-1]}, \quad p_{Ko}(\theta) = \frac{\theta^2(1-2\theta)}{2[(1-\theta)^2K-1 - \theta^2K-1]},
$$

and

$$
p_{io}(\theta) = \frac{\theta^{2(i-1)}(1-\theta)^2(1-2\theta)}{2[(1-\theta)^2K-1 - \theta^2K-1]}, \quad i = 2, \ldots, K - 1.
$$

Further, Assumptions (A1)–(A3) also hold for $P(\theta)$ in (14) with

$$
C = \{(1, 2); (i, i + 1), (i, i), (i, i - 1) \text{ for } i = 2, 3, \ldots, K - 1; (K, K - 1)\},
$$

so that $c = 3K - 4$ and

$$
J(\theta) = [0, 2\theta, 2(1-2\theta), -2(1-\theta), 2\theta, 2(1-2\theta), -2(1-\theta), \ldots, 2\theta, 2(1-2\theta), -2(1-\theta), 0]^t.
$$

Now consider one long sequence $X_T = \{X_0, X_1, \ldots, X_T\}$ observed from this given Markov chain based on which we wish to infer about the target parameter $\theta$. One can easily verify that the MLE of $\theta$ is given by

$$
\hat{\theta}_0 = \frac{\sum_{i=2}^{K-1} [v_{i(i+1)} + v_{ii}/2]}{\sum_{i=2}^{K-1} [v_{i(i-1)} + v_{ii} + v_{i(i+1)}]} = \frac{\sum_{i=2}^{K-1} \hat{\pi}_{io} [\hat{\pi}_{i(i+1)} + \hat{\pi}_{ii}/2]}{\sum_{i=2}^{K-1} \hat{\pi}_{io}}.
$$

On the other hand, the proposed MDPDE of $\theta$ with tuning parameter $\alpha > 0$ can be obtained by solving the estimating equation (6), which simplifies for the present case
as
\[
\sum_{i=2}^{K-1} \left[ \theta^{2\alpha-1} v_{i(i+1)} + 2^{\alpha-1} \theta^{\alpha-1} (1 - \theta)^{\alpha-1} (1 - 2\theta) v_i - (1 - \theta)^{2\alpha-1} v_{i(i-1)} \right] = \left( \sum_{i=2}^{K-1} v_i \right) \left[ \theta^{2\alpha+1} + 2^{\alpha} \theta^{\alpha} (1 - \theta)^{\alpha} (1 - 2\theta) - (1 - \theta)^{2\alpha+1} \right].
\]

Next we derive the asymptotic distribution of the MDPDE at the model using Theorem 2.1. The required assumptions clearly hold for this example and, through some algebra, we obtain \( \Psi_\alpha(P(\theta), \theta) = 4[1 - p_{1\alpha}(\theta) - p_{K\alpha}(\theta)]V_{1,\alpha}(\theta) \) and \( \Omega_\alpha(P(\theta), \theta) = 4[1 - p_{1\alpha}(\theta) - p_{K\alpha}(\theta)]V_{2,\alpha}(\theta) \), where
\[
V_{1,\alpha}(\theta) = (1 - \theta)^{2\alpha} + \theta^{2\alpha} + 2^{\alpha-1} \theta^{\alpha-1} (1 - \theta)^{\alpha-1} (1 - 2\theta)^2,
\]
\[
V_{2,\alpha}(\theta) = (1 - \theta)^{4\alpha} \theta (2 - \theta) + \theta^4 (1 - \theta)^2 + 2^{\alpha+1} (1 - \theta)^{2\alpha+1} + 2^{\alpha+1} \theta^{\alpha+1} (1 - 2\theta)^2.
\]

Then, the asymptotic variance of \( \sqrt{T} \hat{\theta}_\alpha \) is given by
\[
\Sigma_\alpha(P(\theta), \theta) = [1 - p_{1\alpha}(\theta) - p_{K\alpha}(\theta)]^{-1} \frac{V_{2,\alpha}(\theta)}{4V_{1,\alpha}(\theta)^2}.
\]

It is easy to see that this \( \Sigma_\alpha(P(\theta), \theta) \) is symmetric about \( \theta = 1/2 \) for each \( \alpha \geq 0 \), i.e., \( \Sigma_\alpha(P(\theta), \theta) = \Sigma_\alpha(P(1 - \theta), 1 - \theta) \), and is independent of \( \alpha \) at \( \theta = 1/2 \) having value \( \Sigma_\alpha(P(1/2), 1/2) = \frac{3}{4}[1 - p_{1\alpha}(\theta) - p_{K\alpha}(\theta)]^{-1} \). At any other fixed parameter value \( \theta \neq 1/2 \), \( \Sigma_\alpha(P(\theta), \theta) \) is a strictly increasing function of \( \alpha \geq 0 \). In particular, at \( \alpha = 0 \), we have the least asymptotic variance for the MLE (\( \sqrt{T} \hat{\theta}_0 \)) as given by
\[
\Sigma_0(P(\theta), \theta) = \frac{2\theta(1 - \theta)(8\theta^4 - 16\theta^3 + 8\theta^2 + 1)}{[1 - p_{1\alpha}(\theta) - p_{K\alpha}(\theta)]}.
\]

So, the ARE of the proposed MDPDE at any fixed \( \alpha \) can be obtained by comparing \( \Sigma_\alpha(P(\theta), \theta) \) with \( \Sigma_0(P(\theta), \theta) \), which are reported in Table 1 for different parameter values. Note that, the ARE clearly decreases as \( \alpha \) increases but the loss in efficiency is not quite significant at smaller values of \( \alpha > 0 \). With this small price, these MDPDEs gain significant robustness against data contamination as illustrated below through a simulation study.

In our simulation study, sample observations are generated from the Markov chain model having transition probability matrix as in (14) with \( K = 10 \) and \( \theta = 0.25 \). For different values of \( T \), we simulate observed path of length \( (T + 1) \) with \( X_0 = 1 \) and compute the MDPDEs of \( \theta \) for different \( \alpha \geq 0 \). We replicate this experiment 1000 times to compute the empirical mean squared error (MSE) of the MDPDEs with respect to its true value (0.25) for each \( \alpha \). Further, to examine the robustness, a certain percentage, say 100\( \epsilon \)% of the sample path is randomly replaced by observations from another
Fig. 1  Empirical MSEs (×100) of the MDPDEs obtained from the simulation study conducted for Example 1 with $K = 10$, $\theta = 0.25$ and different contamination proportions (solid line: 0%, dotted line: 10%, dashed line: 15%, dash-dotted line: 20%)
### Table 1

ARE (in%) of the MDPDEs for Example 1 at different values of $\alpha > 0$ and $\theta \in (0, 1)$

| $\alpha$ or $(1 - \theta)$ | $\alpha$ | 0.1 | 0.2 | 0.3 | 0.5 | 0.7 | 1  |
|----------------------------|---------|-----|-----|-----|-----|-----|----|
| 0.05                       | 0.1     | 99.1| 97.5| 96.0| 94.2| 93.8| 94.4|
| 0.1                        | 0.2     | 98.9| 96.7| 94.3| 90.8| 89.2| 89.2|
| 0.15                       | 0.3     | 98.9| 96.5| 93.7| 88.8| 85.9| 84.4|
| 0.2                        | 0.4     | 99.1| 96.8| 93.9| 88.2| 83.9| 80.7|
| 0.25                       | 0.5     | 99.3| 97.4| 94.7| 88.8| 83.6| 78.4|
| 0.3                        | 0.6     | 99.5| 98.1| 96.0| 90.7| 85.2| 78.4|
| 0.35                       | 0.7     | 99.7| 98.8| 97.4| 93.5| 88.7| 81.4|
| 0.4                        | 0.8     | 99.9| 99.4| 98.7| 96.6| 93.5| 87.9|
| 0.45                       | 0.9     | 100.0| 99.9| 99.7| 99.0| 98.1| 96.0|
| 0.5                        | 1.0     | 100 | 100 | 100 | 100 | 100 | 100 |

finite Markov chain which always move forward with probability one (i.e., $\theta = 1$ in the present model transition matrix) and repeat the same experiment to compute the MSEs under data contamination. The resulting values of MSEs of the MDPDEs are presented in Fig. 1 for $T = 50$, 100 and for 10%, 15%, 20% contamination proportions, along with the pure data results (0% contamination). Recall that the MDPDE at $\alpha = 0$ is the MLE which provides the least MSE under pure data. The MSE under pure data increases, but very slowly, as $\alpha$ increases, in consistence with their asymptotic AREs (Table 1). However, under contamination, the MSE of the MLE (at $\alpha = 0$) is significantly higher and decreases sharply as $\alpha > 0$ increases; the MSEs remain more stable at larger values of $\alpha$. This clearly indicate the claimed robustness of our proposed MDPDEs at $\alpha > 0$ and that the extent of robustness further increases with increasing values of $\alpha$.

### 3.2 Example 2: a multi-parameter extension of Example 1

We now further extend the Markov chain model described in Example 1, so that the probability defining parameter $\theta$ depends on the current state, leading to the transition matrix

$$P(\theta) = \begin{bmatrix}
0 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 \\
(1 - \theta_2)^2 & 2\theta_2(1 - \theta_2) & \theta_2^2 & 0 & \cdots & 0 & 0 & 0 \\
0 & (1 - \theta_3)^2 & 2\theta_3(1 - \theta_3) & \theta_3^2 & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & \cdots (1 - \theta_{K-1})^2 & 2\theta_{K-1}(1 - \theta_{K-1}) & \theta_{K-1}^2 & \cdots & 0 \\
0 & 0 & 0 & \cdots & 0 & 1 & 0 & 0
\end{bmatrix},$$

(19)

with each $\theta_i \in [0, 1]$ for $i = 2, \ldots, K - 1$. Important models for explaining diffusion between gases or liquids are special cases of this Markov chain; see Sect. 4.3 for an example. Note that, here the target parameter $\theta = (\theta_2, \ldots, \theta_{K-1})^T$ is of dimension $K - 2$.  

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\[ d = (K-2), \text{ but the individual components can be seen to be independent. The Markov chain corresponding to the transition matrix (19) is also stationary and ergodic. Its stationary distribution can be computed easily and is given by (with } \theta_1 = 1, \theta_K = 0) \]

\[
\begin{align*}
\pi_{1o} &= p_{1o}(\theta) = \frac{1}{1 + \sum_{i=2}^{K} \theta_i^2 \cdot \theta_{i-1}^2 (1 - \theta_2)^{-2} (1 - \theta_3)^{-2} \cdots (1 - \theta_i)^{-2}}, \\
\pi_{io} &= p_{io}(\theta) = \frac{\theta_i^2 \cdot \theta_{i-1}^2 (1 - \theta_2)^{-2} (1 - \theta_3)^{-2} \cdots (1 - \theta_i)^{-2}}{1 + \sum_{i=2}^{K} \theta_i^2 \cdot \theta_{i-1}^2 (1 - \theta_2)^{-2} (1 - \theta_3)^{-2} \cdots (1 - \theta_i)^{-2}}, \\
& \quad \quad i = 2, 3, \ldots, K. 
\end{align*}
\]

Firstly, noting the similarity with Example 1, we can see that Assumptions (A1)–(A3) continue to hold for the transition matrix given by (19) with \(C = \{(1, 2); (i, i + 1), (i, i), (i, i - 1) \text{ for } i = 2, 3, \ldots, K - 1; (K, K - 1)\} \). Then, given an observed sequence \(X_T = \{X_0, X_1, \ldots, X_T\} \), one can easily verify that the MDPDE \(\hat{\theta}_{i, \alpha} \) of \(\theta_i\), for each \(i = 2, \ldots, K - 1\), can be obtained separately by solving the respective estimating equation given by

\[
\left[ \theta_i^{2\alpha - 1} v_{i(i+1)} + 2^{\alpha - 1} \theta_i^{\alpha - 1} (1 - \theta_i)^{\alpha - 1} (1 - 2\theta_i) v_{ii} - (1 - \theta_i)^{2\alpha - 1} v_{i(i-1)} \right] = v_i + \left[ \theta_i^{2\alpha + 1} + 2^\alpha \theta^\alpha (1 - \theta)^\alpha (1 - 2\theta) - (1 - \theta)^{2\alpha + 1} \right]. \tag{20}
\]

Further, applying Theorem 2.1, one can verify that the asymptotic distribution of the \((K-2)\) dimensional MDPDE \(\hat{\theta}_\alpha = (\hat{\theta}_{i, \alpha} : i = 2, \ldots, K - 1)^T \) at the model with true parameter value \(\theta_0 = (\theta_{i0} : i = 2, \ldots, K - 1)^T \) is given by

\[
\sqrt{T} (\hat{\theta}_\alpha - \theta_0) \xrightarrow{D} N_{K-2} (0_d, \text{Diag } \left\{ \sigma^{(i)}_\alpha (\theta_0) : i = 2, \ldots, K - 1 \right\}), \quad \text{as } T \to \infty,
\]

with \(\sigma^{(i)}_\alpha (\theta) = [1 - p_{1o}(\theta) - p_{Ko}(\theta)]^{-1} \frac{V_{2, \alpha}(\theta_i)}{4V_{1, \alpha}(\theta_i)^2} \), where \(V_{1, \alpha}\) and \(V_{2, \alpha}\) are as defined in (16) and (17), respectively, but \(p_{io}(\theta)\) is specific to the present example (as computed above). Note that, the AREs of the MDPDEs of each parameter component in the present case are exactly the same as studied in Example 1 (Table 1). Their finite sample robustness advantages are also observed to have a similar pattern as in Example 1 (Fig. 1) via simulations and, hence, they are not reported here for brevity.

### 3.3 Example 3: a Markov chain for epidemic modeling

Our final example would be another practically important Markov chain model, namely the Greenwood model, for epidemic modeling of a contagious disease in a population of fixed size (say \(K\), often small). Suppose that every individual in the population can be in either of two categories, namely infected or uninfected, and the disease evolves in some discrete time unit (a constant latent time period for a person to get infected). Let \(X_t\) denote the number of individuals who are still uninfected at time point \(t = 0, 1, 2, \ldots, T\), so that \(X_0 = K\). If \(\theta \in (0, 1)\) denote the probability of contact
between two individuals (one uninfected and one infected) to produce a new infection at any time point, then $X_t$ is a Markov chain (Gani and Jerwood 1971; Iosifescu 2007) with finite state-space $S = \{0, 1, 2, \ldots, K\}$ and the transition matrix

$$P(\theta) = \begin{bmatrix}
1 & 0 & 0 & \cdots & 0 & 0 \\
\theta & (1-\theta) & 0 & \cdots & 0 & 0 \\
\theta^2 & 2\theta(1-\theta) & (1-\theta)^2 & \cdots & 0 & 0 \\
& \ddots & \ddots & \ddots & \ddots & \ddots \\
& & & & & \theta^K & (K-1)\theta(1-\theta)(K-2) \theta^2 & \cdots & (K-1)\theta(1-\theta)^{K-1} & (1-\theta)^K
\end{bmatrix}.$$  

Note that the underlying Markov chain can easily be seen to be stationary and ergodic. Also Assumptions (A1)–(A3) hold with $C = \{(0, 0); (i, 0), (i, 1), \ldots, (i, i)\}$ for $i = 1, 2, \ldots, K$ so that $c = |C| = (K+1)(K+2)/2$.

Based on an observed sequence $X_T = \{X_0, X_1, \ldots, X_T\}$ from this model, we wish to estimate the target parameter $\theta$ (scalar). We can use the MDPDE as a robust estimator of $\theta$ which can be obtained by solving the estimating equation (7). For the present case, the MDPDE estimating equation (7) can be simplified as

$$\sum_{i=1}^{K} \sum_{j=0}^{i} \binom{i}{j} \alpha [(i-j) - i\theta] \theta^{(i-j)\alpha-1} (1-\theta)^{j\alpha-1} v_{ij}$$

$$= \sum_{i=1}^{K} v_{i} + \sum_{j=0}^{i} \binom{i}{j} 1+\alpha [(i-j) - i\theta] \theta^{(i-j)(1+\alpha)-1} (1-\theta)^{j(1+\alpha)-1}. \quad (21)$$

The asymptotic distribution of the resulting MDPDE, obtained by solving (21), can again be calculated from Theorem 2.1, as in the previous examples; we leave it for the readers as an exercise.

We illustrate the finite sample performance of these MDPDEs and their claimed robustness by another simulation exercise. We simulate observations of a fixed length $(T+1)$ from the present Markov model with $K = 9$ and $\theta = 0.25$. The empirical MSEs of the MDPDEs, obtained based on 1000 replications, are plotted in Fig. 2 over $\alpha \in [0, 1]$ for different amount of contaminations in the sample data. The contaminations are incorporated in the sample path at randomly selected location (say $i$) by taking the next step following $\text{Bin}(i, 1)$ distribution, i.e., by deterministically putting the next location to be 0. Note that, this type of contamination ends the chain there since this Markov chain can not go out of location 0 once it reaches there; hence such a restriction may be considered as heavy contamination in the sample data. Even under such a heavy contamination, we can see from Fig. 2 that the proposed MDPDE with moderately large $\alpha > 0$ provides significantly improved estimator (lower MSE) compared to the usual MLE (at $\alpha = 0$). Under pure data (no contamination), the MSEs show a very mild increasing trend with increasing values of $\alpha$. The MDPDEs with $\alpha$ around the value 0.5 provides the best trade-off in all the cases considered.
Fig. 2. Empirical MSEs (×100) of the MDPDEs obtained from the simulation study conducted for Example 3 with \( K = 9, \theta = 0.25 \) and different contamination proportions (solid line: 0%, dotted line: 10%, dashed line: 15%, dash-dotted line: 20%).
4 Application of the MDPDE in statistical hypothesis testing

4.1 Wald-type tests for general composite hypotheses

Let us now consider the problem of testing statistical hypotheses about the underlying Markov chain defined in terms of the assumed parametric model \( \mathcal{F} \). Under the set-up and notation of previous two sections, let us consider the general composite hypothesis given by

\[
H_0 : \theta \in \Theta_0 \quad \text{against} \quad H_1 : \theta \notin \Theta_0,
\]

where \( \Theta_0 \) is a pre-specified proper subset of \( \Theta \) having rank \( r \). In most applications, the null hypothesis in (22) can be re-expressed in terms of \( r \) linearly independent restrictions of the form

\[
h(\theta) = 0_r.
\]

Let us assume that the \( d \times r \) matrix \( H(\theta) = \frac{\partial h(\theta)}{\partial \theta} \) exists, has rank \( r \) and is continuous in \( \theta \). Further, if the assumptions of Theorem 2.1 hold, there exists the MDPDE \( \hat{\theta}_\alpha \) with tuning parameter \( \alpha \) which satisfies the asymptotic normality result in (11). We can use this MDPDE to construct a Wald-type test statistic for testing (22) as

\[
W_{T,\alpha} = T h' \left( \hat{\theta}_\alpha \right) \left[ H' \left( \hat{\theta}_\alpha \right) \Sigma_\alpha(P(\hat{\theta}_\alpha), \hat{\theta}_\alpha) H(\hat{\theta}_\alpha) \right]^{-1} h \left( \hat{\theta}_\alpha \right),
\]

where \( \Sigma_\alpha \) is as defined in Theorem 2.1. The asymptotic distribution of this proposed test statistic can be obtained from (11) which is presented in the following theorem.

**Theorem 4.1** Assume that the conditions of Theorem 2.1 hold true and the covariance matrix \( \Sigma_\alpha(P(\theta), \theta) \) is continuous in \( \theta \) around the null parameter values. Then, under the null hypothesis in (22), the proposed Wald-type test statistic \( W_{T,\alpha} \) asymptotically follows a chi-square distribution \( (\chi^2_r) \) with \( r \) degrees of freedom.

The above theorem can be used to obtain the asymptotic critical values for testing (22) based on \( W_{T,\alpha} \) for all \( \alpha \geq 0 \). Further properties of these proposed Wald-type tests can be easily obtained in the line of Ghosh et al. (2016) and Basu et al. (2018). In particular, the tests based on \( W_{T,\alpha} \) are consistent, for all \( \alpha \geq 0 \), in the sense that their power at any fixed alternative converges to one as \( T \to \infty \). It can also be shown that, under a contiguous sequence of alternative hypotheses \( H_{1,T} : \theta = \theta_T \), where \( \theta_T = \theta_0 + \frac{d}{\sqrt{T}} \) with \( d \in \mathbb{R}^d \setminus \{0\} \) and \( \theta_0 \in \Theta_0 \), the Wald-type test statistic \( W_{T,\alpha} \) asymptotically (as \( T \to \infty \)) follows a non-central chi-square distribution with degrees of freedom \( r \) and non-centrality parameter \( \delta_\alpha = d' H \left( \theta_0 \right) \Sigma_\alpha^* \left( \theta_0 \right)^{-1} H(\theta_0)' d \), where \( \Sigma_\alpha^*(\theta) = H' \left( \theta \right) \Sigma_\alpha \left( P(\theta), \theta \right) H(\theta) \). This result can be used to obtain the asymptotic power of the proposed Wald-type tests based on \( W_{T,\alpha} \) under contiguous alternatives and, hence, to study their efficiency compared to any other consistent test.
4.2 Robustness analyses for the Wald-type tests

The robustness of the proposed Wald-type tests based on $W_{T,\alpha}$ can also be theoretically justified through the concept of influence function analyses. With the notation of Sect. 2.3, let us first define the statistical functional corresponding to $W_{T,\alpha}$ at the true transition matrix $\Pi$ as given by

$$W_{\alpha}(\Pi) = h'(F_{\alpha}(\Pi)) \Sigma^*_\alpha(F_{\alpha}(\Pi))^{-1} h(F_{\alpha}(\Pi)), \quad (24)$$

where $F_{\alpha}(\Pi)$ is the MDPDE functional with tuning parameter $\alpha$. Then, we can define its first-order influence function as $IF(t; W_{\alpha}, \Pi) = \frac{\partial}{\partial \epsilon} W_{\alpha}(\Pi) \big|_{\epsilon=0}$. Since the influence function of a test statistics is examined at the null hypothesis, let us consider a parameter value $\theta_0 \in \Theta_0$ so that $h(\theta_0) = 0$ and $F_{\alpha}(\Pi^0) = \theta_0$ with $\Pi^0 = P(\theta_0)$. Then, straightforward differentiation yields the first-order IF as

$$IF(t; W_{\alpha}, \Pi^0) = 2h'(F_{\alpha}(\Pi^0)) \Sigma^*_\alpha(F_{\alpha}(\Pi^0))^{-1} H'(F_{\alpha}(\Pi^0)) IF(t; F_{\alpha}, \Pi^0)$$

$$+ h'(F_{\alpha}(\Pi^0)) \left[ \frac{\partial}{\partial \epsilon} \Sigma^*_\alpha(F_{\alpha}(\Pi_\epsilon))^{-1} \right]_{\epsilon=0} h(F_{\alpha}(\Pi^0)), \quad (25)$$

Since this first-order IF is always zero, it is non-informative to indicate the robustness of the test procedure and, hence, we need to consider the second-order IF of the test functional $W_{\alpha}$. By another round of differentiation, we get

$$IF_2(t; W_{\alpha}, \Pi^0) = \frac{\partial^2}{\partial \epsilon^2} W_{\alpha}(\Pi_\epsilon) \big|_{\epsilon=0}$$

$$= 2 IF(t; F_{\alpha}, \Pi^0) I F_1(t; \theta_0) \Sigma^*_\alpha(\theta_0)^{-1} H'(\theta_0) IF(t; F_{\alpha}, \Pi^0). \quad (26)$$

Note that this second-order IF of the Wald-type test functional $W_{\alpha}$ depends directly on the IF of the underlying MDPDE, used in the construction of the test statistics. Therefore, the robustness properties of the MDPDE based Wald-type tests are exactly similar to those of the MDPDE as discussed in Sect. 2.3.

We can also study the IF for the asymptotic level and power of the proposed Wald-type tests in the line of Ghosh et al. (2016) and Basu et al. (2018), which would be a linear function of the IF of the underlying MDPDE. Hence, their robustness would also be implied by the robustness of the MDPDE used in the test statistics (i.e., greater robustness with increasing $\alpha > 0$).

4.3 An example: test for the bernoulli-laplace model of diffusion

The Markov chain associated with the famous Bernoulli-Laplace diffusion model for two incompressible gases or liquids between two containers (Iosifescu 2007) is defined
by the $K \times K$ transition matrix

$$
P_* = \begin{bmatrix}
  r_1 & p_1 & 0 & \cdots & 0 & 0 & 0 \\
  q_2 & r_2 & p_2 & \cdots & 0 & 0 & 0 \\
  0 & q_3 & r_3 & p_3 & \cdots & 0 & 0 \\
  \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
  0 & 0 & 0 & \cdots & q_{K-1} & r_{K-1} & p_{K-1} \\
  0 & 0 & 0 & \cdots & 0 & q_K & r_K
\end{bmatrix},
$$

where $K > 1$ and

$$
p_i = \left(\frac{K - i}{K - 1}\right)^2, \quad q_i = \left(\frac{i - 1}{K - 1}\right)^2, \quad r_i = 2 \left(\frac{K - i}{K - 1}\right) \left(\frac{i - 1}{K - 1}\right),
$$

$i = 1, 2, \ldots, K$.

Suppose that, given a sequence $X_T = \{X_0, X_1, \ldots, X_T\}$ observed from a suitable process, we wish to test if it satisfies the Bernoulli-Laplace model, i.e., if it is generated according to the above transition matrix. As a convenient class of alternatives, we may consider the family $\mathcal{F}$ of parametric transition matrices of the form (19) which was discussed in Sect. 3.2. Note that the transition matrix $P_*$ of the Bernoulli-Laplace model belongs to this parametric family $\mathcal{F}$ for the parameter value $\theta_i = (K-i)/(K-1)$ for each $i = 2, \ldots, K-1$. Then, our targeted hypothesis can be expressed as a (simple) parametric hypothesis (within $\mathcal{F}$) given by

$$
H_0 : \theta_i = \left(\frac{K - i}{K - 1}\right), \quad i = 2, \ldots, K - 1, \quad \text{against} \quad H_1 : H_0 \text{ is not true.}
$$

(27)

Clearly this hypothesis (27) belongs to the class of hypotheses considered in Sect. 4.1 with $r = K - 2$, $h(\theta) = \left(\theta_i - \frac{(K-i)}{(K-1)} : i = 2, \ldots, K - 1\right)$ and hence $H(\theta) = I_{K-2}$, the identity matrix of dimension $(K - 2)$. So, using the (asymptotic) properties of the MDPDEs of $\theta$ derived in Example 2 (Sect. 3.2) and the theory discussed Sect. 4.1, we can construct a robust Wald-type test statistic as defined in (23) for testing the hypothesis is (27). In this case, through the insertion of the particular forms of $h$ and $H$, our proposed test statistic is simplified to be

$$
W_{T, \alpha} = T \sum_{i=2}^{K-1} \frac{(\hat{\theta}_i - \frac{(K-i)}{(K-1)})^2}{\Sigma_\alpha(\theta(\hat{\theta}_{i0}), \hat{\theta}_{i0})}.
$$

(28)

It is easy to see that $W_{T, \alpha}$ coincides with the usual Wald test at $\alpha = 0$, and provide a robust generalization at $\alpha > 0$. Further, for any $\alpha \geq 0$, by Theorem 4.1 and the continuity of the asymptotic variance matrix $\Sigma_\alpha(\theta(\hat{\theta}_{i0}), \hat{\theta}_{i0})$ of the MDPDEs of $\theta$, the test statistic in (28) asymptotically has a $\chi^2_{K-2}$ distribution as $T \to \infty$, under the null hypothesis in (27). Therefore, we reject the null hypothesis in (27) at $\zeta$ level of significance if
$W_{T,\alpha} > \chi^2_{K-2,\xi}$, the $(1 - \xi)$-th quantile of $\chi^2_{K-2}$ distribution.

### 4.4 Test for the similarity of two sequences of Markov chains

We now discuss the problem of comparing two Markov chain sequences. Suppose that we observe two independent sequences $X^{(j)} = \{X_0^{(j)}, X_1^{(j)}, \ldots, X_{T_j}^{(j)}\}$ of length $(T_j+1)$, for $j = 1, 2$, from Markov chains having the same finite state-space $\mathcal{S} = \{1, 2, \ldots, K\}$ and transition probabilities belonging to the parameter family $\mathcal{F} = \{P(\theta) = (p_{ij}(\theta))_{i,j=1,\ldots,K} : \theta \in \Theta \subseteq \mathbb{R}^d\}$. Our aim is to statistically test if the two sequences are generated from the same Markov chain. If we assume that the transition matrix of $X^{(j)}$ is $P(\theta_j)$ for some $\theta_j \in \Theta$, $j = 1, 2$, then our problem corresponds to testing the hypothesis

$$H_0 : \theta_1 = \theta_2 \quad \text{against} \quad H_1 : \theta_1 \neq \theta_2.$$  

In order to develop a robust test statistic for testing (29), let us denote by $\hat{\theta}^{(j)}_{\alpha}$ the MDPDE of $\theta_j$, with tuning parameter $\alpha$, obtained based on the sequence $X^{(j)}$, for $j = 1, 2$, respectively. These two MDPDEs are then independent and each of them is asymptotically normal, under the assumptions of Theorem 2.1, as $T_1, T_2 \rightarrow \infty$. Accordingly, for testing (29), we may consider a Wald-type test statistic defined based on these MDPDEs as

$$W^{(\alpha)}_{T_1, T_2} = T_1 T_2 \left( \hat{\theta}^{(1)}_{\alpha} - \hat{\theta}^{(2)}_{\alpha} \right)^t \times \left[ T_2 \Sigma_{\alpha} \left( P(\hat{\theta}^{(1)}_{\alpha}), \hat{\theta}^{(1)}_{\alpha} \right) + T_1 \Sigma_{\alpha} \left( P(\hat{\theta}^{(2)}_{\alpha}), \hat{\theta}^{(2)}_{\alpha} \right) \right]^{-1} \left( \hat{\theta}^{(1)}_{\alpha} - \hat{\theta}^{(2)}_{\alpha} \right).$$

The critical values for testing (29) using the test statistic $W^{(\alpha)}_{T_1, T_2}$ can be obtained from its asymptotic distribution, which is presented in the following theorem.

**Theorem 4.2** Assume that the conditions of Theorem 2.1 hold true and the covariance matrix $\Sigma_{\alpha}(P(\theta), \theta)$ is continuous in $\theta$ around the null parameter value $\theta_1 = \theta_2$. Suppose that $T_1, T_2 \rightarrow \infty$ in such a way that $T_1/(T_1 + T_2) \rightarrow w$ for some $w \in (0, 1)$. Then, under the null hypothesis in (29), the asymptotic distribution of our MDPDE based Wald-type test statistic $W^{(\alpha)}_{T_1, T_2}$ is $\chi^2_d$.

We can derive other properties of the test based on $W^{(\alpha)}_{T_1, T_2}$ by extending the theory of usual two-sample Wald-type tests in the line of Ghosh et al. (2018). In particular, this test is also consistent for all $\alpha \geq 0$ and its power under pure data as well as its robustness depend directly on the relative efficiency and the robustness of the MDPDE used in constructing the test statistics.
5 Further extensions

5.1 Multiple sequences of Markov chain observations

Extending the notation from Sect. 4.4, let us now consider \( n (\geq 2) \) sequences of Markov chain observations denoted by \( X^{(j)} = \{X_0^{(j)}, X_1^{(j)}, \ldots, X_{T_j}^{(j)}\} \), for \( j = 1, 2, \ldots, n \). Suppose that all of them are generated from the same Markov chain having finite state-space \( S = \{1, 2, \ldots, K\} \) and transition probability matrix \( \Pi \) to be modeled by \( P(\theta) \). Our aim is to estimate the parameter \( \theta \) from the combined information from all these \( n \) sequences of observations.

Here, we define the (nonparametric) probability estimates \( \hat{\pi}_{ij} \) and \( \hat{\pi}_{i+} \) from the combined (average) frequency counts \( \nu_{ij}^{(n)} \) and \( \nu_{i+}^{(n)} \) obtained from all the \( n \) chains in place of \( \nu_{ij} \) and \( \nu_{i+} \), respectively, in (1), where

\[
\nu_{ij}^{(n)} = \frac{1}{n} \sum_{j=1}^{n} \sum_{t=0}^{T_j-1} I(X_t^{(j)} = i, X_{t+1}^{(j)} = j), \quad \nu_{i+}^{(n)} = \sum_{j=1}^{K} \nu_{ij}^{(n)}, \quad i, j = 1, \ldots, K.
\]

(30)

Then, we can proceed exactly as in the case of one sequence, described in Sect. 2.1, with these new definitions of \( \hat{\pi}_{ij} \) and \( \hat{\pi}_{i+} \) to define the MDPDE of \( \theta \) with tuning parameters \( \alpha \). The robustness analyses of Sect. 2.3 would also be valid in this case. However, the asymptotic results derived in Sect. 2.2 are needed to be modified appropriately for the present case. For simplicity in discussion, in the following, we will assume that \( T_1 = T_2 = \cdots = T_n = T \); the results can be easily extended for the case of different \( T_j \)'s.

Note that, there can be two directions of asymptotic derivation. Firstly, when the number of sequences \( n \) is a small finite number and the length of the sequences \( T \to \infty \), the main asymptotic results (8) can be modified easily leading to the result

\[
\eta := \sqrt{nT} \left( \hat{\Pi}_C - \Pi_C \right) \overset{D}{\to} N_c \left( \theta_c, \Lambda(\Pi) \right), \quad \text{as } T \to \infty,
\]

(31)

where \( \hat{\Pi} = (\hat{\pi}_{ij}) \) is now defined from the modified (average) frequency counts \( \nu_{ij}^{(n)} \) and \( \nu_{i+}^{(n)} \) given in (30) and the asymptotic variance matrix \( \Lambda(\Pi) \) is exactly the same as defined in Sect. 2.2.

In the second practically relevant case, we may observe a large number \( (n) \) of sequences, each of which has a small finite length \( T \), so that the asymptotics has to be done as \( n \to \infty \). This second type of asymptotics is studied in detail by Anderson and Goodman (1957) under finite Markov chains with two different initial conditions on \( n_i = \sum_{j=1}^{n} I(X_0^{(j)} = i) \), the number of observations in state \( i \) at time \( t = 0 \), for each \( i = 1, 2, \ldots, K \). For non-random \( n_is \) one needs to assume that \( n_i/n \to w_i \in (0, 1) \) with \( \sum_i w_i = 1 \), whereas for random \( n_is \) they were assumed to have a multinomial distribution with probabilities \( w_i \) and sample size \( n \). In either cases, a modified version
of (8) has been derived in Anderson and Goodman (1957) for a stationary ergodic chain starting from the stationary state, which is exactly the same as (31) but now as \( n \to \infty \).

Therefore, in both the directions of asymptotics, we can use the same result (31) to derive the asymptotic distribution of our MDPDEs in the present case. Proceeding exactly as in the proof of Theorem 2.2, we now have the following result

\[
\sqrt{nT} \left( \hat{\theta}_n - \theta_0 \right) \xrightarrow{D} \mathcal{N}(0_d, \Sigma_{\alpha}(P^0, \theta_0)),
\]

under both directions of asymptotic, i.e., either as \( T \to \infty \) or as \( n \to \infty \). Therefore, all the subsequent properties of the MDPDE and the associated Wald-type tests can also be extended in the present case of multiple sequence of Markov chain observations in a straightforward manner.

5.2 Finite Markov chains of higher order

Our proposed statistical methodologies can also be extended for higher order Markov chains. Let us now illustrate it for a second order Markov chain sequence \( X_T = \{X_0, X_1, \ldots, X_T\} \) having finite state-space \( S = \{1, 2, \ldots, K\} \) and stationary transition probabilities

\[
\pi_{ijl} = P(X_t = l|X_{t-1} = j, X_{t-2} = i), \quad i, j, l = 1, 2, \ldots, K.
\]

Suppose we wish to model these transition probabilities by some parametric family of \( K \times K \times K \) transition (3D)-matrices \( \tilde{F} = \{P(\theta) = (p_{ijl}(\theta))_{i,j,l=1,...,K} : \theta \in \Theta \subseteq \mathbb{R}^d\} \) so that our objective is to estimate the unknown parameter \( \theta \) from the observed sequence.

To define the MDPDE of \( \theta \) for this second-order Markov chain, we re-express it as a first-order Markov chain with the state-space \( S \times S = \{(i, j) : i, j = 1, 2, \ldots, K\} \). This resulting first-order Markov chain over \( S \times S \) will have a \( K^2 \times K^2 \) transition matrix of the form \( \Pi = (\pi(i,j)(h,l))(i,j),(h,l)\in S\times S \), where \( \pi(i,j)(h,l) = \delta_{jh}\pi_{ijl} \). The parametric model family \( \tilde{F} \) can also be converted similarly to a parametric family of \( K^2 \times K^2 \) transition matrices given by

\[
\mathcal{F} = \left\{ P(\theta) = ((p_{(i,j)(h,l)}(\theta)))_{(i,j),(h,l)\in S\times S} : \theta \in \Theta \subseteq \mathbb{R}^d \right\},
\]

where \( p_{(i,j)(h,l)}(\theta) = \delta_{jh}p_{ijl}(\theta) \).

Then, the MDPDE of \( \theta \) can be defined as in 2.1 by minimizing the appropriate DPD measure between the modified model transition matrix \( P(\theta) \) and the (nonparametric) estimate of \( \Pi \). In this case, the nonparametric estimates of the original transition probabilities \( \pi_{ijl} \)'s are given by

\[
\hat{\pi}_{i,j,l} = \frac{\sum_{T=2}^{T} I(X_{t-2} = i, X_{t-1} = j, X_t = l)}{\sum_{l=1}^{K} \sum_{j=1}^{K} \sum_{t=2}^{T} I(X_{t-2} = i, X_{t-1} = j, X_t = l)}, \quad i, j, l = 1, 2, \ldots, K.
\]
Therefore, an estimate of the element of the modified transition matrix \( \Pi \) is given by

\[
\hat{\pi}(i,j)(h,l) = \delta_{jh} \hat{\pi}_{ijl} = \frac{\delta_{jh} \sum_{t=2}^{T} I(X_{t-2} = i, X_{t-1} = j, X_{t} = l)}{\sum_{j=1}^{K} \sum_{t=1}^{T} \sum_{l=1}^{L} I(X_{t-2} = i, X_{t-1} = j, X_{t} = l)},
\]

\((i, j), (h, l) \in S \times S,\)

and the estimate of the associated stationary probabilities \( \pi(i,j) \) are given by

\[
\hat{\pi}(i,j) = \frac{1}{T} \sum_{l=1}^{K} \sum_{h=1}^{K} \hat{\pi}(i,j)(h,l) = \frac{1}{T} \sum_{l=1}^{K} \hat{\pi}_{ijl}, \quad (i, j) \in S \times S.
\]

Then, the MDPDE of \( \theta \) is defined as a minimizer of the objective function in (5), which now reads as

\[
H_{T,\alpha}^{(2)}(\theta) = \frac{1}{1 + \alpha} \sum_{(i,j) \in S \times S} \sum_{(h,l) \in S \times S} \hat{\pi}(i,j) \cdot \left( p(i,j)(h,l)(\theta)^{1+\alpha} - \left( 1 + \frac{1}{\alpha} \right) p(i,j)(h,l)(\theta)^{\alpha} \hat{\pi}(i,j)(h,l) \right)
\]

\[
= \frac{1}{1 + \alpha} \sum_{i=1}^{K} \sum_{j=1}^{K} \sum_{l=1}^{K} \rho(i,j) \cdot \left( p(i,j)(\theta)^{1+\alpha} - \left( 1 + \frac{1}{\alpha} \right) p(i,j)(\theta)^{\alpha} \hat{\pi}(i,j)(h,l) \right).
\]

(33)

In analogue to (6), the estimation equation of the MDPDE will now have the form

\[
U_{T,\alpha}^{(2)}(\theta) := \sum_{i=1}^{K} \sum_{j=1}^{K} \sum_{l=1}^{K} \pi(i,j) \cdot \left( p(i,j)(\theta) - \hat{\pi}(i,j)(h,l) \right) \cdot \left( p(i,j)(\theta)^{\alpha} - \pi(i,j) \right) = 0_d.
\]

(34)

All the asymptotic properties of the resulting MDPDE can be easily obtained from the results of Sect. 2.2 via the first-order Markov chain representation over \( S \times S \). Then, the subsequent testing procedures can also be developed in a similar fashion.

Note that, the objective function (33) and the estimating Eq. (34), corresponding to the MDPDE in a second-order Markov chain, have quite general structures that can easily be extended for Markov chains of any higher order. Suppose we have a sequence \( X_T = \{X_0, X_1, \ldots, X_T\} \) of observations from a Markov chain of order \( r \geq 2 \) having finite state-space \( S = \{1, 2, \ldots, K\} \) and stationary transition probabilities

\[
\pi_{i_1i_2\cdots i_{r+1}} = P(X_t = i_{r+1}|X_{t-r} = i_1, X_{t-r+1} = i_2, \cdots, X_{t-1} = i_r),
\]

\( i_j = 1, \ldots, K; \quad j = 1, \ldots, (r + 1).\)

If these transition probabilities are modeled by some parametric model of the form \( p_{i_1i_2\cdots i_{r+1}}(\theta) \), the MDPDE of the corresponding parameter \( \theta \) would be defined as the minimizer of the objective function.
\[
H^{(r)}_{T,\alpha}(\theta) = \frac{1}{1+\alpha} \sum_{i_1=1}^{K} \cdots \sum_{i_r=1}^{K} \sum_{i_{r+1}=1}^{K} \pi_{(i_1, \ldots, i_r)} \sum_{i_{r+1}=1}^{K} \pi_{(i_1, \ldots, i_r, i_{r+1})} \\
\times \left\{ p_{l_1l_2 \cdots l_{r+1}}(\theta)^{1+\alpha} - \left( 1 + \frac{1}{\alpha} \right) p_{l_1l_2 \cdots l_{r+1}}(\theta)^{\alpha} \hat{\pi}_{l_1l_2 \cdots l_{r+1}} \right\},
\]

or the solution of the estimating equation

\[
U^{(r)}_{T,\alpha}(\theta) := \sum_{i_1=1}^{K} \cdots \sum_{i_r=1}^{K} \sum_{i_{r+1}=1}^{K} \psi_{l_1l_2 \cdots l_{r+1}}(\theta) \left( p_{l_1l_2 \cdots l_{r+1}}(\theta) - \hat{\pi}_{l_1l_2 \cdots l_{r+1}} \right)
\]

where

\[
\hat{\pi}_{l_1l_2 \cdots l_{r+1}} = \frac{\sum_{t=r}^{T} I(X_{t-r} = i_1, X_{t-r+1} = i_2, \ldots, X_t = i_{r+1})}{\sum_{i_1=1}^{K} \cdots \sum_{i_r=1}^{K} \sum_{i_{r+1}=1}^{K} \sum_{t=r}^{T} I(X_{t-r} = i_1, X_{t-r+1} = i_2, \ldots, X_t = i_{r+1})},
\]

\[
\hat{\pi}_{(i_1, \ldots, i_r)} = \frac{1}{T} \sum_{i_{r+1}=1}^{K} \hat{\pi}_{l_1l_2 \cdots l_{r+1}}, \quad \text{for } i_j = 1, 2, \ldots, K; \ j = 1, 2, \ldots, r.
\]

Further in-depth investigations of the MDPDEs under such higher order Markov chains as well as their applications would be interesting future research. Among others, an important application would be the robust test for the order of a Markov chain based on the given observations, i.e., to test if the given sequence of observations is coming from a Markov chain of order \( r \) via the hypothesis \( H_0 : \pi_{l_1l_2 \cdots l_{r+1}} = \pi_{l_2 \cdots l_{r+1}} \) with \( i_j \in \{1, \ldots, K\} \), for each \( j = 1, \ldots, (r+1) \). There have been several approaches for determination of the order of a Markov chain including the information criteria like AIC and BIC (Zhao et al. 2001), divergence based test of the above \( H_0 \) (Menendez et al. 2001) and mutual information based procedures (Papapetrou and Kugiumtzis 2013).

In the same spirit, we can also use the MDPDE and the associated DPD measure to develop appropriate robust test for the above \( H_0 \) corresponding to the order selection of Markov chain observations which we hope to study in detail in a sequel work.

### 5.3 Finite Markov chains with time-dependent transition probabilities

In several practical applications, the Markov chain may not be stationary, i.e., the transition probabilities depend on time. We can also extend the concept of MDPDE for robust parameter estimation for such non-stationary cases. First note that, if we have one large sequence of observations from a non-stationary Markov chain, without loss of generality, the observations far away from the starting point can often be treated as stationary, under appropriate assumptions, for the inference purpose. This is because, in many common situations, such a chain mixes very fast (exponential or geometric mixing) and, hence, behave like a stationary chain in long run. So, here, we discuss...
the extension of the MDPDE only for the case of several small-length sequence of observations from a non-stationary Markov chain model.

Let us consider the set-up and notation of Sect. 5.1, where we have observed \( n \) sequence of observations each of length \((T + 1)\) (for simplicity), with large enough \( n \) \((\rightarrow \infty)\) and relatively small \( T \). Suppose that the underlying Markov chain has transition probabilities \( \pi_{ij}(t) \) for a given time-point \( t = 0, 1, \ldots, T \), and we model it by a parametric family of transition matrices depending on time \( t \), i.e., by the family \( \mathcal{F} = \{ P(t; \theta) = (p_{ij}(t; \theta))_{i,j=1,\ldots,K} : \theta \in \Theta \subseteq \mathbb{R}^d \} \), where \( p_{ij}(t; \theta) \) are known functions depending on the unknown \( d \)-dimensional parameter vector \( \theta = (\theta_1, \ldots, \theta_d)' \in \Theta \) for each time point \( t \). We want to estimate \( \theta \) based on the observed sequences \( X^{(l)}_t \) for \( l = 1, 2, \ldots, n \).

In this context, the nonparametric MLEs of the transition probabilities \( \pi_{ij}(t) \) are given by

\[
\hat{\pi}^{(n)}_{ij}(t) = \frac{\sum_{l=1}^{n} I(X^{(l)}_{t-1} = i, X^{(l)}_t = j)}{\sum_{j=1}^{K} \sum_{l=1}^{n} I(X^{(l)}_{t-1} = i, X^{(l)}_t = j)}, \quad i, j = 1, \ldots, K; t = 0, 1, \ldots, T.
\]

If \( \hat{\Pi}^{(n)}(t) = (\hat{\pi}^{(n)}_{ij}(t))_{i,j=1,\ldots,K} \) denote the corresponding estimate of \( \Pi(t) \) for each \( t = 0, 1, \ldots, T \), then the MDPDE of \( \theta \) can be defined as the minimizer of an appropriate generalization of the DPD measures between \( \hat{\Pi}^{(n)}(t) \) and \( P(t; \theta) \). The most intuitive choice (extending the idea from Ghosh and Basu (2013)) is to minimize the total discrepancy measure \( \sum_{t=0}^{T} \sum_{i=1}^{K} \hat{\pi}^{(n)}_{io}(t) \cdot d_q(\hat{\Pi}^{(n)}_i(t), P_i(t; \theta)) \), where \( \hat{\Pi}^{(n)}_i(t) \) and \( P_i(t; \theta) \) denote the \( i \)th row of \( \hat{\Pi}^{(n)}(t) \) and \( P(t; \theta) \), respectively, and

\[
\hat{\pi}^{(n)}_{io}(t) = \frac{1}{n} \sum_{j=1}^{K} \sum_{l=1}^{n} I(X^{(l)}_{t-1} = i, X^{(l)}_t = j), \quad i = 1, 2, \ldots, K; \ t = 0, 1, \ldots, T.
\]

This leads to the simpler MDPDE objective function, in analogue of (5), as given by

\[
H_{n, \alpha}(\theta) = \frac{1}{1 + \alpha} \sum_{t=0}^{T} \sum_{i=1}^{K} \sum_{j=1}^{K} \hat{\pi}^{(n)}_{io}(t) \sum_{j=1}^{K} \left\{ p^{(n)}_{ij}(t; \theta)^{1+\alpha} - \left( 1 + \frac{1}{\alpha} \right) p^{(n)}_{ij}(t; \theta)^{\alpha} \hat{\pi}^{(n)}_{ij}(t) \right\}.
\] (35)

The resulting MDPDE can be studied asymptotically as \( n \to \infty \) (fixed \( T \)) in a similar fashion as in Sect. 5.1, provided we have a result similar to (31). Such results are available in the literature of Markov chain under suitable assumptions (e.g., Anderson and Goodman (1957)) which would lead to the asymptotic distribution of MDPDE as a suitable extension of (32). Considering the length and content of the present manuscript, we have deferred the detailed investigation of the properties and applications of the MDPDE in such non-stationary context for a future work.
6 Real-life application: credit-rating migration data

We now describe a real-life application of the finite Markov chain models in modelling credit-risk migration data. In a recent work, Mostel et al. (2020) statistically modeled Moody’s corporate ratings migration data with finite Markov chain models for statistical inference. Here, we illustrate the usefulness of robust inference procedures for the finite Markov chain models in analyzing the average one year corporate transition rates as reported in Table 22 of Richhariya et al. (2019). They presented the average transition rates for seven rating categories AAA, AA, A, BBB, BB, B, CCC/C, along with the default (D), computed based on the rating changes of different corporate entities till 2018 separately for three international markets, namely USA, Europe and Emerging Markets; see pages 66-67 of Richhariya et al. (2019) for definitions (Sources: S&P Global Fixed Income Research and S&P Global Market Intelligence’s CreditPro.). For USA, the data from the year 1981 are considered while for Europe and Emerging markets data from 1996 are used, taking into account the sample size issues. The entities which were listed at the beginning of the time period but not listed at the final year of 2018, are reported in a separate category NR (not-rated). Our aim is to get parametric estimate of the upgrade and downgrade probabilities for each rating categories.

We model these data, after conditioning by removal of the NR category, with a Markov chain model having $K = 8$ states corresponding to the seven ratings and the default (D); these states are ordered from AAA to CCC/C with D being the lowest category (which is an absorbing state). We fit a parametric model with transition matrix $P(\theta) = (p_{ij}(\theta))_{i,j=1,...,K}$, having a binomial-type form as in Example 2 (Sect. 3.2) with slight modifications. With an aim of predicting the probability of upgrade and downgrade from each states, we indeed club the transition probabilities to all states above and below the current state; these combined data are presented in Table 1 of the Online Supplement (Sect. C), for all the three markets. Since the transition rate from any state to itself is the highest, the parametric model of Example 2 (Sect. 3.2) always yield an estimate of $\theta_i$ near about 0.5 for all $i$, which is clearly not suited to model our data. So, we consider a slightly modified model given by

$$p_{ii}(\theta) = \theta_i^2, \quad \sum_{j<i} p_{ij}(\theta) = (1 - \theta_i)^2, \quad \sum_{j>i} p_{ij}(\theta) = (1 - \theta_i), \quad i = 2, \ldots, K - 1.$$  

The model for the first state (AAA) is considered as $p_{11}(\theta) = \theta_1^2$ and $\sum_{j>1} p_{1j}(\theta) = (1 - \theta_1)$, whereas the last state (D) is an absorbing state so that $p_{KK}(\theta) = 1$ and $\sum_{j<K} p_{1j}(\theta) = 0$. Here, the parameter vector is $\theta = (\theta_1, \ldots, \theta_{K-1})^t \in [0, 1]^{K-1}$, which we estimate from the given data (separately for the three markets) using the usual MLE and the proposed MDPDE with $\alpha = 0.5$ (suggested choice of the tuning parameter). Given an estimate $\hat{\theta}_i$ of $\theta_i$ for the $i$th state ($i = 2, \ldots, K - 1$), the corresponding estimates of the upgrade and downgrade probabilities are obtained by $(1 - \hat{\theta}_i)^2$ and $2\hat{\theta}_i(1 - \hat{\theta}_i)$, respectively. The resulting parameter estimates for all three markets are reported in Table 2, and the corresponding upgrade and downgrade
Table 2  The MLE and the MDPDE at $\alpha = 0.5$ of the parameters under the assumed Markov chain models for the Credit rating migration data of three international markets

| Rating     | USA MLE | USA MDPDE | Europe MLE | Europe MDPDE | Emerging Markets MLE | Emerging Markets MDPDE |
|------------|---------|-----------|------------|--------------|----------------------|------------------------|
| AAA ($\theta_1$) | 0.9516  | 0.9540   | 0.9422     | 0.9418       | 0.9454               | 0.9524                 |
| AA ($\theta_2$)  | 0.9505  | 0.9638   | 0.9489     | 0.9629       | 0.9553               | 0.9683                 |
| A ($\theta_3$)   | 0.9376  | 0.9686   | 0.9311     | 0.9676       | 0.9462               | 0.9653                 |
| BBB ($\theta_4$) | 0.8959  | 0.9322   | 0.8937     | 0.9354       | 0.9184               | 0.9529                 |
| BB ($\theta_5$)  | 0.8988  | 0.9349   | 0.8897     | 0.9399       | 0.8895               | 0.9382                 |
| CCC/C ($\theta_7$) | 0.6803  | 0.7054   | 0.6666     | 0.6993       | 0.6563               | 0.7183                 |

probability estimates are presented (in%) in Fig. 1 in the Online Supplement (due to page restriction).

It can be easily seen from the results that the MDPDE and the MLE are more close for the higher-rating categories and for developed markets; their difference increases for lower rating categories and also from USA to Europe followed by the emerging markets. It is known that these ratings are more stable for the higher categories and more developed markets; so, in these cases, there is no drastic effects of outlying observations and the proposed MDPDE yields similar parameter estimate as the MLE. But, for the other group of lower rating category and developing markets, these ratings are known to be unstable due to sudden changes in economic conditions and the MDPDE provides more stable results compared to the MLE which is quite far off in such cases. Similar patterns are also observed for the estimated upgrade and downgrade probabilities. Of particular interest is the downgrade probability from rating CCC/C, which is nothing but the default probability of a corporate entity after a year starting with a rating of CCC/C. Based on the MLE, this default probability is highest for the emerging markets (45.11%) followed by Europe (44.45%) and USA (43.50%), whereas these estimates are 40.47%, 42.06% and 41.57%, respectively, based on the proposed MDPDE. It is then evident that the higher default probability of the emerging markets in the MLE based inference is only due to some outlying entities (sudden default due to external factors within these markets), although it indeed have a lowest (stable) default rate (starting from CCC/C) compared to Europe and USA which is more intuitive and can be correctly obtained from the proposed MDPDE based inference yielding robust estimates. The same is also observed for the upgrade probability from CCC/C and for other lower ranking categories as well (see Fig. 1 in the Online Supplement).

7 Concluding remarks

This paper develops a robust estimator, namely the minimum density power divergence estimator, of the underlying parameter in finite Markov chain models and several important extensions. The advantages of the proposed estimator is illustrated theo-
retically and empirically along with its applications in statistical hypotheses testing. Several possible extensions and future works are pointed out throughout the paper. We would like to further mention that, although the simplest Wald-type tests based on the MDPDE are discussed here, one might also want to construct robust versions of the other two types of tests, namely the likelihood-ratio and the score type tests. Such constructions can also be done using the MDPDE and its asymptotic distributions (Theorems 2.1 and 2.2) under the present set-up of finite Markov chains, extending the corresponding works done for independent observations (Basu et al. 2018, 2019) and will be investigated further in future.

Additionally, the present work opens up a new direction of research to further extend the concept of MDPDE for robust inference in more complex stochastic processes. In particular, extensions for the Markov chains having countably infinite or continuous state-spaces, discrete time stochastic processes and more generally continuous time stochastic processes would have significant advantages for robust insight generations in several real-life applications. Although the definition of the MDPDE can easily be extended for such general stochastic processes, their theoretical study and practical implementations would need substantive additional (non-trivial) works. We hope to pursue some of these important extensions in future.

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