Stability of the manifold boundary approximation method for reducing the nuclear structure models

M. Imbrišak and K. Nomura
Department of Physics, Faculty of Science, University of Zagreb, HR-10000 Zagreb, Croatia

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The framework of nuclear energy density functionals has been employed to describe nuclear structure phenomena for a wide range of nuclei. Recently, statistical properties of a given nuclear model, such as parameter confidence intervals and correlations, have received much attention, particularly when one tries to fit complex models. We apply information-theoretic methods to investigate stability of model reductions by the manifold boundary approximation method (MBAM). In an illustrative example of the density-dependent point-coupling model of the relativistic energy density functional, utilizing Monte Carlo simulations, it is found that main conclusions obtained from the MBAM procedure are stable under variation of the model parameters. Furthermore, we find that the end of the geodesic occurs when the determinant of the Fisher information metric vanishes, thus effectively separating the parameter space into two disconnected regions.

I. INTRODUCTION

The nuclear energy density functional (EDF) framework is a promising, unified theoretical approach for a global description of nuclear structure phenomena. One of the successful EDFs has been the one that is based on the relativistic mean-field Lagrangian in the finite-range meson-exchange model [1], with the density-dependent meson-nucleon couplings providing an improved description of asymmetric nuclear matter [2]. Moreover, it has been found that simpler, point-coupling models [3, 4] produce comparable results to the finite-range ones, even if the point-coupling interactions are being adjusted to nuclear matter and ground-state properties of finite nuclei [5]. These density-dependent point-coupling models, however, have been shown to exhibit an exponential range of sensitivity to parameter variations, prompting the application of model reduction methods based on concepts of information geometry [6, 7].

The Universal Nuclear Energy Density Functional (UNEDF) project was a large-scale collaborative effort primarily focused on a wide range of pioneering developments in EDF, including uncertainty quantification of nuclear theory [8, 9]. In the last decade, statistical error analysis, either employing classical or Bayesian inference, has started to be recognized in EDF research for its ability to quantify theoretical errors, distinguish safe and risky extrapolations, provide sensitivity analysis, and offer insight into model instabilities [10–20].

Information geometry is an interdisciplinary field that introduces differential geometry concepts to statistical problems [21, 22] with its initial applications centered around machine learning and neural networks [23, 24]. Recently, the manifold boundary approximation method (MBAM) [25, 27] has been developed to study complex and sloppy problems occurring in physics, chemistry and biology [25, 28] in order to either classify or reduce complex models, such as the nuclear EDFs [20, 27, 31].

The complexity of nucleon-nucleon interaction in the nuclear medium, coupling between single-nucleon and collective degrees of freedom, and finite-size effects present obstacles to numerous attempts to establish a single theoretical framework to treat the nuclear many-body problem. The nuclear EDFs, and structure models based on them, have become a promising tool for the description of ground-state properties and low-energy collective excitation spectra of medium-heavy and heavy nuclei. A variety of structure phenomena have been successfully described using the nuclear EDF framework with a high level of global precision and accuracy over the entire chart of nuclides, and at a very moderate computational cost.

The unknown exact nucleon EDF is approximated by functionals of powers and gradients of ground-state nucleon densities and currents, representing distributions of matter, spin, isospin, momentum, and kinetic energy. A generic density functional is not necessarily microscopic, i.e., it is related to the underlying inter-nucleon interactions, but some of the most successful functionals are entirely empirical. However, one can also follow the middle way between fully microscopic and entirely empirical EDFs, and consider semi-empirical functionals that start from a microscopically motivated ansatz for the nucleonic density dependence of the energy of a system of protons and neutrons. Most of the parameters of such a functional are adjusted, in a local density approximation, to reproduce a given microscopic equation of state (EoS) of infinite symmetric and asymmetric nuclear matter, and eventually neutron matter. The remaining, usually few, terms that do not contribute to the energy density at the nuclear matter level, are then adjusted to selected ground-state data of an arbitrarily large set of spherical and/or deformed nuclei. A number of semi-empirical functionals have been developed over the last decade [8, 32, 41], and very successfully applied to studies of a diversity of structure properties, from clustering in relatively light nuclei to the stability of superheavy systems, and from bulk and spectroscopic properties of stable nu-
cnel to the physics of exotic nuclei at the particle drip
lines.

In the previous studies [6, 7], the authors have used
concepts from information geometry to demonstrate
that nuclear EDFs are, in general, “sloppy” [25–28, 42].
The term “sloppy” refers to the fact that the predictions
of nuclear EDFs and related models are really sensitive to
only a few combinations of parameters (stiff parameter
combinations) and exhibit an exponential decrease of sen-
sitivity to variations of the remaining combinations of
parameters (soft parameter combinations). This means
that the soft combinations of parameters are only loosely
constrained by the available data, and that most nuclear
EDFs in fact contain models of lower effective dimen-
sionality associated with the stiff combinations of model
parameters. In Ref. [6], by employing the MBAM [27] the
authors have deduced the most effective functional form
of the density-dependent coupling parameters of a repre-
sentative model EDF. The data used in this calculation
included a set of points on a microscopic EoS of symmetric
nuclear matter and neutron matter. This choice was
motivated by the necessity to calculate the derivatives of
observables with respect to model parameters which is,
of course, much more efficiently accomplished for nuclear
matter in comparison to finite nuclei. In Ref. [7] we have ex-
tended this calculation by employing a simple numerical
approximation to calculate the derivatives of observables
with respect to model parameters. Thus we were able
to apply the MBAM to realistic models constrained not
only by the nuclear matter EoS but also by observables
measured in finite nuclei.

In this work, we study the stability of the MBAM with
respect to the variation of the model parameters. In Sec.
[II] we give an introduction to information-geometric
concepts. In Sec. [III] we describe the numerical imple-
mentation for finding the Dirac mass and binding en-
ergy, aided by algorithmic differentiation. The results of
our investigation are given in Sec. [IV] while further ap-
lications of information geometry to nuclear EDFs are
discussed in Sec. [V].

II. INFORMATION GEOMETRY AND MODEL
REDUCTION

A selection of the model is usually made through
the maximum likelihood method, with the assumption
that at the a-th measurement the data \((x^a, y^a)\) can
be described using a normal distribution, denoted by
\(\mathcal{N}\), by a model function \(f(x^a, p) \equiv f^a(p)\) as
\(y^a \sim \mathcal{N}(f^a(p), (\sigma^a)^2)\). Here, \(\sigma^a\) is the uncertainty of each
measurement, and \(p\) is chosen from an appropriate pa-
rameter space, denoted by \(\mathcal{M}\). Finding the best-fitting
model is equivalent to maximizing the following log-
likelihood function \(l(p)\) over \(p \in \mathcal{M}\),

\[
l(p) = \sum_a \ln \phi \left( \frac{y^a - f^a(p)}{\sigma^a} \right)
\]

with \(\phi\) a Gaussian probability density. To simplify the
notations, we shall use indices from the beginning of the Latin
alphabet for measurements, and the Greek letters for
derivatives \(\frac{\partial}{\partial p}\), shortened to \(\partial_p\). The log-likelihood
function can then be Taylor expanded to the second order to find
parameter uncertainties by the Cramer-Rao bound [22]
using the Hessian of the log-likelihood,

\[
g_{\mu\nu}(p) = \sum_a \frac{\partial f^a}{\partial_p^\mu} \frac{\partial f^a}{\partial_p^\nu} \left(\sigma^a\right)^2
\]

The above quantity is referred to as the Fisher informa-
tion matrix (FIM).

A. Information geometry

The simple picture described above can be reinterpre-
ted by using information geometry. The function \(i(p)\)
connects \(\mathcal{M}\) and \(\mathcal{N}\), now interpreted as manifolds.
Furthermore, the differential form, i.e., \(dl = \partial_p \log \mathcal{M}\),
forms a basis for the cotangent bundle on \(\mathcal{N}\), labeled as \(T^*\mathcal{N}\),
while the FIM serves as a metric on \(\mathcal{N}\). Here, we note
that the appearance of the same index \(\mu\) more than
once in the mathematical expression indicates summation
with respect to that index, and shall follow this con-
vention from now on. The functional form of the log-
likelihood is then used to induce a metric on the param-
eter space, \(\mathcal{M}\). This is achieved by computing the ex-
pectation value taken with respect to \(\mathcal{N}\): \(g \equiv E[dl \otimes dl]\)
[22]. The pullback operation, \(l^*\), then induces a met-
ric \(g(p) \in (T^*\mathcal{M})^2\) on \(\mathcal{M}\), as \(g(p) = g_{\mu\nu}(p) \otimes dp^\mu \otimes dp^\nu = E[\partial_p l^* \otimes l^* dp^\mu \otimes dp^\nu] = l^* g\). This procedure equips the
model manifold \(\mathcal{M}\) with a tangent bundle spanned by
the basis \(\partial_p \in T \mathcal{M}\) and its cotangent bundle by the dual
basis \(dp^\mu \in T^* \mathcal{M}\). Since the normal family is a subset of
the exponential family, the model manifold \(\mathcal{M}\) is there-
fore a submanifold embedded in \(\mathcal{N}\) and belongs to the
curved exponential family [21].

In differential geometry, tangent spaces of nearby
points in \(\mathcal{M}\) are connected via the covariant derivative,
usually expressed as \(\nabla_X\) with an arbitrary direction \(X\).
The action of the covariant derivative on a tangent vec-
ctor \(Y \in T \mathcal{M}\) is simply given by \(\nabla_X(Y) = \nabla_X(Y^\mu \partial_{\mu}) = X^\nu \partial_{\nu}(Y^\mu) \partial_{\mu} + \Gamma^\alpha_{\mu\nu} X^\mu Y^\nu \partial_{\alpha}\). The quantity \(\Gamma^\alpha_{\mu\nu}\) stands
for the Christoffel symbol when the metric-compatible
connection with the condition \(\nabla_X(g) = 0\) is chosen (for
details see, e.g., Ref. [43]). For the FIM, the Christoffel
symbols are given by

\[
\Gamma^\alpha_{\mu\nu}(p) = g^{\kappa\rho} \sum_a \frac{\partial f^a}{\partial_{\mu}^\kappa} \frac{\partial f^a}{\partial_{\nu}^\rho} \left(\sigma^a\right)^2
\]

where \(g^{\kappa\rho} = (g^{-1})_{\kappa\rho}\) denotes the inverse of the metric.

Additionally, along the geodesic, we compute the Riem-
ann curvature tensor, and the scalar curvature. We
implement the Riemann curvature tensor, defined for
\(X, Y, Z \in T \mathcal{M}\), as \(R(X, Y)Z = [\nabla_X, \nabla_Y]Z - \nabla_{[X,Y]}Z\).
The components of the Riemann tensor are expressed as

$$ R_{\mu\nu\rho\kappa} = \sum_{ab} P^{ab} \left( \partial_{\mu} f^{a}_{\sigma\alpha} \partial_{\kappa} f^{b}_{\sigma\beta} - \partial_{\mu} f^{a}_{\sigma\beta} \partial_{\kappa} f^{b}_{\sigma\alpha} \right), \quad (4) $$

where $P^{ab}$ denotes the projection operator

$$ P^{ab} = \delta^{ab} - g^{\mu\nu} \partial_{\mu} f^{a}_{\sigma\alpha} \partial_{\nu} f^{b}_{\sigma\beta}. \quad (5) $$

The Ricci scalar (or scalar curvature) is computed simply as

$$ R_{\mu\nu\rho\kappa} g^{\mu\rho} g^{\nu\kappa}. \quad (6) $$

B. The manifold boundary approximation method

Complex models might have large parameter uncertainties, i.e., a large covariance matrix. In the cases where the covariance matrix, and therefore the corresponding FIM, have a spectrum spanning many orders of magnitude, model reduction procedures can improve parameter estimates. The MBAM [27] allows for better constraining parameters of such models across many physical disciplines [28]. The method computes the geodesic by solving the geodesic equation, $\nabla_{\dot{p}} \dot{p} = 0$, by starting from the best-fitting (bf) point in the model manifold, $p_{bf} \equiv p_{bf}^\mu \partial_{\mu}$. Note that the dot on $p$ represents the differentiation with respect the affine parametrization of the geodesic. The geodesic equation, written in parameter components as

$$ \ddot{p}^\kappa + \Gamma_{\mu\nu}^{\kappa} \dot{p}^\mu \dot{p}^\nu = 0, \quad (7) $$

is solved with the $\dot{p}$ initial conditions pointing in the direction of the FIM eigenvector, $v^0$, corresponding to its smallest eigenvalue. This is the largest eigenvalue of the covariance matrix and the biggest contributor to the uncertainty of the derived model parameters. The behavior of $v^0$ is followed along the geodesic until the parameter, or combination of parameters, contributing most to $v^0$ can be easily determined. This parameter is then eliminated from the model, resulting in a simpler model with smaller parameter uncertainties. This procedure can be repeated as long as the reduced model describes the data set sufficiently well.

III. ILLUSTRATIVE CALCULATION

The density-dependent point-coupling (DD-PC1) interaction [5] is a semi-empirical relativistic EDF that involves the point coupling [15], and has been used in many contemporary studies of nuclear structure and dynamics. The DD-PC1 functional explicitly includes nucleon degrees of freedom and considers only second-order interaction terms. Its applicability to a wide range of atomic nuclei has been demonstrated, e.g., in Refs. [16] [17].

We use the Dirac mass and energy density data shown in Table I to constrain the density-dependent coupling constants of the DD-PC1 functional, $\alpha_s(\rho)$, $\alpha_v(\rho)$ and $\alpha_{tv}(\rho)$, modeled as

$$ \alpha_i = a_i + \left( b_i + c_i \frac{\rho}{\rho_{sat}} \right) e^{-d_i \frac{\rho}{\rho_{sat}}}, \quad i \in \{ s, v, tv \}, \quad (8) $$

where the indices $i = s$, $v$, and $tv$ correspond to the isoscalar-scalar, isoscalar-vector, and isovector-vector channels respectively, while $\rho_{sat}$ is the saturation density. In this paper, we take a closer look at the reduced version of the model with $\alpha_{tv} = 0$ and $c_v = 0$, which results in a seven-parameter model involving $a_s$, $b_s$, $c_s$, $d_s$, $a_v$, $b_v$, and $d_v$.

| index | $\rho_s$, fm$^{-3}$ | $y^s$ | $\sigma_y$ |
|-------|---------------------|-------|------------|
| 1     | 0.152               | 0.58  | 0.055      |
| 2     | 0.04                | -6.48 | 0.648      |
| 3     | 0.08                | -12.13| 1.213      |
| 4     | 0.12                | -15.04| 1.504      |
| 5     | 0.16                | -16   | 1.6        |
| 6     | 0.2                 | -15.09| 1.509      |
| 7     | 0.24                | -12.88| 1.288      |
| 8     | 0.32                | -5.03 | 0.503      |

*first row in $M_D/m$, otherwise in MeV units

A. Numerical implementation

We solve the equation for the Dirac mass $M_D$, that is given by

$$ M_D = m + \alpha_s \rho_s, \quad (9) $$

where $m$ is the bare nucleon mass, and $\rho_s$ the scalar density

$$ \rho_s = \frac{2}{\pi^2} M_D \int_0^{p_F} \frac{x^2 dx}{\sqrt{x^2 + M_D^2}}, \quad (10) $$

with $p_F$ being the Fermi momentum

$$ p_F(\rho_s) = \left( \frac{3}{2} \rho_s \pi^2 \right)^{\frac{1}{3}}. \quad (11) $$

The equation (9) is solved numerically by using the Newton-Raphson algorithm. We have also tested the Halley’s method, but found no improvement of the results in accuracy.

Upon finding $M_D$, we compute the binding energy of symmetric nuclear matter

$$ E_a = \frac{2}{\pi^2} \int_0^{p_F} \frac{x^2 dx}{\sqrt{x^2 + M_D^2}} + m(\rho_s - \rho_c) + \frac{1}{2} \alpha_s \rho_s^2 + \frac{1}{2} \alpha_v \rho_v^2. \quad (12) $$
The best-fitting DD-PC1 parameter set is then found by computing the least-square solution to the set of measurements of $M_D/m$ and $E_a$ presented in Table IV (see Ref. [7]). Differential equations are solved with the aid of the SciPy implementation of the ordinary differential equation integration (odeint) library [18]. These values are then used to compute the FIM and the Christoffel symbols using algorithmic differentiation implemented via the autograd package. We thus eliminate numerical errors due to the approximations arising from numerical differentiations.

IV. INVESTIGATING STABILITY OF THE MBAM METHOD

In some cases, the numerical integration of the geodesic equation might slow down, or even fail. This behavior is due to the divergence of the metric tensor determinant that implicitly appears in the geodesic equation [7] through the metric inverse necessary for computing the Christoffel symbols [see Eq. (3)]. However, this divergent behavior is confined to only a small region in the parameter space, and therefore it might be easily missed by choosing too imprecise an integrator. Therefore, in Sec. IV A we investigate the impact of the size of the integration step on the MBAM procedure by artificially extrapolating the geodesic beyond the divergent region in the parameter space. Moreover, as the parameter uncertainties become larger, small perturbations to the starting point of the geodesic might influence the end result of the MBAM. In Sec. IV B we describe the impact of parameter uncertainties on the MBAM conclusions for the nuclear EDF DD-PC1 by numerical error propagation of the MBAM geodesics. Finally, in Sec. IV C we investigate the impact of using a common, physically-motivated restrictive reparametrization of the DD-PC coupling constants on the MBAM model manifold.

A. Geodesic extrapolation

We extrapolate the geodesic by using the last point having det $g > 0$ (labeled as $\tau_2$) and the point before it ($\tau_1$). We first extrapolate $\tau(t) = \tau_1(1-t) + \tau_2t$ for $t > 0$, i.e., a straight line joining $\tau_1$ and $\tau_2$. We then compute the $p^\mu(t)$ and $\dot{p}^\mu(t)$ using their corresponding values at $\tau_1$ and $\tau_2$ as

$$p^\mu(t) = p^\mu(\tau_1)(1-t) + p^\mu(\tau_2)t$$
$$\dot{p}^\mu(t) = \dot{p}^\mu(\tau_1)(1-t) + \dot{p}^\mu(\tau_2)t$$

This procedure produces a linear extrapolation of the geodesics in the region where the geodesic equation does not hold because det $g = 0$. The variable $t$ is just an interpolation parameter, not connected to $\tau$, so $\dot{p}$ is not coupled as $dp/d\tau$ in this region. We find that one can safely continue integrating the geodesic equation after $t = 2$, where there are no more singularities along the path.

In Fig. 1 the resulting model parameters along the extended geodesic (a), the corresponding model evaluation (b), the FIM eigenvalues (c), the $v^0$ eigenvector (d), the Ricci scalar (e), and the metric determinant (f) are shown. After the $t = 2$ point along the extrapolated geodesic, the metric tensor determinant starts to rise again. In the same figure, the extrapolated geodesic is shown with dashed, and the new MBAM continuation with dotted lines. The initial odeint solutions (solid lines), which produce results for a few points after $\tau = 1.3$, differ significantly from the interpolated solution, indicating numerical problems due to singularity. Upon restarting the odeint procedure after the singular region, we find that the MBAM solution yields different contributions to the $v^0$ eigenvector, indicating an equal contribution of $\partial_{\delta_{\mu}}$, $\partial_{\delta_{\nu}}$, and $\partial_{\delta_{\rho}}$ directions, while before $\tau = 1.3$, the MBAM method finds that the most significant contribution is from $\partial_{\delta_{\mu}}$. The Ricci scalar diverges at $\tau \sim 1.3$, but starts to fall and change signs at $\tau > 1.3$. Since the Ricci scalar is related to the volume element, its divergence to positive values would produce a compressed region of the parameter manifold, that begins to expand after the singularity.

The conclusion drawn from the results given in Fig. 1 is that one must be careful with the models where the metric tensor determinant shows significant variations, as choosing too big steps for the odeint integrator might result in “skipping” to another portion of the parameter space and continuing along it. This yields completely different contributions to the FIM eigenvector corresponding to its smallest eigenvalue and hence might lead to a completely different model reduction than expected from the simple MBAM case.

B. Parameter uncertainties

Further extension of the basic model might be the propagation of its parameter uncertainties, and this can be facilitated by looking into how the uncertainties of the best-fitting parameters propagate along the geodesics. For this purpose, we perform Monte Carlo simulations. To analyze the error propagation one would have to compute the geodesic equation many times, which is not cost-effective. We, therefore, adopt a simplified approach that makes use of the Jacobi equation, which computes differences $\delta p$ between neighboring geodesics along the already computed MBAM geodesic.

We use the covariance matrix $\Sigma$ to produce Monte Carlo simulations of $\delta p$ from the normal distribution, $\delta p \sim \mathcal{N}(0, \Sigma)$. For each simulated $\delta p$, we compute its propagation by using the Jacobi equation

$$\delta p^\mu + R^\mu_{\alpha\beta\gamma} \dot{p}^\alpha \delta p^\beta \delta p^\gamma = 0 .$$

We find 1300 points to sample the DD-PC1 parameter space reasonably well. Figure 2 shows the distributions
FIG. 1. Results of extrapolating the geodesic after the $\det g = 0$ point. Shown are (a) the behavior of the evaluated model for different $\tau$-s along the geodesic, (b) the model parameters, (c) the FIM eigenvalues as functions of $\tau$, (d) the squares of the FIM eigenvector $v^0$ components, (e) the Ricci scalar, and (f) the FIM determinant along the geodesic. Solid, dashed, and dotted lines stand for, respectively, the initial odeint solutions, the linear interpolation, and the values derived using odeint starting from the endpoint of the interpolated solutions.

of the parameters at the beginning (denoted by black symbols and contours) and at $\tau = 1.3$ (red symbols and contours). These two distributions are almost identical since the simulated parameters are more dispersed than the gradual changes in parameter values along the geodesic.

Even though the parameter uncertainties in the full model are large, we can estimate the error on the eigenvalues of the FIM along the geodesic. The results of this procedure along the geodesic are shown in the top row of Fig. 3. We see that, while the results using the simulated sample are consistently ordered when compared to the MBAM solution, there is a small offset between the median and the MBAM solution. The simulated scalar curvature and the metric determinant along the geodesic show a larger difference in their values along the geodesic. In panel (c) [(d)] of Fig. 3 we also observe that the 5th (95th) percentile of $\det g$ (scalar curvature) does follow the value along the geodesic, indicating that only the geodesics starting at the vicinity of the best-fitting point encounter the region corresponding to $\det g = 0$.

Furthermore, in Figs. 4 and 5 we show, respectively,
the distributions of eigenvalues and components of \( v^0 \) at the beginning and at the end of the geodesic. These large differences in eigenvalues and eigenvector components propagating along the geodesic are in stark contrast to the parameter values in Fig. 2. This discrepancy can be explained by the sensitivity of the FIM eigenproblem to small changes in DD-PC1 parameters, since diagonalization results are not expected to change linearly with inputs. We conclude that the offset is due to the non-Gaussianity of the distribution of eigenvalues and \( v^0 \) components, which arises even though the parameters were sampled using the normal distribution. Even though there is a change in the shape of these distributions, the overall qualitative MBAM conclusions remain the same along the geodesic.

C. Model reparametrization

The authors of Ref. [6] have considered an exponential reparametrization of the seven-parameter DD-PC1 coupling constants centered at their best-fitting values [5]. This reparametrization transformation can be schematically represented as a vector

\[
\mathbf{p(\tilde{\mathbf{p}})} = \begin{pmatrix}
a_s(p_{a_s}) \\
b_s(p_{b_s}) \\
c_s(p_{c_s}) \\
d_s(p_{d_s}) \\
a_v(p_{a_v}) \\
b_v(p_{b_v}) \\
d_v(p_{d_v})
\end{pmatrix} = \begin{pmatrix}
a_{s, bf} e^{-p_{a_s}} \\
b_{s, bf} e^{-p_{b_s}} \\
c_{s, bf} e^{-p_{c_s}} \\
d_{s, bf} e^{-p_{d_s}} \\
a_{v, bf} e^{-p_{a_v}} \\
b_{v, bf} e^{-p_{b_v}} \\
d_{v, bf} e^{-p_{d_v}}
\end{pmatrix}, \quad (16)
\]

where \( \mathbf{\tilde{p}} \) indicates multivariate distribution of parameters \( p_{a_s}, \cdots, p_{d_s} \), and the quantities such as \( a_{s, bf}, b_{s, bf}, \) etc.
Using these constraints the scalar mean-field potential remains attractive and the vector mean-field repulsive for all allowed parameter values [9].

We repeat the Monte Carlo analysis described in Sec. [14] for the reparametrized model. The resulting error estimates are shown in Fig. 6 in the same manner as in Fig. [5]. By comparing the two figures panel-by-panel, we conclude that both methods produce MBAM geodesics that are stable under perturbations, even though the two FIMs do not behave in the same way along their respective geodesics. The reparametrized FIM determinant and the Ricci scalar change gradually, compared to the initial model.

One may ask whether this discrepancy is due to using a too simplistic description of the reparametrized distributions. We then employ the Bayesian statistics to check whether the multivariate distribution \( \tilde{p} \) has pronounced non-Gaussian features. To this end, we use the Markov chain Monte Carlo (MCMC) technique to sample the \( \chi^2 \) posterior distribution, as implemented in the package emcee [14]. In Fig. 7, we show the behavior of the chosen 200 Markov chains as two-dimensional sections of the parameter space. The chains have been run for a long enough time to avoid the initial “burn-in” phase characteristic of the algorithm during which they follow mostly the (uniform) prior distribution instead of sampling the \( \chi^2 \) posterior distribution. From the fact that the classical covariance ellipses (represented by red contours in Fig. 7) are well-aligned with the MCMC estimates, we conclude that one can proceed with using the simple Monte Carlo Gaussian mock sample for error propagation instead of the computationally more expensive Bayesian MCMC mock sample.

The theoretical argument for the discrepancy between the two geodesics is based on the properties of the applied transformation. Since the exponential transformations are not bijections, the geodesics on the manifold spanned by \( \tilde{p} \) need not have the same behavior as the geodesics on the manifold spanned by \( p \). To better understand the connection between these two geodesics, we derive the FIM determinant on the \( \tilde{p} \)-manifold by using the transformation of Eq. (16),

\[
\det g(\tilde{p}) = a_s^2(a_s) b_s^2(b_s) c_s^2(c_s) d_s^2(d_s) a_v^2(a_v) b_v^2(b_v) d_v^2(d_v) \det g(p(\tilde{p})).
\]

The determinant of the metric is not an invariant quantity under reparametrizations, hence the additional multiplicative scaling is required. Equation (17) shows that, if the value of \( \det g \) approaches zero for particular values of \( p \), both geodesics terminate. However, additional singularities appear if any of the coupling constants is allowed to change sign along a particular geodesic. In contrast to the FIM determinant, the Ricci scalar is not affected by reparametrizations. The scalar curvature distributions for different points on the geodesic in Fig. 6(d) do not have the same values as those in Fig. 3(d). The effects of reparametrizations on the scalar curvature can be clearly seen from the comparison between these figures.

The general conclusion is, therefore, that the MBAM method is sensitive to the way the reparametrization is made, as has been shown above in the case of the reparametrization tied to domain restrictions. This is related to the fact that different reparametrizations do not
lead to the same, but similar, models describing the common physical problem. Since the EDF has an arbitrarily-chosen functional form, there is no \textit{a priori} way of identifying which parametrization is optimal.

V. CONCLUSION

Methods of information geometry have been applied to investigate the stability of reducing the nuclear structure models. We have constrained the error estimates of the manifold boundary approximation method (MBAM) solutions by means of the Monte Carlo simulations. In the illustrative application to the DD-PC1 model of the nuclear EDF, it has been found that the main conclusions obtained by using the MBAM method are stable under the variation of the parameters within the 1\(\sigma\) confidence interval of the best-fitting model. Moreover, we have found that the end of the geodesic occurs when the determinant of the FIM approaches zero, thus effectively separating the parameter space into two disconnected regions.

Further applications of information geometry to nuclear EDFs could be analyzing possible phase transitions in models of finite nuclei using scalar curvature and their impact on nuclear properties. The analysis could even be expanded to include an extended temperature-dependent model or to look for model instabilities. It would be worth investigating whether information-theoretic optimizations, like the natural-gradient descent, could accelerate computer codes to solve nuclear many-body problems.
FIG. 5. Same as Fig. 2 but for Monte Carlo simulated sample components of the FIM $v^0$ eigenvector.

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[1] M. Bender, P.-H. Heenen, and P.-G. Reinhard, Reviews of Modern Physics 75, 121 (2003).
[2] D. Vretenar, A. Afanasjev, G. Lalazissis, and P. Ring, Physics Reports 409, 101 (2005).
[3] B. A. Nikolaus, T. Hoch, and D. G. Madland, Physical Review C 46, 1757 (1992).
[4] T. Bürvenich, D. G. Madland, J. A. Maruhn, and P.-G. Reinhard, Physical Review C 65, 10.1103/PhysRevC.65.044308 (2002).
[5] T. Nikšić, D. Vretenar, G. A. Lalazissis, and P. Ring, Phys. Rev. C 77, 034302 (2008) [arXiv:0802.2442 [nucl-th]]
[6] T. Nikšić and D. Vretenar, Physical Review C 94, 10.1103/PhysRevC.94.024333 (2016).
[7] T. Nikšić, M. Imbrisak, and D. Vretenar, Physical Review C 95, 10.1103/PhysRevC.95.054304 (2017).
[8] M. Kortelainen, T. Lesinski, J. Moré, W. Nazarewicz, J. Sarich, N. Schunck, M. V. Stoitsov, and S. Wild, Phys. Rev. C 82, 024313 (2010) [arXiv:1005.5145 [nucl-th]].
FIG. 6. Same as Fig. 3, but for the reparametrized model described in Sec. IV C.
FIG. 7. Monte Carlo simulations of posterior distributions of the error estimates for the reparametrized model, based on the MCMC algorithm. The figure shows the 1σ, 2σ and 3σ covariance ellipses in red, as estimated from the FIM inverse, and the estimates of the covariance ellipses based on the MCMC sample points in blue.

[48] P. Virtanen, R. Gommers, T. E. Oliphant, M. Haberland, T. Reddy, D. Cournapeau, E. Burovski, P. Peterson, W. Weckesser, J. Bright, S. J. van der Walt, M. Brett, J. Wilson, K. J. Millman, N. Mayorov, A. R. J. Nelson, E. Jones, R. Kern, E. Larson, C. J. Carey, I. Polat, Y. Feng, E. W. Moore, J. VanderPlas, D. Laxalde, J. Perktold, R. Cimrman, I. Henriksen, E. A. Quintero, C. R. Harris, A. M. Archibald, A. H. Ribeiro, F. Pedregosa, P. van Mulbregt, and SciPy 1.0 Contributors, Nature Methods 17, 261 (2020).

[49] D. Foreman-Mackey, D. W. Hogg, D. Lang, and J. Goodman, Publications of the ASP 125, 306 (2013) arXiv:1202.3665 [astro-ph.IM]