NONPARAMETRIC BAYESIAN ESTIMATION IN A MULTIDIMENSIONAL DIFFUSION MODEL WITH HIGH FREQUENCY DATA

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ABSTRACT. We consider nonparametric Bayesian inference in a multidimensional diffusion model with reflecting boundary conditions based on discrete high-frequency observations. We prove a general posterior contraction rate theorem in $L^2$-loss, which is applied to Gaussian priors. The resulting posteriors, as well as their posterior means, are shown to converge to the ground truth at the minimax optimal rate over Hölder smoothness classes in any dimension. Of independent interest and as part of our proofs, we show that certain frequentist penalized least squares estimators are also minimax optimal.

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1. INTRODUCTION

Diffusion models are widely used in applications, including in the physical and biological sciences, economics and finance, as well as for particle filters and emulators amongst many others purposes. Denote by \( u(t, x) \) the density of a quantity that is diffusing in a closed system at time \( t > 0 \) and location \( x \in \Omega \) in bounded convex domain \( \Omega \subseteq \mathbb{R}^d \) with smooth boundary \( \partial \Omega \). Fick’s laws of diffusion state that the resulting dynamics are governed by the evolution equation

\[
\frac{\partial u}{\partial t} = \nabla \cdot (f \nabla u),
\]

with Neumann boundary conditions and where \( f > 0 \) is the diffusivity of the possibly inhomogeneous medium \( \Omega \). This describes the macroscopic behaviour of many particles in \( \Omega \) undergoing diffusion governed by Brownian dynamics.

On a microscopic level, the individual behaviour of a single such particle can be modelled as the multidimensional diffusion process \((X_t)_{t \geq 0}\) on \( \Omega \) that is reflected upon hitting the boundary \( \partial \Omega \) and arises as the solution to the SDE:

\[
\begin{align*}
X_t &= X_0 + \int_0^t \nabla f(X_s)ds + \int_0^t \sqrt{2f(X_s)}dB_s + \ell_t, \\
\ell_t &= \int_0^t n(X_s)d|\ell_s|, \quad |\ell_t| = \int_0^t 1_{\{X_s \in \partial \Omega\}}d|\ell_s|,
\end{align*}
\]

where \((B_t)_{t \geq 0}\) is a standard \(d\)-dimensional Brownian motion, \((\ell_t)_{t \geq 0}\) a bounded variation process with \( \ell_0 = 0 \) that accounts for the boundary reflection and \( n(x) \) denotes the unit inward normal to the boundary \( \partial \Omega \) at \( x \). We assume

\[
f : \Omega \to [f_{\text{min}}, \infty)
\]

is a positive function with \( f_{\text{min}} > 0 \) and take \( X_0 \) to be uniformly distributed on \( \Omega \), which is the invariant measure of the SDE (2), and hence \( X \) is started at stationarity. If \( \partial \Omega \) and \( \nabla f \) are continuously differentiable, existence and uniqueness of the solution to (2) follows from [37]. These
conditions, together with the convexity of the domain $\mathcal{O}$, can be relaxed, but will be sufficient for the level of generality intended here.

Consider observations regularly collected at discrete time points, resulting in data of the form

$$X^N = (X_0, X_D, \ldots, X_{ND})$$

with sampling interval $D > 0$. The statistical problem at hand is then to make inference on the diffusivity $f$ based on discrete observations of the location of a single particle corresponding to the macroscopic diffusion model (1). We study nonparametric Bayesian estimation of $f$ in model (2) using Gaussian process priors in the high-frequency and long term sampling regime, where $D = DN \to 0$ such that the time-horizon $NDN \to \infty$. In particular, we establish minimax optimal frequentist contraction rates for the posterior for $f$ about the ‘ground truth’ $f_0$ generating the data, thereby establishing theoretical guarantees for this method.

A statistical feature of model (2) is that its generator $L_f \phi = \nabla \cdot (f \nabla \phi)$ is a divergence form operator, which implies that the invariant measure $\mu_f$ is simply the uniform measure on the domain $\mathcal{O}$ for all $f$:

$$\mu_f(A) = \lim_{T \to \infty} \frac{1}{T} \int_0^T 1_A(X_t)dt \propto \text{vol}(A),$$

for any measurable $A \subset \mathcal{O}$, so that the average asymptotic time spent by the process $X$ in different regions does not contain information about $f$. By Markovianity, all information about $f$ is thus contained in the transitions $X_{(i-1)D} \rightarrow X_iD$, which motivates using a likelihood based approach, such as the Bayesian one we pursue here. In particular, this contrasts with several other well-studied diffusion models where one can identify the relevant model parameters from the invariant measure $\mu_f$, see e.g. [17, 58, 29, 2].

To better understand our approach, it is helpful to consider the one-dimensional diffusion model,

$$dX'_t = b(X'_t)dt + \sigma(X'_t)dW_t,$$

where $b : \mathbb{R} \to \mathbb{R}$ is the drift and $\sigma : \mathbb{R} \to \mathbb{R} \otimes \mathbb{R}^d$ is the diffusion coefficient. In the high frequency case where $b$ and $\sigma$ are both $s$-smooth, their minimax estimation rates scale like $(ND)^{-s/(2s+1)}$ and $N^{-s/(2s+1)}$, respectively, and one can thus estimate the diffusivity $\sigma$ at a faster rate than the drift $b$ [32]. In model (2), where these parameters are coupled, the diffusivity term is similarly more informative about $f$ than the drift, which must be exploited to obtain minimax optimal rates. While the Bayesian methodology does not explicitly make this distinction, simply placing a prior on $f$ as usual, our proofs themselves heavily rely on this idea. One can therefore view rate-optimal estimation of $f$ in model (2) as qualitatively analogous to estimation of $\sigma$ in model (5). Our work is thus relevant to the literature on estimating the diffusion coefficient [32, 14, 56] under high-frequency sampling. Our results indicate that Bayesian methods can correctly pick up this feature of the data via the likelihood.

We prove a general contraction rate theorem for $f$ under approximation-theoretic conditions on the prior following the classic testing approach of Bayesian nonparametrics [25], which requires:

(i) the integrated log-likelihood process is not too small with high probability;

(ii) the existence of suitable tests with exponentially decaying type-II errors.

Since the present high-frequency setting involves increasingly correlated observations, establishing (i) is much more involved than in the i.i.d. setting, where the log-likelihood tensorizes [24].
In particular, we must deal with the full dependent log-likelihood ratio process as a whole. Following the intuition from the continuous observation setting [65, 41, 29], we employ martingale techniques to study an approximation of the log-likelihood which allows to deal with the dependence structure of the Markov chain. Making this approximation both precise and uniform is a key challenge, and our proof relies on refined small time expansions of the transition density or heat kernel via Riemannian geometry [4, 8, 10].

Turning to (ii), we construct suitable tests by establishing concentration inequalities for frequentist estimators [26]. Given the above discussion regarding model (5), our estimators must draw information from the diffusivity term to be minimax optimal. For this task, we follow the ideas of Comte et al. [14] in the scalar case of using penalized least squares estimators. As a by-product, we obtain frequentist estimators that we prove to be optimal in a minimax sense. To the best of our knowledge, these are the first minimax results for estimating the diffusion coefficient in a multidimensional setting. We finally apply our general contraction rate theorem to concrete Gaussian priors, such as the Matérn process. Gaussian priors are widely used in practice [47] and have been applied in multiple ways to diffusion models, see for instance [46, 54, 7]. While we do not focus on computational issues here, note that posterior sampling based on discrete data is possible using Euler–Maruyama schemes [33] or other methods [9, 43, 11, 63, 55].

Regarding related works, theoretical properties of Bayesian nonparametric methods in the scalar ($d = 1$) diffusion model (5) have been well-studied, see for instance [65, 46, 64, 67, 42, 1]. In the multivariate setting, contraction rates were recently obtained under continuous observations [41, 29] and only consistency for discrete observations [31, 40]. While the continuous observation model provides some high-level intuition regarding the use of martingales techniques in our proofs, we note it is fundamentally unsuited as a model for statistical estimation of diffusion coefficients, see Section 3.3 in [29] for further discussion. For discrete observations, [40] extends the one-dimensional results of [30, 42] to establishes posterior consistency in the same multidimensional model (2) in the low-frequency setting using PDE and spectral techniques, showing that Bayesian methods can in principle adapt to the sampling regime, see [1] for further discussion. In the present high-frequency setup, a spectral approach will not give sharp rates and we instead use refined tools from stochastic analysis (in turn unsuited to the low-frequency setting) to obtain minimax optimal contraction rates.

Inference for the diffusivity $f$ has also been studied in other contexts, notably in the inverse problems literature where one often studies a time-independent version of the PDE (1) corresponding to a ‘steady state’ measurement of diffusion, see Section 1.1.2 of [39]. One can then consider an idealized statistical model where one observes the solution to this PDE under additive noise that does not typically depend on $f$ [59, 39]. As well as being a simplified observation model, this will typically yield ill-posed convergence rates in terms of the number of observations $N$. In contrast, we show here that in the high-frequency Markovian setting, one recovers the ‘usual’ (and faster) nonparametric convergence rate $N^{-s/(2s+d)}$ for an $s$-smooth $f$. As discussed above, this is possible because our methods exploit information about $f$ contained in the noise structure of (2) that is absent in these simplified models. While not surprising from a high-frequency diffusion perspective, this does highlight how studying simplified noise models in inverse problems can lead to qualitatively different statistical behaviour, and that embedding unknown parameters into the noise model need not make the problem more difficult, and can even do the opposite.
2. Main results

2.1. Preliminary setup for a reflected diffusion model in $\mathbb{R}^d$. We now rigorously set up the statistical framework for our results in model (2). To account for the boundary behaviour, we assume that $f$ is known to be 1 in an open neighbourhood of $\partial \mathcal{O}$. More precisely, for $\mathcal{K} \subset \mathcal{O}$ a known compact set with $\text{dist}(\mathcal{K}, \partial \mathcal{O}) > 0$, define the parameter space

\begin{equation}
\mathcal{F}_0 = \mathcal{F}_0(\mathcal{K}, d, f_{\text{min}}) = \left\{ f \in C^\alpha(\mathcal{O}) : \inf_{x \in \mathcal{O}} f(x) \geq 2 f_{\text{min}} \text{ and } f(x) = 1 \text{ for all } x \in \mathcal{O} \setminus \mathcal{K} \right\},
\end{equation}

where $0 < f_{\text{min}} < 1/2$ and the minimal smoothness equals

\begin{equation}
\alpha = \alpha_d = \max(4, 2 \lfloor d/4 + 1/2 \rfloor).
\end{equation}

The minimal value $\alpha_d$ scales like $d/2$ for large dimension $d$ and is needed to employ suitable bounds on the transition densities of the diffusion [16], see Section 4.1 for further discussion about the parameter space $\mathcal{F}_0$. In particular, since $\alpha \geq 4$, this implies existence and uniqueness of the solution to (2).

We consider the statistical experiment generated by the discrete observations

\[ X^N = (X_0, X_D, \ldots, X_{ND}) \]

from (2) with sampling rate $D_N = D > 0$. We work in the high-frequency and long-term sampling regime as stated in the following assumption.

**Assumption (Sampling regime).** Suppose that $D = D_N \to 0$ such that $ND \to \infty$, but $ND^2 \to 0$ as $N \to \infty$.

This is the minimal assumption for all our results and will be assumed throughout the paper without further mention.

Let $P_f$ (simply $P$ when no confusion may arise) denote the unique law of the Markov process $(X_t)_{t \geq 0}$ arising from (2). Consider the corresponding infinitesimal generator

\begin{equation}
L_f(\phi) = \nabla \cdot (f \nabla \phi) = \nabla f \cdot \nabla \phi + f \Delta \phi = \sum_{j=1}^d \frac{\partial}{\partial x_j} \left( f \frac{\partial}{\partial x_j} \phi \right),
\end{equation}

densely defined on continuous functions. For such a divergence form operator, the unique invariant probability measure can be explicitly computed as the uniform measure on $\mathcal{O}$ as in (4), see p. 46 of [5], so that the process $(X_t)_{t \geq 0}$ in (2) is stationary. Without loss of generality, we will assume that $\text{vol}(\mathcal{O}) = 1$. Let $(P_{f,t})_{t \geq 0}$ denote the family of transition operators associated to $(X_t)_{t \geq 0}$, each of which admits a transition density $p_{f,t}(x, y)$ on $\mathcal{O} \times \mathcal{O}$, so that for every real-valued and bounded function $\phi : \mathcal{O} \to \mathbb{R}$,

\[ P_{f,t} \phi(x) = \mathbb{E}_f[\phi(X_t) \mid X_0 = x] = \int_\mathcal{O} \phi(y) p_{f,t}(x, y) dy. \]

In particular $p_{f,t}$ arises as the fundamental solution to the heat equation (1) with Neumann boundary conditions. It can be shown that there exists $\lambda_f > 0$ such that $\|P_{f,t} \phi\|_2 \leq e^{-\lambda_f t} \|\phi\|_2$ for every $\phi : \mathcal{O} \to \mathbb{R}$ such that $\int_\mathcal{O} \phi d\mu_f = \int_\mathcal{O} \phi dx = 0$, where $\lambda_f$ satisfies $\lambda_f \geq \lambda_{\text{min}}/\rho_0 > 0$ with $\rho_0 > 0$ the Poincaré constant for the domain $\mathcal{O}$, see for example Section 3.1 of [40]. This implies that the transition operator $P_{f,D}$ of the discrete time Markov chain $X_0, X_D, X_{2D}, \ldots$ has first non-trivial eigenvalue

\begin{equation}
1 - e^{-D \lambda_f} \geq rD > 0,
\end{equation}

where $rD$ is known to be 1 in an open neighbourhood of $\partial \mathcal{O}$.
for some $r = r(f_{\text{min}}, p_0) > 0$, namely the Markov chain has a spectral gap decreasing linearly in the step size $D \to 0$.

From the above, we obtain the likelihood
\[
e^{\ell_N(f)} = e^{\ell(f; X_0, \ldots, X_{ND})} = \prod_{i=1}^{N} p_{f,D}(X_{(i-1)D}, X_{iD})
\]

based on observations $X^N = (X_0, X_D, \ldots, X_{ND})$. We consider a Bayesian approach by placing on $f$ a possibly $N$-dependent prior $\Pi = \Pi_N$, supported on some set $\mathcal{F} \subset \{ f \in \mathcal{C}^2(\mathcal{O}) : \inf_{x \in \mathcal{O}} f(x) \geq f_{\text{min}} \}$, leading to the posterior distribution
\[
\Pi(A|X_0, X_D, \ldots, X_{ND}) = \frac{\int_\mathcal{F} \prod_{i=1}^{N} p_{f,D}(X_{(i-1)D}, X_{iD})d\Pi(f)}{\int_\mathcal{F} \prod_{i=1}^{N} p_{f,D}(X_{(i-1)D}, X_{iD})d\Pi(f)}, \quad A \subseteq \mathcal{F} \text{ measurable.}
\]

In the following, we will study frequentist contraction rates for the posterior for $f$ about the ‘ground truth’ $f_0$ assumed to generate the data $X^N$ in (2).

**Additional notation and function spaces.** Let $\| \cdot \|$ denote the usual Euclidean norm on $\mathbb{R}^d$. For a multi-index $j = (j_1, \ldots, j_d) \in \mathbb{N}^d$, set $|j| = j_1 + \cdots + j_d$ and consider the resulting partial differential operator $\partial^j = \frac{\partial^{j_1}}{\partial x_1^{j_1}} \cdots \frac{\partial^{j_d}}{\partial x_d^{j_d}}$. For integer $k \geq 0$, let $\mathcal{C}^k(\mathcal{O})$ denote the space of $k$-times differentiable functions on $\mathcal{O}$ with uniformly continuous derivatives, while $\mathcal{C}(\mathcal{O}) = \mathcal{C}^0(\mathcal{O})$ denotes the space of continuous function equipped with the supremum norm $\| \cdot \|_{\infty}$. For non-integer $\beta > 0$, set
\[
\mathcal{C}^\beta(\mathcal{O}) = \left\{ f \in C^{|\beta|}(\mathcal{O}) : \sup_{x,y \in \mathcal{O} : x \neq y} \frac{|\partial^j f(x) - \partial^j f(y)|}{|x - y|^{|\beta| - |j|}} < \infty \quad \text{for all } |j| = |\beta| \right\},
\]

where $|\beta|$ denotes the largest integer less than or equal to $\beta$. For $\beta \geq 0$, $\mathcal{C}^\beta(\mathcal{O})$ is equipped with the usual norm
\[
\|f\|_{\mathcal{C}^\beta(\mathcal{O})} = \|f\|_{\mathcal{C}^{|\beta|}(\mathcal{O})} = \sum_{|j| = 0}^{\lfloor \beta \rfloor} \sup_{x \in \mathcal{O}} |\partial^j f(x)| + \sum_{|j| = |\beta|} \sup_{x,y \in \mathcal{O} : x \neq y} \frac{|\partial^j f(x) - \partial^j f(y)|}{|x - y|^{|\beta| - |j|}},
\]

where the second sum is removed for integer $\beta$. In particular, $\|f\|_{\mathcal{C}^0} = \|f\|_{\mathcal{C}\mathcal{C}}$, and the norms $\| \cdot \|_{\mathcal{C}^\beta}$ are non-decreasing in $\beta$.

Write $\langle \cdot, \cdot \rangle_2$ for the usual inner product for $L^2 = L^2(\mathcal{O})$. For integer $s \geq 0$, define the Sobolev space on $\mathcal{O}$ by
\[
H^s(\mathcal{O}) = \{ f \in L^2(\mathcal{O}) : \partial^j f \text{ exists weakly and } \partial^j f \in L^2(\mathcal{O}) \text{ for all } |j| \leq s \}
\]
equipped with the inner product
\[
\langle f, g \rangle_{H^s(\mathcal{O})} = \sum_{|j| \leq s} \langle \partial^j f, \partial^j g \rangle_2.
\]

For non-integer $s \geq 0$, one defines $H^s(\mathcal{O})$ by interpolation [36, 61]. When no confusion may arise, we will often drop the explicit reference to the domain $\mathcal{O}$ in the notation.

We will repeatedly use positive quantities that do depend on some parameters of the model, and that we informally call constants, and that may vary from line to line. These never depend on $N$, but do usually depend on the dimension $d$ of the ambient space. Other relevant dependences may be emphasised by a subscript, such as $C_{f}, C_{\|f\|_{L^p}}$ or $C_{f, \ell_0}$. The notation $A_N \lesssim B_N$ means $A_N \leq C B_N$ for every $N \geq 1$, where $C$ is a "constant" according to our informal terminology. For
2.2. Gaussian process priors. Gaussian priors are widely used in diffusion models and we investigate here their theoretical frequentist convergence rates. We assign to \( f \) a prior based on a Gaussian process, which must be modified to account for the constrained parameter space \( F_0 \) in (6), in particular that \( f \geq 2f_{\min} \) and \( f = 1 \) near the boundary. We therefore employ an exponential link function \( \Phi: \mathbb{R} \to (f_{\min}, \infty) \), similar to those used in density estimation [25] or inverse problems [59]:

\[
\Phi(x) = f_{\min} + (1 - f_{\min})e^x,
\]

which is strictly increasing on \( \mathbb{R} \) with \( \Phi(0) = 1 \).

We now detail our full prior construction, starting from an underlying Gaussian process \( V \). For definitions and background material on Gaussian processes and their associated RKHS, see Chapter 11 of [25] or [47].

**Condition 1.** Let \( \Pi_V = \Pi_{V,N} \) be a mean-zero Gaussian Borel probability measure on the Banach space \( \mathcal{C}(O) \) that is supported on a separable measurable linear subspace of \( \mathcal{C}^4(O) \), and assume that its reproducing kernel Hilbert space (RKHS) \( (H_V, \| \cdot \|_{H_V}) \) embeds continuously into the Sobolev space \( H^s(O) \) for some \( s \geq 4 \), i.e. \( H_V \hookrightarrow H^s(O) \).

Recall that any \( f_0 \in F_0 \) satisfies \( \{ x \in O : f_0(x) \neq 1 \} \subseteq \mathcal{K} \) by (6), where \( \mathcal{K} \subset O \) is a known compact set with \( \text{dist}(\mathcal{K}, \partial O) > 0 \). There thus exists \( \delta > 0 \) and an open set \( O_0 \) having smooth \( \mathcal{C}^\infty \)-boundary \( \partial O_0 \) such that \( \mathcal{K} \subseteq O_0 \subseteq O \) and

\[
\text{dist}(\mathcal{K}, \partial O_0) \geq \delta \quad \text{and} \quad \text{dist}(O_0, \partial O) \geq \delta,
\]

see, e.g., the proof of Proposition 8.2.1 in [18]. A simple example showing the relationship between such sets is plotted in Figure 1.

![Figure 1. A simple example of a suitable domain \( O \) (black), the region \( K \) (red) where the ground truth \( f_0 \in F_0 \) is not equal to 1, and a set \( O_0 \) (blue) that \( \delta \)-separates these sets as in (11). The \( \delta/2 \)-enlargement \( O_{\Delta} \) (dashed blue) of \( O_0 \) given in (20) is also plotted.](image)
Let $\chi \in C^\infty(\mathcal{O})$ be a smooth bounded cutoff function such that $\chi = 1$ on $\mathcal{X}$ and $\chi = 0$ outside $\mathcal{O}_0$. We take as prior distribution $\Pi = \Pi_N$ for $f$ the law of the random function
\begin{equation}
(12) \quad f(x) = \Phi(\chi(x)W(x)), \quad W(x) = \frac{V(x)}{N^{d/(4s + 2d)}}.
\end{equation}
It follows that $W$ is again a mean-zero Gaussian process with the same support and RKHS as $V$, but with rescaled covariance function. The cutoff function $\chi$ ensures that $f$ transitions smoothly to take value 1 near the domain boundary. Since the sample paths of $V$ are in $C^4(\mathcal{O})$ almost surely under the prior by Condition 1, then $\Pi(\mathcal{F}) = 1$ for
\begin{equation}
(13) \quad \mathcal{F} = \left\{ \ f \in C^4(\mathcal{O}) : \inf_{x \in \mathcal{D}} f(x) \geq f_{\min} \text{ and } f(x) = 1 \text{ for all } x \in \mathcal{O} \setminus \mathcal{O}_0 \right\}.
\end{equation}
Note that $\mathcal{F}_0 \subseteq \mathcal{F}$ since $\mathcal{X} \subseteq \mathcal{O}_0$, so that the prior lives on a slightly larger parameter space than $\mathcal{F}_0$, see Section 4.1 for further discussion. Moreover, since $\Phi^{-1}(y) = \log \frac{y - f_{\min}}{1 - f_{\min}}$ has uniformly bounded derivatives of all orders on $(2f_{\min}, \infty)$, we have that for any $f_0 \in \mathcal{F}_0 \cap C^4(\mathcal{O})$, the function $w_0 = \Phi^{-1}(f_0)$ is also in $C^4(\mathcal{O})$ with supp$(w_0) \subseteq \mathcal{X}$.

The following is the main result of our paper, establishing contraction rates for these rescaled Gaussian priors.

**Theorem 2.** Consider the sampling interval $D = N^{-a}$ for some $a \in (1/2, 1)$ and suppose $s > s^*_{d,a}$, where
\begin{equation}
(14) \quad s^*_{d,a} = \max \left( 4 + \frac{d}{2} \frac{2 - ad}{2a - 1}, \frac{d(1 + a)}{2(1 - a)} \right).
\end{equation}
Let $\Pi = \Pi_N$ denote the prior (12) with mean-zero Gaussian process $V \sim \Pi_V$ having RKHS $H_V$ and satisfying Condition 1 for this $s$. Let $f_0 \in \mathcal{F}_0 \cap C^4(\mathcal{O})$, set $w_0 = \Phi^{-1}(f_0)$ and suppose that there exists a sequence of functions $v_{0,N} \in H_V$ in the RKHS of $V$ such that
\begin{enumerate}
\item $\|v_{0,N}\|_{H_V} = O(1)$,
\item $\|\chi v_{0,N}\|_{C^\alpha} = O(1)$ for $\alpha = \max\{4, 2(\lfloor d/4 \rfloor + 1/2)\}$,
\item $\|w_0 - \chi v_{0,N}\|_{C^k} = O(N^{-\frac{s-k}{2+\alpha}})$ for $k = 0, 1, 2, 3$,
\end{enumerate}
as $N \to \infty$. Then for $M > 0$ large enough, as $N \to \infty$,
\[\mathbb{E}_{F_0} \Pi(f : \|f - f_0\|_2 \geq MN^{-\frac{s-k}{2+\alpha}} | X_0, X_D, \ldots, X_{ND}) \to 0.\]

Since $N^{-\frac{s-k}{2+\alpha}}$ is the minimax estimation rate in the high-frequency sampling regime (see Theorem 6 below for the corresponding lower bound), this result says that the posterior contracts about the truth at the minimax-optimal rate in any dimension $d$. Given the invariant measure is uninformative here, being the uniform distribution on $\mathcal{O}$ for all $f \in \mathcal{F}_0$, this confirms that the Bayes method can indeed perform optimal inference by picking up sufficient information from the transitions $X_{(1-d)} \mapsto X_{(d)}$ via the likelihood.

The minimal smoothness condition $s^*_{d,a}$ in (14) can be rewritten as
\[s_{d,a}^* = \begin{cases} 
\max \left( 4 + \frac{d}{2} \frac{2 - ad}{2a - 1}, \frac{d(1 + a)}{2(1 - a)} \right) & \text{if } d = 1, 2 \text{ and } a \in (1/2, 1), \text{ or } d = 3 \text{ and } a \in (1/2, 2/3), \\
\max \left( 4 + \frac{d}{2} \frac{2 - ad}{2a - 1}, \frac{d(1 + a)}{2(1 - a)} \right) & \text{if } d = 3 \text{ and } a \in [2/3, 1), \\
\frac{d(1 + a)}{2(1 - a)} & \text{if } d \geq 4 \text{ and } a \in (1/2, 1). 
\end{cases}\]
This becomes more stringent as $a \to 1$, namely the frequency $D = N^{-a} \to N^{-1}$ increases, since the time horizon $ND = N^{1-a}$ then grows more slowly. The term $\frac{d(1 + a)}{2(1 - a)}$ should be thought of as the main condition, with the extra terms for $d = 1, 2, 3$ coming from minimal smoothness assumptions needed to use various expansions and bounds.
Theorem 2 requires that the true \( w_0 = \Phi^{-1}(f_0) \) can be very well approximated by elements \( v_{0,N} \) of the RKHS \( \mathbb{H}_V \) of \( V \). Under Condition 1, an \( s \)-smooth truth almost lies in \( \mathbb{H}_V \) as needed, but this in turn implies that the Gaussian process \( V \) will typically have \((s - d/2)\)-smooth sample paths (e.g. Proposition 1.4 of [25] for the Matérn process), thereby undersmoothing the truth. When the prior mismatches the true smoothness, suitably rescaling the prior as in (12) has been shown to still yield optimal rates in several benchmark statistical models [66, 34]. This rescaling has also recently been used in the Bayesian inverse problems literature, where it is typically used to control stability estimates [28, 39].

We now consider two examples of Gaussian process priors satisfying the assumptions of Theorem 2. Let \( V = \{V(x) : x \in \mathcal{O}\} \) denote a Matérn process on \( \mathcal{O} \) with regularity parameter \( s - d/2 > 0 \), that is \( V \) is a mean-zero stationary Gaussian process with covariance function

\[
K(x, y) = K(x - y) = \int_{\mathbb{R}^d} e^{-i(x-y)\cdot \xi} (1 + |\xi|^2)^{-s} d\xi, \quad x, y \in \mathcal{O}.
\]

The covariance function can alternatively be represented in terms of special functions, see e.g. p.84 of [47]. While the Matérn process models (almost) \((s - d/2)\)-smooth functions in a Hölder sense, its rescaled version \( W = V/N^{d/(4s+2d)} \) in (12) concentrates on \( s \)-smooth functions.

**Corollary 3.** Let \( D = N^{-a} \) for some \( a \in (1/2, 1) \), and let \( \Pi = \Pi_N \) denote the prior (12) with \( V \) a Matérn process of regularity \( s - d/2 \) with \( s > s_{d,a}^* \) for \( s_{d,a}^* \) as in (14). If \( f_0 \in \mathcal{F}_0 \cap \mathcal{C}^{s}(\mathcal{O}) \), then for \( M > 0 \) large enough,

\[
E_{f_0, \Pi}(f : \|f - f_0\|_2 \geq MN^{-\frac{a}{2s}}|X_0, X_D, \ldots, X_{ND}) \to 0 \quad \text{as } N \to \infty.
\]

As a second example, we consider a truncated Gaussian wavelet series prior. Let \( \{\psi_l : l \geq J_0, r \in \mathbb{Z}^d\} \) denote an orthonormal basis of \( L^2(\mathbb{R}^d) \) composed of sufficiently regular, compactly supported Daubechies wavelets, where \( J_0 \in \mathbb{N} \) is the base resolution level of the scaling functions, which we also denote by \( \{\psi_{l,r}\} \) to simplify notation (see Chapter 4 of [27] for details). Let \( R_l \) denote the set of indices \( r \) for which the support of \( \psi_{l,r} \) intersects \( \mathcal{O}_0 \). For \( J_0 \) large enough (see Section 3), consider the Gaussian series expansion

\[
V(x) = \sum_{l=0}^J \sum_{r \in R_l} 2^{-ls} g_{l,r} \psi_{l,r}(x), \quad g_{l,r} \sim \text{iid } N(0, 1),
\]

where \( 2^J \simeq N^{\frac{1}{2s}} \). Note we could extend the second index set from \( r \in R_l \) to \( r \in \mathbb{Z}^d \) to cover all of \( \mathbb{R}^d \) since wavelet functions \( \psi_{l,r} \) supported outside \( \mathcal{O}_0 \) ultimately play no role in the prior (12) due to the cutoff function \( \chi \).

**Corollary 4.** Let \( D = N^{-a} \) for some \( a \in (1/2, 1) \), and let \( \Pi = \Pi_N \) denote the prior (12) with \( V \) a Gaussian wavelet series as in (15) with \( s > s_{d,a}^* \) for \( s_{d,a}^* \) as in (14). If \( f_0 \in \mathcal{F}_0 \cap \mathcal{C}^{s}(\mathcal{O}) \), then for \( M > 0 \) large enough,

\[
E_{f_0, \Pi}(f : \|f - f_0\|_2 \geq MN^{-\frac{a}{2s}}|X_0, X_D, \ldots, X_{ND}) \to 0 \quad \text{as } N \to \infty.
\]

Using a uniform integrability argument (e.g. Theorem 2.3.2 of [39]), this implies the same convergence rate for the posterior mean.

**Corollary 5.** Let \( \bar{f}_N = E_{\Pi}[f|X_0, X_D, \ldots, X_{ND}] \) denote the posterior mean based on the Matérn process or Gaussian wavelet series prior. Under the conditions of Corollary 3 (Matérn) or Corollary 4 (Gaussian wavelet series), there exists a constant \( M > 0 \) such that as \( N \to \infty \),

\[
\mathbb{P}_{f_0}(\|\bar{f}_N - f_0\|_2 \geq MN^{-\frac{a}{2s}}) \to 0.
\]
We thus have two concrete examples of Gaussian priors for which the posterior (means) converge to the true $f_0 \in \mathcal{F}_0 \cap \mathfrak{F}$ at rate $N^{-\frac{\alpha}{2d}}$. The following lower bound shows that this is indeed the minimax rate of convergence.

**Theorem 6 (Minimax lower bound).** Let $D = N^{-\alpha}$ for some $\alpha \in (1/2, 1)$. For any $s > \alpha_d$ (the minimal smoothness (7)) and $M > 0$, the following frequentist lower bound holds:

$$\lim inf\inf_{N \to \infty} \sup_{f \in \mathcal{F}_0} N \frac{s}{2} \mathbb{E}_f \left[ \|\tilde{f}_N - f\|_2^2 \right] > 0,$$

where the infimum is taken among all estimators based on data (3).

In particular, we extend the univariate minimax lower bound of [32]. The proof is given in Appendix 10.1.

### 3. A GENERAL CONTRACTION THEOREM

We now state and discuss the abstract contraction rate theorem used to derive the convergence results for Gaussian process priors in Section 2.2 above. This is based on the general testing approach of Bayesian nonparametrics [25], which requires (i) that the prior puts sufficient mass on a neighbourhood of the truth and (ii) the existence of suitable tests with exponentially decaying type-II errors.

For $0 < \varepsilon_N \leq \varepsilon_{1,N} \leq \varepsilon_{2,N} \leq \varepsilon_{3,N} \to 0$ positive sequences with $N\varepsilon_N^2 \to \infty$, $r > 0$ and $\alpha = \alpha_d$ as in (7), define the following neighbourhood of $f_0$:

$$\mathcal{E}_N = \mathcal{E}_N(f_0, \varepsilon_N, \varepsilon_{1,N}, \varepsilon_{2,N}, \varepsilon_{3,N}, r)$$

$$= \left\{ f \in \mathcal{F} : \|f\|_{\mathcal{E}^r} \leq r, \|f - f_0\|_{\infty} \leq \varepsilon_N, \|f - f_0\|_{\mathcal{E}^k} \leq \varepsilon_{k,N} \text{ for } k = 1, 2, 3 \right\},$$

which can be related to the information theoretic distance of the model induced by the log-likelihood ratio process. Further define

$$E_N := \varepsilon_N^2 \left( 1 + \frac{\varepsilon_{2,N}}{\varepsilon_N} D + \frac{\varepsilon_{3,N}}{\varepsilon_N^2} D^{3/2} \right)$$

$$V_N := N\varepsilon_N^2 + N\varepsilon_{2,N}^2 D^{-1} + N^2 \varepsilon_{2,N}^2 D + N^2 \varepsilon_{3,N}^2 D^3 + N^2 D^4.$$  

The quantities $NE_N$ and $V_N$ control the expectation and variance, respectively, of the integrated log-likelihood ratio process restricted to the small-ball $\mathcal{E}_N$, which is used to lower bound the normalized denominator of the Bayes formula. This is the content of the next result, which is the most technically involved part of our proof.

**Theorem 7 (Evidence lower bound).** Let $f_0 \in \mathcal{F}_0$ and $\nu$ be a probability measure supported on $\mathcal{E}_N$ as in (16) with $r > 0$ and sequences $0 < \varepsilon_N \leq \varepsilon_{1,N} \leq \varepsilon_{2,N} \leq \varepsilon_{3,N} \to 0$ satisfying $N\varepsilon_N^2 \to \infty$ as $N \to \infty$. Then the integrated log-likelihood ratio process

$$\Lambda_D^N = \int_{\mathcal{E}_N} \log \prod_{i=1}^{N} \frac{p_{f_0,D}(X_{i-1,D}, X_{i,D})}{p_{f,D}(X_{i-1,D}, X_{i,D})} \nu(df)$$

satisfies

$$\sup_{f \in \mathcal{E}_N} \mathbb{E}_{f_0} \left[ \log \frac{p_{f_0,D}(X_0, X_D)}{p_{f,D}(X_0, X_D)} \right] \preceq E_N,$$

$$\text{Var}_{f_0}(\Lambda_D^N) \preceq V_N.$$
where $E_N, V_N$ are defined in (17) and the constants depend only on $f_0, r, d, \delta, f_{\min}$. This implies that for every $c > 0$,
\begin{equation}
P_{f_0} \left( \prod_{i=1}^{N} \int_{\mathbb{R}^d} \frac{p_{f,D}(X_{(i-1)D}, X_{iD})}{p_{f_0,D}(X_{(i-1)D}, X_{iD})} \nu(df) \leq e^{-cN\epsilon_N^2 - C_0 N E_N} \right) \leq \frac{V_N}{c^2 N^2 \epsilon_N^4},
\end{equation}
where $C_0 > 0$ is a fixed constant depending only on $f_0, r, d, \delta, f_{\min}$.

Theorem 7 shows that the Bayesian evidence is at least $e^{-CN\epsilon_N^2}$ with $P_{f_0}$-probability tending to one if
\begin{equation}
E_N \lesssim \epsilon_N^2 \quad \text{and} \quad V_N/(N^2 \epsilon_N^4) \to 0.
\end{equation}
An overview of the proof of Theorem 7 is found in Section 5.

Remark 8. For $a \in (1/2, 1)$, consider the ‘usual’ nonparametric choices of sequences for a $C^a$-smooth truth:
$$D = N^{-a}, \quad \epsilon_N = N^{-\frac{a}{2+a}}, \quad \epsilon_{k,N} = N^{-\frac{a}{2+a}}, \quad k = 1, 2, 3.$$ 
Then (19) is implied by
$$s > \begin{cases} \frac{2-ad}{2a-1} & \text{if } d = 1, 2, a \in (1/2, 1), \text{ or } d = 3, a \in (1/2, 2/3), \\ 0 & \text{if } d = 3, a \in (2/3, 1), \text{ or } d \geq 4, a \in (1/2, 1). \end{cases}$$ 

For comparison, consider the i.i.d model $Y_1, \ldots, Y_N \sim \text{iid } P$ with $P$ having density $p$, so that $(Y_1, \ldots, Y_N) \sim \text{\iids } P^N = \otimes_{i=1}^{N} P$. The corresponding neighbourhood can then be expressed in terms of the Kullback-Leibler divergence and its $2nd$-variation [24],
\begin{equation}
B_2(p_0, E_N, V_N) = \left\{ p : p_0^N \log(p_0^N / p^N) \leq NE_N, \text{Var}_{p_0}(\log(p_0^N / p^N) \leq V_N) \right\} 
= \left\{ p : p_0 \log(p_0/p) \leq E_N, \text{Var}_{p_0}(\log(p_0/p)) \leq V_N/N \right\},
\end{equation}
where the last equality follows from the densities tensorizing in the i.i.d. model. In this model, one can take $E_N \simeq \epsilon_N^2$ and $V_N \simeq N^2 \epsilon_N^2$ ([25], Lemma 8.10 with $k = 2$), which gives some intuition behind the roles of $E_N$ and $V_N$. In contrast, the present diffusion setting induces a Markovian dependence structure in the data and hence the likelihood. In the low frequency regime where $D > 0$ is fixed, the spectral gap of the Markov chain is bounded away from zero by (9) and hence one can use spectral techniques [44, 42, 40] to show that the model dependence is not too dissimilar from i.i.d. However, in the present high frequency setting, the spectral gap shrinks rapidly as $D \to 0$ inducing a much stronger dependence, thereby making such techniques unsuitable. We must therefore deal with the full dependent log-likelihood ratio process $\Lambda_D^N$ as a whole, rendering this computation much more involved.

Our strategy is to use second-order small time expansions of the transition densities [4, 8, 10], which heuristically corresponds to replacing $p_{f,D}$ in $\Lambda_D^N$ with the corresponding Euler scheme without drift, that is a $N_d(x, 2Df(x)I_d)$ density. This reflects the property of model (2) that the drift is of smaller order than the diffusivity, and hence does not affect the leading order terms in $\Lambda_D^N$ as $D \to 0$. Such expansions can also be viewed as a quantitative form of local asymptotic normality (LAN) with uniform remainders over $C_N$. We then further approximate the resulting process by a martingale difference, which allows us to deal with the dependence of the process. Note that we require control of the derivatives of $f - f_0$ up to third order in $C_N$ in (16) to ensure the higher order terms of these expansions are negligible, uniformly over $C_N$.

Turning to the existence of tests with exponentially decreasing type-II errors, we employ plug-in tests based on estimators satisfying suitable concentration inequalities as was done for i.i.d.
models in [26], see also [48, 42, 1, 38]. As estimators, we follow the ideas of Comte et al. [14] who use penalized least squares estimators in the scalar case. We therefore extend the results of [14] to the multidimensional setting with domain boundary, exploiting the structure of the $L^2$-loss function to obtain the required concentration inequalities.

Our proofs require certain wavelet-based approximations, which must be adapted to deal with the boundary as we now make precise. Let

\begin{equation}
\mathcal{O}_0^J = \{ x \in \mathcal{O}, \text{dist}(x, \mathcal{O}_0) \leq \delta/2 \}
\end{equation}

denote the $\delta/2$-enlargement of $\mathcal{O}_0$, and note that $\mathcal{O}_0^J \subsetneq \mathcal{O}$ since $\text{dist}(\mathcal{O}_0, \partial \mathcal{O}) \geq \delta$ by assumption (11), see Figure 1 for an example. As in Section 2.2, let $\{ \psi_{l,r} : l \geq J_0, r \in \mathbb{Z}^d \}$ denote an orthonormal basis of $L^2(\mathbb{R}^d)$ composed of sufficiently regular, compactly supported Daubechies wavelets, where $J_0 \in \mathbb{N}$ is the base resolution level of the scaling functions, which we also denote by $\{ \psi_{J_0,r} \}$ to simplify notation. Let $R_l$ denote the set of indices $r$ for which the support of $\psi_{lr}$ intersects $\mathcal{O}_0$, in which case $|R_l| = O(2^{Jl})$ since $\mathcal{O}_0$ is a bounded domain in $\mathbb{R}^d$. Since dist($\mathcal{O}_0, \partial \mathcal{O}$) $\geq \delta/2 > 0$ and $\text{diam}(\text{supp}(\psi_{lr})) = O(2^{-l})$, we may take $J_0$ large enough such that no wavelet function $\psi_{lr}, l \geq J_0$, has support intersecting both $\mathcal{O}_0$ and $(\mathcal{O}_0^J)^c$. Any function $g \in L^2(\mathcal{O})$ with supp($g$) $\subseteq \mathcal{O}_0$ can then be uniquely represented as

\begin{equation}
g(x) = \sum_{l=J_0}^{\infty} \sum_{r \in R_l} \langle g, \psi_{lr} \rangle_2 \psi_{lr}.
\end{equation}

Even though the wavelets $\{ \psi_{lr} : l \geq J_0, r \in R_l \}$ do not form an orthonormal basis of $L^2(\mathcal{O})$ due to their behaviour on $\mathcal{O} \setminus \mathcal{O}_0$, any $g$ as above can be extended to a function on $\mathbb{R}^d$ (or any set containing $\mathcal{O}_0$) by setting it to zero outside $\mathcal{O}_0$. In particular, the Sobolev and Hölder norms on $\mathcal{O}$ and $\mathbb{R}^d$ coincide for such functions and we may therefore use all the usual wavelet characterizations and embeddings for Sobolev and Hölder norms. This fact will be used without mention in the proofs.

For $J \geq J_0$, set

\begin{equation}
V_J = V_J(\mathcal{O}_0) = \left\{ f = \sum_{l=J_0}^{J} \sum_{r \in R_l} f_{lr} \psi_{lr} \right\} \subset \mathcal{C}(\mathcal{O})
\end{equation}

to be the linear space of all functions in the wavelet projection space of resolution level $J$, restricted to those wavelets with support intersecting $\mathcal{O}_0$ but not $(\mathcal{O}_0^J)^c$. Note that

\begin{equation}
g(x) = g(x)1_{x \in \mathcal{O}_0^J} \quad \text{for every } g \in V_J
\end{equation}

since supp($g$) $\subseteq \mathcal{O}_0^J$ for $g \in V_J$. We must slightly modify the usual notion of a wavelet projection to account for the behaviour near the boundary in $\mathcal{F}$ in (13). To that end, note that supp($f - 1$) $\subseteq \mathcal{O}_0$ for any $f \in \mathcal{F}$ and thus $f - 1$ has a wavelet expansion as in (21). Setting $P_J : L^2(\mathcal{O}) \to V_J$ to be the $L^2$-projection operator onto $V_J$, we define the projection operator $\overline{P}_J : \mathcal{F} \to \mathcal{F}$ by

\begin{equation}
\overline{P}_J[f](x) := 1 + P_J[f - 1](x) = 1 + \sum_{l=J_0}^{J} \sum_{r \in R_l} \langle f - 1, \psi_{lr} \rangle_2 \psi_{lr}(x), \quad x \in \mathcal{O}.
\end{equation}

Since supp($f - 1$) $\subseteq \mathcal{O}_0$, $P_J[f - 1](x) = \sum_{l=J_0}^{J} \sum_{r \in R_l} \langle f - 1, \psi_{lr} \rangle_2 \psi_{lr}(x)$ coincides with the usual wavelet projection of $f - 1$ on all of $\mathbb{R}^d$. Intuitively, $\overline{P}_J[f]$ should be thought of as the usual wavelet projection of resolution level $J$ adapted to account for the boundary conditions of $\mathcal{F}$. 


We are now ready to define our projection estimator following Comte et al. [14]. Let
\[
\hat{g}_N \in \arg \min_{g \in V_J} \sum_{i=1}^N \left( (Y_{i,D} - 1)1_{A_{i,D}} - g(X_{(i-1)D}) \right)^2,
\]
with \(A_{i,D} = \{X_{(i-1)D} \in \mathcal{O}_0^J\}\) and
\[
Y_{i,D} = \frac{1}{2dD} |X_{iD} - X_{(i-1)D}|^2.
\]
Note that by (23), the sum in (25) actually spans over \(i\) such that \(X_{(i-1)D}\) lies in \(\mathcal{O}_0^J\). We then consider the estimator
\[
\hat{f}_N(x) = 1 + \hat{g}_N(x), \quad x \in \mathcal{O},
\]
The idea behind (25) is that for small \(D > 0\), by Itô’s formula, we have the signal plus noise representation
\[
Y_{i,D} - 1 = f(X_{(i-1)D}) - 1 + \varepsilon_{i,D} + r_{i,D},
\]
where \(\varepsilon_{i,D}\) is a martingale error term with variance of order 1 and \(r_{i,D}\) is a small remainder term combining stochastic expansions and boundary effects, see (66) in the proofs for a precise definition. Thus \(\hat{g}_N\) is an estimate of \(f - 1\), which has support contained in \(\mathcal{O}_0\) for all \(f \in \mathcal{F}\). Indeed, one needs only estimate \(f\) on \(\mathcal{O}_0\), since \(f \equiv 1\) is already known on \(\mathcal{O} \setminus \mathcal{O}_0\) for all \(f \in \mathcal{F}\). This permits to separate estimation on the interior of \(\mathcal{O}\), where the function \(f\) is unknown, with the behaviour near the boundary \(\partial \mathcal{O}\), where the reflecting boundary conditions alter the diffusion dynamics. We next establish a concentration inequality for the estimator \(\hat{f}_N\).

**Theorem 9** (Exponential inequality). Let \(\hat{f}_N = \hat{f}_N(X_0, X_1, \ldots, X_{ND})\) be the estimator (26). Let \(\varepsilon_N, \xi_N \to 0, 2^J = 2^{JN} \to \infty\) and \(R_J\) be sequences such that \(N\varepsilon_N^2 \to \infty\) as \(N \to \infty\). Define the sets
\[
\mathcal{U}_N = \{ f \in \mathcal{F} : \|f\|_{C^1} \leq r, \|f - \mathcal{P}_{\mathcal{F}} f\|_2 \leq C\varepsilon_N, \|f - \mathcal{P}_{\mathcal{F}} f\|_\infty \leq R_J \},
\]
where \(C, r > 0\) and \(\mathcal{P}_{\mathcal{F}} f\) denotes the projection (24). Assume further that \(2^{Jd} = o(\sqrt{ND})\),
\[
R_J^2 \varepsilon_N^2 \lesssim D\xi_N, \quad 2^{3d/2} N^{-1} + 2^{d/2} N^{-1/2} + 2^{d/2} \varepsilon_N^2 + \varepsilon_N \lesssim \xi_N,
\]
as \(N \to \infty\). Then there exist events \(\mathcal{B}_N\) satisfying
\[
\sup_{f \in \mathcal{F}} \mathbb{P}_f(\mathcal{B}_N^c) \to 0
\]
as \(N \to \infty\), such that for every \(L > 0\),
\[
\sup_{f \in \mathcal{F}_N} \mathbb{P}_f(\|\hat{f}_N - \mathcal{P}_{\mathcal{F}} f\|_2 \geq K\xi_N, \mathcal{B}_N) \leq C'e^{-LN\varepsilon_N^2},
\]
where \(K\) depends on \(L\).

The proof can be found in Section 8. Theorem 9 says that if the underlying function \(f\) can be well-enough approximated by its projection \(\mathcal{P}_{\mathcal{F}} f\) as quantified by the conditions in \(\mathcal{U}_N\), then the estimator \(\hat{f}_N\) will concentrate around this projection with all but exponentially small \(\mathbb{P}_f\)-probability.

As far as we are aware, this extension of [14] in Theorem 9 is the first frequentist estimator of the diffusion function \(f\) in the multivariate setting and thus may be of independent interest. Combined with the lower bound of Theorem 6, we obtain
**Theorem 10.** Let \( D = N^{-a} \) for some \( a \in (1/2, 1) \), \( s > \alpha_d \), and let \( M > 0 \). Define \( \hat{f}_N = \min(\hat{f}_N, M)_+ \), where \( \hat{f}_N \) is as in (26) constructed with Daubechies wavelets with at least \( |s| - 1 \) vanishing moments, and \( 2^J \approx N^{1/(2s+d)} \). Then

\[
\sup_{f \in \mathcal{F}_0, \|f\|_{c^s} \leq M} \mathbb{E}_f \left[ \|\hat{f}_N - f\|_2^2 \right] \lesssim N^{-2s/(2s+d)}.
\]

Combined with Theorem 6, we obtain that the (normalised) rate \( N^{-s/(2s+d)} \) is asymptotically minimax for estimating \( f \) over \( \{f \in \mathcal{F}_0 : \|f\|_{c^s} \leq M\} \).

**Remark 11** (Minimax rates in related diffusion models). The minimax rates for estimating a drift with smoothness \( s_b \) and a diffusion coefficient with smoothness \( s \) when both terms are decoupled are \((ND)^{-s_b/(2s_b+1)} \) and \( N^{-s/(2s+d)} \) in dimension \( d = 1 \), see [32]. Theorem 6 extends the lower bound for the diffusion coefficient to an arbitrary dimension and, together with Theorem 10, shows that the rate \( N^{-s/(2s+d)} \) is indeed minimax optimal. While we prove our results in a coupled model for which the drift has the form \( \nabla f(x) \), a glance at the proofs of the upper bound and the lower bound, where we use the control of the KL divergence from Theorem 7 in an extended model, shows that the result is actually valid in a more general setting with decoupled drift and diffusion coefficient.

The proof of Theorem 10 is given in Appendix 10.2. We emphasize that while this estimator plays a key role in our proof of minimax optimal posterior contraction rates using the Gaussian prior (12), it is not actually involved in the prior construction or Bayesian method itself. Using Theorems 7 and 9, we obtain the following general posterior contraction theorem for our setting, whose proof is found in Section 9.1.

**Theorem 12** (General contruction theorem). Let \( \Pi = \Pi_N \) be a sequence of prior distributions supported on \( \mathcal{F} \) in (13), let \( r, K_0 > 0 \) be fixed constants and \( 0 < \varepsilon_N \leq \varepsilon_{1,N} \leq \varepsilon_{2,N} \leq \varepsilon_{3,N} \to 0 \), \( \xi_N \to 0 \), \( 2^J = 2^{J_0} \to \infty \) and \( R_J \) be sequences satisfying \( N\varepsilon_N^2 \to \infty \), \( 2^{J_0} = o(\sqrt{ND}) \) and

\[
R_J^2 \varepsilon_N^2 \lesssim D \xi_N^2, \quad 2^{3J_0/2}N^{-1} + 2^{J_0/2}2^{-1/2} + 2^{J_0/2}2^2 + \varepsilon_N \lesssim \xi_N,
\]

as \( N \to \infty \). Further suppose that \( E_N \) and \( V_N \) in (17) satisfy

\[
E_N \leq K_0 \varepsilon_N^2, \quad \text{and} \quad V_N/(N^2 \varepsilon_N^2) \to 0.
\]

Let

\[
\mathcal{F}_N = \left\{ f \in \mathcal{F} : \|f\|_{c^s} \leq r, \|f - f_0\|_{\infty} \leq \varepsilon_N, \|f - f_0\|_{c^s} \leq \varepsilon_{k,N} \text{ for } k = 1, 2, 3 \right\}
\]

be the set defined in (16),

\[
\mathcal{F}_N \subseteq \left\{ f \in \mathcal{F} : \|f\|_{c^s} \leq r, \|f - P_J f\|_2 \lesssim \xi_N, \|f - P_J f\|_{\infty} \lesssim R_J \right\},
\]

where \( P_J \) denotes the projection (24), and \( C_0 > 0 \) be the fixed constant in Theorem 7, which depends only on \( f_0, r, d, 0, \delta, f_{\min} \). Assume the true \( f_0 \in \mathcal{F}_0 \) satisfies \( \|f_0 - P_J f_0\|_2 \lesssim \xi_N \) and \( \|f_0 - P_J f_0\|_{\infty} \lesssim R_J \). Suppose that for some \( C, L > 0 \),

(i) \( \Pi(\mathcal{F}_N) \leq L e^{-(C + C_0 K_0 + 2)N\varepsilon_N^2} \),

(ii) \( \Pi(\mathcal{E}_N) \geq e^{-CN\varepsilon_N^2} \).

Then for \( M > 0 \) large enough, as \( N \to \infty \),

\[
\mathbb{E}_{f_0} \Pi(f : \|f - f_0\|_2 \geq M\xi_N | X_0, X_D, \ldots, X_{ND}) \to 0.
\]

To summarize, in order to apply Theorem 12 in examples, we must verify that the prior places most of its mass on functions \( f \in \mathcal{F}_N \) that are well-approximable by their projections \( P_J f \), and also that the prior places at least an exponentially small amount of mass in a neighbourhood of the truth in the sense of \( \mathcal{E}_N \), i.e. conditions (i) and (ii) of Theorem 12, respectively.
4. Discussion and generalizations

4.1. The parameter space $\mathcal{T}_0$. The parameter space $\mathcal{T}_0$ in (6) captures relevant features of the underlying physical model, while allowing us to focus on the inferential task of estimating the diffusivity $f_0$ in the interior of the domain $\mathcal{O}$ without being overly encumbered by boundary technicalities. We consider reflecting boundary conditions, rather than say a simpler periodic model [41, 29], to better represent the microscopic process corresponding to diffusion as in (1). However, estimation near boundaries often behaves in qualitatively different ways [49, 51], for instance exhibiting different convergence rates. Since this is not the focus of the present work, we assume $f_0 \in \mathcal{T}_0$ is known near the boundary $\partial \mathcal{O}$ to avoid such statistical issues (note we must still deal with probabilistic aspects of the boundary in our proofs). We set $f = 1$ on $\mathcal{O}\setminus \mathcal{K}$ for simplicity and clarity of presentation, but our theory could accommodate more general constraints of the form $f = g$ on $\mathcal{O}\setminus \mathcal{K}$ for some known smooth $g \geq 2f_{\min}$ by considering a modified prior $f(x) = \Phi(\chi(x))W(x) + \Phi^{-1}(g(x)))$. Our proofs can straightforwardly be adapted by considering wavelet projections of the form $\mathcal{P}_j[f](x) := g + P_j[f-g](x)$ instead of (24), since this still separates out the boundary because $\text{supp}(f-g) \subseteq \mathcal{O}_0^d$ for any $f$ in the prior support.

The lower bound $f_0 \geq 2f_{\min}$ is arbitrary, but provides uniformity for our results in terms of the constants in the convergence rates. While our prior link function depends on this unknown quantity, this is purely for our proof arguments and in any case one can take $f_{\min}$ as close to zero as desired. In practice, we would expect the standard exponential link function $\Phi(x) = e^x$ (i.e. with $f_{\min} = 0$) often used in inverse problems [59, 39] to work equally well. The class $\mathcal{T}_0$ also assumes minimal smoothness $f_0 \in C^{\alpha_d}$, where $\alpha_d$ in (7) grows roughly like $\max(4, d/2)$. The $d/2$-dependence is needed to establish suitable bounds on the transition densities as in (35), which follow from results in [19, 16]. The minimal smoothness $\alpha_d \geq 4$ dominates for small dimensions and is an artifact of our proof, which requires expansions of the transition densities to third order with suitable control of the remainder terms.

4.2. Extensions to other models. While the model (2) we consider here is motivated by physical considerations, our results conceptually extend to SDEs with more general drifts of the form

$$dX_t = b(\nabla f(X_t), X_t)dt + \sqrt{2f(X_t)}dW_t + d\ell_t,$$

where $b$ is suitably regular, see (28) in the proofs below for the exact formulation. Indeed, many of our probabilistic results are actually proved for this more general framework, which includes the present model with $b(x, y) = x$, while also allowing an independent drift $G(X_t)$ by taking $b(x, y) = G(y)$. Our results and techniques should thus be extendable to estimation of the diffusion coefficient $f$ in these more general models where either the drift is viewed as a nuisance parameter or is less informative than the diffusion term regarding $f$.

To deal with the boundary, we first show that in small time $D \to 0$, a particle started away from the boundary will hit it with very small probability (Step 1 in Section 5.1). Our proof then approximates the present model by one without boundary on the whole of $\mathbb{R}^d$, see (31) below, so that our probabilistic expansions actually treat this unbounded diffusion case. Our techniques should thus extend to diffusion models where one can show that with high probability, the particle is constrained to a compact set, for instance unbounded domains in $\mathbb{R}^d$ with sufficiently strong confining drifts. In this way, our proof essentially separates out the boundary problem (corresponding to either reflecting boundary conditions or confining drifts) from statistical inference in the interior of the effective domain.

One can also consider the problem of simultaneous estimation of the drift and diffusion coefficient when these are in principle uncoupled as in (5). However, in the one-dimensional case $d = 1,$
it is known that these estimation problems interact with each other and it can still be helpful to
couple the priors, for instance by first modelling the diffusion coefficient \( f \) and then modelling
the drift \textit{conditional} on \( f \), see Remark 7 in [42]. This is an interesting direction, but is beyond the
scope of the present work.

5. \textbf{Proof of Theorem 7: Expectation and Variance of the Integrated Log-Likelihood Restricted to \( \mathcal{C}_N \)}

The proof of the variance and expectation of the log-likelihood is split into several approxi-
mation steps employing different techniques. Following the suggestion of a referee, we write the
proof of Theorem 8 and its technical auxiliary results in a slightly more general setting: we replace
\( (2) \) by the extended model

\[
X_t = X_0 + \int_0^t b(\nabla f(X_s), X_s) ds + \int_0^t \sqrt{2f(X_s)} dB_s + \ell_t,
\]

\[
\ell_t = \int_0^t n(X_s) d|\ell|_s, \quad |\ell|_t = \int_0^t 1_{\{X_s \in \partial D\}} d|\ell|_s,
\]

The drift function: \( b = (b^1, \ldots, b^d) : \mathbb{R}^{2d} \to \mathbb{R}^d \) belongs to the class

\[
\mathcal{B} = \left\{ b : \mathbb{R}^{2d} \to \mathbb{R}^d, \sum_{i=1}^d \|b^i\|_{C^1} \leq b \right\}
\]

for some \( b > 0 \). In particular, we recover model \( (2) \) for the choice \( b(x, y) = x \) and putting \( b(x, y) = \nabla G(y) \) for some arbitrary sufficiently smooth \( G : \mathbb{R}^d \to \mathbb{R}^d \) enables us to have a generic drift vector
field that can be considered as a nuisance.

We provide here an overview of the proof, deferring the detailed technical arguments to later
in the paper to aid readability. We first prove the more difficult variance bound for \( \Lambda_N^\gamma \) in Theorem
7.

5.1. \textbf{Proof of the variance bound of Theorem 7.} For an integer \( m \geq 1 \), real-valued random vari-
able \( (Z_{f,k} : f \in \mathcal{F}, k \geq 1) \) and a probability measure \( \nu(df) \) with support \( A \subset \mathcal{F} \), we will repeatedly use the inequalities

\[
\text{Var}_{f_0} \left( \sum_{k=1}^m Z_{f,k} \nu(df) \right) \leq \int_{\mathcal{F}} \text{Var}_{f_0} \left( \sum_{k=1}^m Z_{f,k} \nu(df) \right) \leq m \sum_{k=1}^m \sup_{f \in A} \mathbb{E}_{f_0} |Z_{k,f}^2|.
\]

\textbf{Step 1: Restricting observations away from the boundary.} We first decompose the log-likelihood according to whether \( X_{(i-1)D} \in \partial_0 \) or not. On the event \( A_{i,D} = \{X_{(i-1)D} \in \partial_0^d\} \), where \( \partial_0^d \) is the \( \delta/2 \)-enlargement of \( \partial_0 \) defined in (20) above, the process does not hit the boundary during \([i-1)D, iD]\) with overwhelming probability, and hence we may use analytic approximation techniques that ignore the boundary reflection. Since \( f = f_0 = 1 \) near the boundary for \( f, f_0 \in \mathcal{F} \), on \((A_{i,D})^c\) the likelihood ratio is already close to one and thus makes a negligible contribution. We quantify this last observation in the following result.

\textbf{Lemma 13.} Let \( \mathcal{F}' = \{ f \in \mathcal{F} : \|f\|_{C^{\alpha}} \leq r \} \) for \( \alpha = \max(4, 2|d/4 + 1/2|) \). Then, in Model \( (28) \), for \( k = 1, 2 \), any \( f, f_0 \in \mathcal{F}' \) and any \( \gamma > 0 \),

\[
\int_{x \in \mathcal{D} \setminus \partial_0^d, y \in \mathcal{D}} \left( \log \frac{p_{f_0,D}(x, y)}{p_{f,D}(x, y)} \right)^k p_{f_0}(x, y) dx dy 
\leq C_1 D^{-d/2} (1 + \gamma^2 k (\log N)^k) N^{-C_2 \gamma^2} + C_3 N^{C_4 \gamma^2} \exp(-cD^{-1}),
\]
where the constants $C_1 - C_4, c > 0$ are uniform over $(0, d, f_{\text{min}}, r, \delta, b)$.

The proof is based on explicit bounds for the heat kernel in small time, for instance Theorem 3.2.9 in [19] for the upper bound and Theorem 3.1 in [16] for the lower bound. It is delayed until Section 6.1. Abbreviating $X_t^D = (X_{(i-1)D}, X_{iD})$ and applying Lemma 13 with $k = 2$ together with (30) yields

$$\text{Var}_f(\int \sum_{i=1}^{N} \log \frac{P_{f,D}}{P_{f_0,D}}(X_t^D)1_{(A_{i,D})} \nu(df))$$

$$\leq N^2 \int_{x \in \mathcal{O} \setminus \mathcal{O}^{(d/2)}_0, y \in \mathcal{O}} \left( \log \frac{P_{f,D}(x,y)}{P_{f_0,D}(x,y)} \right)^2 p_{f_0,D}(x,y)dxdy$$

$$\lesssim D^{-d/2}(\log N)^2 N^{-C_2\mu} + N^{C_4\mu} \exp(-cD^{-1})$$

for large enough $\mu > 0$ and constants uniform over $\mathcal{O}_N$. In view of the statement of Theorem 7, it remains to consider the variance of $\int_{\mathcal{O}_N} \sum_{i=1}^{N} \log \frac{P_{f,D}}{P_{f_0,D}}(X_t^D)1_{(A_{i,D})} \nu(df)$, i.e. we may restrict to the events $A_{i,D}$.

Step 2: Approximation by an unbounded diffusion model on $\mathbb{R}^d$. We can smoothly extend any $f \in \mathcal{F}$ to all of $\mathbb{R}^d$ by setting $f = 1$ outside $\mathcal{O}$. Consider a diffusion process $(\tilde{X}_t)_{t \geq 0}$ taking values on all of $\mathbb{R}^d$ arising as the solution to the stochastic differential equation

$$\tilde{X}_t = x + \int_0^t b(\nabla f(\tilde{X}_s), \tilde{X}_s)ds + \int_0^t (2f(\tilde{X}_s))^{1/2} dB_s,$$

defined on the same probability space with the same driving Brownian motion $(B_t)_{t \geq 0}$ as $(X_t)_{t \geq 0}$. Thus in this section, $\mathbb{P}_f$ denotes a probability measure defined on a rich enough probability space to accommodate a Brownian motion $(B_t)_{t \geq 0}$ and the strong solutions $(X_t)_{t \geq 0}$ of (28) and $(\tilde{X}_t)_{t \geq 0}$ of (31) driven by the parameters $f, b$.

The process $(\tilde{X}_t)_{t \geq 0}$ in turn generates a family of transition densities $\tilde{p}_{f,D} : \mathbb{R}^d \times \mathbb{R}^d \to [0, \infty)$. We may pick a continuous version of $\tilde{p}_{f,D}$ so that in particular, for any $x \in \mathcal{O}$,

$$\tilde{p}_{f,D}(x, y)dy = \mathbb{P}_f(\tilde{X}_D \in dy | X_0 = x).$$

Consider the decomposition

$$\int_{\mathcal{O}_N} \sum_{i=1}^{N} \log \frac{P_{f,D}}{P_{f_0,D}}(X_t^D)1_{(A_{i,D})} \nu(df) = \int_{\mathcal{O}_N} \sum_{i=1}^{N} \log \frac{P_{f,D}}{P_{f_0,D}}(X_t^D)1_{(A_{i,D})} \nu(df)$$

$$+ \int_{\mathcal{O}_N} \sum_{i=1}^{N} \left( \log \frac{P_{f,D}}{P_{f_0,D}} + \log \frac{P_{f_0,D}}{P_{f,D}} \right)(X_t^D)1_{(A_{i,D})} \nu(df).$$

We have an analogous result to Lemma 13 for controlling the expectation and variance of the approximation of $\log p_{f,D}$ by $\log \tilde{p}_{f,D}$ starting from $x \in \mathcal{O}_0$.

**Lemma 14.** Let $\mathcal{F}' = \{ f \in \mathcal{F} : \|f\|_{\mathcal{C}_0} \leq r \}$ for $\alpha = \max(4, 2 \lfloor d/4 + 1/2 \rfloor)$. Then for small enough $D$, $k = 1, 2$, in Model (28), any $g = f$, $f_0 \in \mathcal{F}'$ and any $\gamma > 0$,

$$\int_{x \in \mathcal{O}_0^d, y \in \mathcal{O}} \left( \log \frac{p_{f,D}(x,y)}{p_{f_0,D}(x,y)} \right)^k p_{f_0}(x,y)dx dy$$

$$\leq C_1 D^{-d/2}(1 + \gamma^k (\log N)^k) N^{-C_2\gamma^2} + C_3 N^{C_4\gamma^2} \exp(-cD^{-1}),$$
where the constants $C_1 - C_4, c > 0$ are uniform over $(0, d, f_{\min}, r, \delta, b)$. The same estimate holds replacing $(\log \frac{p_{2N,0}(x,y)}{p_{2N,0}(x,y)})^k$ by $(\log \frac{\tilde{p}_{2N,0}(x,y)}{\tilde{p}_{2N,0}(x,y)})^k$.

The proof uses similar tools as for Lemma 13 and is delayed until Section 6.3. Using (30) and Lemma 14 with $k = 2$ and $\gamma > 0$ large enough, the $\mathbb{P}_{f_0}$-variance of the second term in the RHS of (33) is bounded above by

$$N^2 \sup_{f \in \mathcal{F}_N} \mathbb{E}_{f_0}\left[ \left( \log \frac{\tilde{p}_{f_0,0}(X_0^D)}{p_{f_0,0}(X_0^D)} \right)^2 \right]$$

$$\lesssim D^{-d/2} (\log N)^2 N^{-C_2 \mu} + N^{C_4 \mu} \exp(-cD^{-1}),$$

for large enough $\mu > 0$ and constants uniform over $\mathcal{E}_N$. We have thus established that for any large enough but fixed $\mu > 0$,

$$\text{Var}_{f_0}(A^N_{D}) \lesssim \text{Var}_{f_0}\left( \int_{\mathcal{E}_N} \log \frac{\tilde{p}_{f_0,0}(X_i^D)}{p_{f_0,0}(X_i^D)} (X_i^D) 1_{A_{i,D}} \nu(df) \right) + D^{-d/2} (\log N)^2 N^{-C_2 \mu} + N^{C_4 \mu} \exp(-cD^{-1}).$$

**Step 3:** Approximating $\tilde{p}_{f,D}$ by a Gaussian transition density in small-time. We approximate $\tilde{p}_{f,D}$ by the transition density of the corresponding Euler scheme $N_d(x, 2Df(x)I_d)$ without drift, namely

$$q_{f,D}(x,y) = \frac{1}{(4\pi Df(x))^{d/2}} \exp\left( -\frac{|y-x|^2}{4Df(x)} \right).$$

Note that while $q_{f,D}$ is defined on $\mathbb{R}^d \times \mathbb{R}^d$, it will be evaluated at $X_i^D$ which lies in $\mathcal{O} \times \mathcal{O}, \mathbb{P}_{f_0}$ almost surely. Define

$$A^N_{q,D} = \int_{\mathcal{E}_N} \log \frac{q_{f_0,0}(X_i^D)}{q_{f_0,0}(X_i^D)} (X_i^D) 1_{A_{i,D}} \nu(df),$$

again writing $X_i^D = (X_{i-1,D}, X_i^D)$. The key estimate to prove Theorem 7 is the following result, which quantifies this approximation.

**Proposition 15.** For $f_0 \in \mathcal{F}_0$ and any probability measure $\nu$ supported on $\mathcal{E}_N$ as in (16), in Model (28), it holds that

$$\text{Var}_{f_0}\left( \int_{\mathcal{E}_N} \log \frac{q_{f_0,0}(X_i^D)}{q_{f_0,0}(X_i^D)} (X_i^D) 1_{A_{i,D}} \nu(df) \right)$$

$$\lesssim \text{Var}_{f_0}(A^N_{q,D}) + N^2 \varepsilon_{1,N} (D + ND^2) + N^2 \varepsilon_{2,N} D^2 + N^2 \varepsilon_{3,N} D^3 + N^2 D^4 + N^2 \varepsilon_{1,N} D \exp(-cD^{-1}),$$

where the constants are uniform over $(0, d, f_{\min}, r, \delta, b)$.

The proof of Proposition 15 relies on second-order small time expansions of the heat-kernel and is deferred to Section 7.2.

**Step 4:** Variance of the proxy log-likelihood. It remains to control the final variance term in the RHS of the last estimate. It involves the proxy density $q_{f,D}$ but is evaluated at the points of the original diffusion $X$ given by (2) with reflection at the boundary.
Proposition 16. For \( f_0 \in \mathcal{F} \) and any probability measure \( \nu \) supported on \( \mathcal{C}_N \) as in (16), in Model (28), it holds that

\[
\text{Var}_{\nu}(\Lambda_{N,D}^N) \lesssim N e_N^2 \left( 1 + D + ND^2 + D^{-1} e_N^2 + Ne^{-C f_0 D^{-1}} \right),
\]

where the constants are uniform over \((0, d, f_{\text{min}}, r, \delta, b)\).

The proof of Proposition 16 is given in Section 7.3 and relies on martingale arguments, which are key to dealing with the dependence structure of the Markov chain. Combining the bounds from Steps 1-4 and keeping track of the leading order terms establishes the desired variance bound for \( \Lambda_{N,D}^N \) in Theorem 7.

5.2. Proof of the expectation bound of Theorem 7. The proof follows along similar, though easier, lines as the variance bound and is written in the extended Model (28) likewise. The expectation bounds will be proved uniformly over \( f \in \mathcal{C}_N \), which will sometimes be implied without explicit reference.

Step 1: Restricting observations away from the boundary. Applying Lemma 13 above with \( k = 1 \) gives

\[
\mathbb{E}_{f_0} \left[ \log \frac{\tilde{p}_{f_0,D}(X_0^D)}{p_{f,D}(X_0^D)} \mathbf{1}_{A_1,D} \right] \leq \mathbb{E}_{f_0} \left[ \log \frac{\tilde{p}_{f_0,D}(X_0^D)}{p_{f,D}(X_0^D)} \mathbf{1}_{A_1,D} \right] + C_1 D^{-d/2} (\log N) N^{-C f_2 \mu} + C_3 N^{C_4 \mu} \exp(-c D^{-1})
\]

for large enough \( \mu > 0 \), and where the constants \( C_1, C_2, c > 0 \) are uniform over \( \mathcal{C}_N \) and \( \mathcal{B} \).

Step 2: Local approximation by an unbounded diffusion model on \( \mathbb{R}^d \). Let \( \tilde{p}_{f,D} : \mathbb{R}^d \times \mathbb{R}^d \to [0, \infty) \) denote the transition density defined in (32) above, corresponding to the unbounded diffusion model (28) over the whole space \( \mathbb{R}^d \). Consider \( \mathbb{E}_{f_0} \)-expectation of the integrands in (minus) the decomposition (33). Using Lemma 14 above with \( k = 1 \) and large enough \( \gamma > 0 \), the \( \mathbb{E}_{f_0} \)-expectation of (minus) the integrand in the second term in (33) is bounded above by

\[
\sup_{f \in \mathcal{C}_N, b \in \mathcal{B}} \mathbb{E}_{f_0} \left[ \log \frac{\tilde{p}_{f,D}(X_0^D)}{p_{f,D}(X_0^D)} \mathbf{1}_{A_1,D} \right] \leq D^{-d/2} (\log N) N^{-C f_2 \mu} + N^{C_4 \mu} \exp(-c D^{-1}),
\]

for large enough \( \mu > 0 \). Arguing in the same way, an identical bound also holds for the \( \mathbb{E}_{f_0} \)-expectation of the integral of minus the third term in (33). Therefore,

\[
\mathbb{E}_{f_0} \left[ \log \frac{\tilde{p}_{f_0,D}(X_0^D)}{p_{f,D}(X_0^D)} \mathbf{1}_{A_1,D} \right] \lesssim \mathbb{E}_{f_0} \left[ \log \frac{\tilde{p}_{f_0,D}(X_0^D)}{p_{f,D}(X_0^D)} \mathbf{1}_{A_1,D} \right] + D^{-d/2} (\log N) N^{-C f_2 \mu} + N^{C_4 \mu} \exp(-c D^{-1}).
\]

Step 3: Approximating \( \tilde{p}_{f,D} \) by a Gaussian transition density in small-time. Recalling the definition (34) of the proxy density \( q_{f,D} \) from above, we now approximate the expected log-likelihood. The proof of the following proposition is deferred to Section 7.2.

Proposition 17. For \( f_0 \in \mathcal{F}_0 \) and any probability measure \( \nu \) supported on \( \mathcal{C}_N \) as in (16), in Model (28), it holds that

\[
\sup_{f \in \mathcal{C}_N, b \in \mathcal{B}} \mathbb{E}_{f_0} \left[ \log \frac{\tilde{p}_{f_0,D}(X_0^D)}{p_{f,D}(X_0^D)} \mathbf{1}_{A_1,D} \right] \lesssim \mathbb{E}_{f_0} \left[ \log \frac{q_{f_0,D}(X_0^D)}{q_{f,D}(X_0^D)} \mathbf{1}_{A_1,D} \right] + e_N^2 \left( \frac{\varepsilon_3 N}{e_N} D + \frac{\varepsilon_3 N}{e_N} D^3 / 2 + \frac{\varepsilon_3 N}{e_N} D^{3/2} \exp(-c D^{-1}) \right).
\]
where the constants are uniform over \((\emptyset, d, f_{\text{min}}, r, \delta, b)\).

**Step 4: Expectation of the proxy log-likelihood.** It finally remains to control the remaining expectation in Proposition 17 involving the proxy density \(q_{f, D}\). The proof of the following estimate can be found in Section 7.3.

**Proposition 18.** For \(f_0 \in \mathcal{F}\) and any probability measure \(\nu\) supported on \(C_N\) as in (16), in Model (28), it holds that

\[
\sup_{f \in C_N, b \in \mathcal{B}} \mathbb{P}_{f_0} \left[ \log \frac{q_{f_0, D}}{q_{f, D}} (X_0^D) \mathbf{1}_{A_{1, D}} \right] \lesssim \varepsilon_N^2 + \varepsilon_N D + \varepsilon_N D^{1/2} \exp(-cD^{-1}),
\]

where the constants are uniform over \((\emptyset, d, f_{\text{min}}, r, \delta, b)\).

Combining the bounds from Steps 1-4 and keeping track of the leading order terms establishes the expectation bound for \(\Lambda^N_{p,D}\).

It remains to show the evidence lower bound (18). By Jensen’s inequality, the desired probability in (18) is upper bounded by

\[
\mathbb{P}_{f_0} \left( \int_{C_N} \sum_{i=1}^N \log \frac{p_{f,D}(X_i^D)}{p_{f_0,D}(X_i^D)} \nu(df) \right) \leq -cN\varepsilon_N^2 - NE_N^2.
\]

Using the expectation bound just derived, the \(\mathbb{E}_{f_0}\)-expectation of the left-hand side is lower bounded by \(-NE_N^2\). Using Chebychev’s inequality and the variance bound just derived, the last probability is then bounded by

\[
\mathbb{P}_{f_0} \left( \int_{C_N} \sum_{i=1}^N \left( \log \frac{p_{f,D}(X_i^D)}{p_{f_0,D}(X_i^D)} - \mathbb{E}_{f_0} \left[ \log \frac{p_{f,D}(X_i^D)}{p_{f_0,D}(X_i^D)} \right] \right) \nu(df) \leq -cN\varepsilon_N^2 \right)
\leq \frac{1}{c^2N^2}\mathbb{E}_{f_0} \left( \int_{C_N} \sum_{i=1}^N \log \frac{p_{f,D}(X_i^D)}{p_{f_0,D}(X_i^D)} \nu(df) \right) \leq \frac{V_N}{c^2N^2\varepsilon_N^2},
\]

which completes the proof of Theorem 7.

### 6. Heat kernel estimates in small time

In this section of independent interest, we use various estimates for the transition densities of diffusions to study the expectation and variance of the integrated log-likelihood process \(\Lambda^N_{p,D}\) in Theorem 7. This is the key part of the paper where we combine stochastic calculus and perturbations of small time expansions for the transition density of a multidimensional diffusion process with reflections.

For terms near the boundary (the events \((A_{i,D})^c\)), it suffices to use upper and lower bounds of the same order. Combining the upper bound from Theorem 3.2.9 of [19] with the lower bound from Theorem 3.1 of [16], one has that for \(x, y \in \emptyset\), the transition densities of \((X_t)\) generated by (28) satisfy:

\[
c_f^- D^{-d/2} \exp \left( -C_f^+ \frac{|y - x|^2}{D} \right) \leq p_{f,D}(x, y) \leq c_f^+ D^{-d/2} \exp \left( -C_f^- \frac{|y - x|^2}{D} \right),
\]

where these estimates are uniform over \(f \in C_N \subset \{ f : f \geq f_{\text{min}}, \|f\|_{C^0} \leq r \}\) and \(b \in \mathcal{B}\) for any positive even integer \(\alpha > d/2 - 1\), see also the proof of Proposition 4 of [40] for the case of the conductivity equation with \(b(x, y) = x\). In particular, the smallest such integer is \(2 \lceil d/4 + 1/2 \rceil\), which is exactly the minimal smoothness assumption used to define \(\alpha = \alpha_d\) in (7). For the main
terms in the interior of $\emptyset$ (the events $A_{i,D}$), we will require more precise estimates, which are developed in Section 6.4 below.

6.1. **Proof of Lemma 13.** Using (35), we have

$$
\log \frac{c_{f_0^-}}{c_f} - (C_{f_0} - C_f^+) \frac{|y - x|^2}{D} \leq \log \frac{p_{f_0,D}(x,y)}{p_{f,D}(x,y)} \leq \log \frac{c_{f_0}^+}{c_f} - (C_{f_0}^+ - C_f^-) \frac{|y - x|^2}{D},
$$

which implies for $k = 1, 2$,

$$
(36) \quad \left( \log \frac{p_{f_0,D}(x,y)}{p_{f,D}(x,y)} \right)^k p_{f_0}(x,y) \leq \left( c_{f_0,f} + C_{f_0,f} \frac{|y - x|^{2k}}{D^k} \right) D^{-d/2} \exp \left( -C_{f_0}^+ \frac{|y - x|^2}{D} \right)
$$

for all $x, y \in \emptyset$. Since all constants above are uniform over $3'$ by (35), so too are all constants below, which will not be explicitly mentioned. For $\gamma > 0$, the region of the integral such that $|y - x| \geq \gamma \sqrt{D \log N}$ thus satisfies

$$
\int_{x \in \emptyset \setminus \emptyset, |y - x| \geq \gamma \sqrt{D \log N}} \left( \log \frac{p_{f_0,D}(x,y)}{p_{f,D}(x,y)} \right)^k p_{f_0,D}(x,y) \, dx \, dy \leq C_{f_0,D} D^{-d/2} (1 + \gamma^{2k} \log N)^k N^{-C_{f_0}^+ \gamma^2}.
$$

Using that $\log(1 + z) \leq |z|$ for $z \geq -1$ and (35), for $k = 1$,

$$
\log \frac{p_{f_0,D}(x,y)}{p_{f,D}(x,y)} p_{f_0,D}(x,y) \leq |p_{f,D}(x,y) - p_{f_0,D}(x,y)| \left| \frac{p_{f_0,D}(x,y)}{p_{f,D}(x,y)} - 1 \right| \leq \frac{c_{f_0}^+}{c_f} |p_{f,D}(x,y) - p_{f_0,D}(x,y)| \exp \left( (C_f^- - C_{f_0}^+) \frac{|y - x|^2}{D} \right).
$$

We obtain

$$
(37) \quad \int_{x \in \emptyset \setminus \emptyset, |y - x| \leq \gamma \sqrt{D \log N}} \log \frac{p_{f_0,D}(x,y)}{p_{f,D}(x,y)} p_{f_0,D}(x,y) \, dx \, dy \leq C_{f_0,D} N^{C_{f_0}^+ \gamma^2} \int_{x \in \emptyset \setminus \emptyset} \|p_{f,D}(x, \cdot) - p_{f_0,D}(x, \cdot)\|_{TV} \, dx,
$$

where $\| \cdot \|_{TV}$ denotes total variation norm and $p_{f,D}(x,A) = \int_A p_{f,D}(x,y) \, dy$ for any Borel set $A \subseteq \emptyset$ with a slight abuse of notation. In order to obtain a similar estimate as (38) for $k = 2$, we introduce the set

$$
\mathcal{E} = \left\{ (x,y) \in \emptyset \times \emptyset : \left| \frac{p_{f_0,D}(x,y)}{p_{f,D}(x,y)} - 1 \right| \leq 1 \right\}.
$$

Using $(\log(1 + z))^2 \leq 4z^2$ for $|z| \leq \frac{1}{2}$, for every $(x,y) \in \mathcal{E}$, we have

$$
\left( \log \frac{p_{f_0,D}(x,y)}{p_{f,D}(x,y)} \right)^2 \leq 4 \left( \frac{p_{f,D}(x,y) - p_{f_0,D}(x,y)}{p_{f,D}(x,y)} \right)^2 \min \left( p_{f,D}(x,y), p_{f_0,D}(x,y) \right)^2.
$$

$$
\leq 4 \left( p_{f,D}(x,y) - p_{f_0,D}(x,y) \right)^2 \min(c_f, c_{f_0}^+)^{-2} D^d \exp \left( 2 \max(C_f^+, C_{f_0}^+) \frac{|y - x|^2}{D} \right)
$$

$$
\leq C_{f_0,D}^\prime |p_{f,D}(x,y) - p_{f_0,D}(x,y)| D^{d/2} \exp \left( C_{f_0} \frac{|y - x|^2}{D} \right).
$$
using the rough bound
\[(p_{f,D}(x,y) - p_{f_0,D}(x,y))^2 \leq |p_{f,D}(x,y) - p_{f_0,D}(x,y)\| |(p_{f,D}(x,y) + p_{f_0,D}(x,y)\|)
\]
with (35). We now obtain
\[
\int_{x \in \Omega_0^d \setminus [y-x] \leq \gamma D \log N} \left( \log \frac{p_{f_0,D}(x,y)}{p_{f,D}(x,y)} \right)^2 p_{f_0,D}(x,y) dx dy
\]
(39) \[
\leq C_f f_0 D^{d/2} N^{C_f'} f_0 \gamma^2 \int_{x \in \Omega_0^d \setminus [y-x] \leq \gamma D \log N} \left\| p_{f,D}(x,) - p_{f_0,D}(x,) \right\|_{TV} dx dy.
\]
For \((x,y) \in \mathcal{E}_c\), thanks to (36), we have
\[
\int_{x \in \Omega_0^d \setminus [y-x] \leq \gamma D \log N, (x,y) \in \mathcal{E}_c} \left( \log \frac{p_{f_0,D}(x,y)}{p_{f,D}(x,y)} \right)^2 p_{f_0,D}(x,y) dx dy
\]
\[
\leq (c_{f_0} + C_{f_0} \gamma^2 (\log N)^k) D^{-d/2} \int_{x \in \Omega_0^d \setminus [y-x] \leq \gamma D \log N} dx dy.
\]
Moreover, the lower bound of (35) enables to write
\[
\mathcal{E}_c \cap \{|y - x| \leq \gamma D \log N\}
\]
\[
= \{|p_{f,D}(x,y) - p_{f_0,D}(x,y)| > \frac{1}{2} p_{f,D}(x,y)\} \cap \{|y - x| \leq \gamma D \log N\}
\]
\[
\subset \{|p_{f,D}(x,y) - p_{f_0,D}(x,y)| > \frac{1}{2} c_f D^{-d/2} \exp \left(-C_f \frac{|y - x|^2}{D}\right)\} \cap \{|y - x| \leq \gamma D \log N\}
\]
\[
\subset \{|p_{f,D}(x,y) - p_{f,D}(x,y)| > \frac{1}{2} c_f D^{-d/2} (\log N)^{-C_f}\},
\]
and this entails
\[
(c_{f_0} + C_{f_0} \gamma^2 (\log N)^k) D^{-d/2} \int_{x \in \Omega_0^d \setminus [y-x] \leq \gamma D \log N} dx dy
\]
\[
\leq (c_{f_0} + C_{f_0} \gamma^2 (\log N)^k) 2(c_f^{-1} (\log N)^C_f) \int_{x \in \Omega_0^d \setminus [y-x] \leq \gamma D \log N} \left| p_{f_0,D}(x,y) - p_{f,D}(x,y) \right| dx dy
\]
(40) \[
\leq C_f f_0 (1 + \gamma^2) (\log N)^{C_f'} f_0 \int_{x \in \Omega_0^d \setminus [y-x] \leq \gamma D \log N} \left\| p_{f,D}(x,\cdot) - p_{f_0,D}(x,\cdot) \right\|_{TV} dx.
\]
Putting together (38), (39) and (40), we obtain, for \(k = 1, 2\)
\[
\int_{x \in \Omega_0^d \setminus [y-x] \leq \gamma D \log N} \left( \log \frac{p_{f_0,D}(x,y)}{p_{f,D}(x,y)} \right)^k p_{f_0,D}(x,y) dx dy
\]
\[
\leq C_f f_0 N^{C_f'} f_0 \gamma^2 \int_{x \in \Omega_0^d \setminus [y-x] \leq \gamma D \log N} \left\| p_{f,D}(x,\cdot) - p_{f_0,D}(x,\cdot) \right\|_{TV} dx dy
\]
Thanks to Lemma 19 right below, the last display is then bounded by \(C_f f_0 \pi \gamma^2 \exp(-c_4 D^{-1})\), which completes the proof.

6.2. The behaviour of the transition density near the boundary. The following lemma shows that the transition densities for different functions in \(\mathcal{F}\) are similar for points near the boundary.

Lemma 19. For \(x \in \Omega \setminus \Omega_0^d\) and \(f, f_0 \in \mathcal{F}\), it holds that
\[
\|p_{f,D}(x,\cdot) - p_{f_0,D}(x,\cdot)\|_{TV} \leq \frac{16}{\sqrt{\pi} d} e^{-d^2/(16D)}.
\]
Proof. Write \( \mathbb{P}_x^f \) for the law of the solution \( X_t \) to (28) with parameter \( f \), conditional on \( X_0 = x \). Let \( \tau = \inf\{ t \geq 0, X_t \in \partial \Omega_0 \} \) denote the hitting time of the boundary of \( \Omega_0 \). For a Borel set \( \mathcal{A} \subset \Omega \), by the strong Markov property,
\[
p_{f,D}(x,A) = \mathbb{E}_x^f[1_{\{X_{\tau} \in \mathcal{A}\}}1_{\{\tau > D\}}] + \mathbb{E}_x^f[p_{f,D-\tau}(X_\tau, \mathcal{A})1_{\{\tau \leq D\}}],
\]
where, as before, we write \( p_{f,D}(x,A) = \int_A p_{f,D}(x,y)dy \) for any Borel set \( \mathcal{A} \subset \Omega \) with a slight abuse of notation. Since \( x \in \Omega \setminus \Omega_0^\delta \), we have
\[
\mathbb{E}_x^f[1_{\{X_{\tau} \in \mathcal{A}\}}1_{\{\tau > D\}}] = \mathbb{E}_x^f[1_{\{X_{\tau} \in \mathcal{A}\}}1_{\{\tau > D^\delta\}}]
\]
and
\[
\mathbb{E}_x^f[1_{\{X_{\tau} \in \mathcal{A}\}}1_{\{\tau \leq D\}}] = \mathbb{E}_x^f[1_{\{X_\tau \in \mathcal{A}\}}1_{\{\tau \leq D\}}]
\]
which implies
\[
\|p_{f,D}(x,\cdot) - p_{f_0,D}(x,\cdot)\|_{TV} \leq 2\mathbb{P}_x(\tau \leq D).
\]
Here, for \( x \in \Omega \setminus \Omega_0^\delta \), the hitting time \( \tau \) of the boundary of \( \Omega_0 \) by the process \( (x + \sqrt{2}B_t + \xi_t)_{t \geq 0} \) has law that does not depend on \( f \) nor \( f_0 \). Introduce now the two stopping times \( 0 \leq S \leq T \):
\[
S = \inf\{ t \geq 0, X_t \in \partial \Omega_0^\delta \}, \quad T = \inf\{ t \geq S, |X_t - X_S| \geq \delta \},
\]
the first hitting time of the boundary \( \partial \Omega_0^\delta \) and the first exit time of the ball of center \( X_S \) and radius \( \delta/2 \), respectively. Necessarily,
\[
\{\tau \leq D\} \subset \left\{ \sup_{0 \leq t \leq D} |X_{(t+S)\wedge T} - X_S| = \delta/2 \right\}.
\]
Moreover, the process \( (X_{(t+S)\wedge T} - X_S)_{t \geq 0} \) has the same law as \( (\sqrt{2}B_{t\wedge T})_{t \geq 0} \). It follows that
\[
\mathbb{P}_x(\tau \leq D) \leq \mathbb{P}_x\left( \sup_{0 \leq t \leq D} |B_{t\wedge T}| \geq \delta/2^{3/2} \right) \leq \mathbb{P}_x\left( \sup_{0 \leq t \leq D} |B_t| \geq \delta/2^{3/2} \right)
\]
\[
\leq 4\mathbb{P}_x\left( B_D \geq \delta/2^{3/2} \right) \leq \frac{4}{\sqrt{2\pi}} \frac{2^{3/2}}{\delta} \exp\left( \frac{-\delta^2}{16D} \right),
\]
where the third inequality follow from the reflection principle for Brownian motion and the last inequality from the standard Gaussian tail bound. Combining (41) with the last display proves the lemma. \( \square \)

6.3. Proof of Lemma 14. Let \( g = f \) or \( f_0 \) in the notation below. For \( \bar{p}_{g,D}(x,y) \), an estimate of the kind (35) is classical (see e.g. [3, 23]) for diffusion processes over the whole space \( \mathbb{R}^d \). Using the analogous estimate to (35), one can then argue exactly as in the proof of Lemma 13, again splitting the integral according to whether \( |y - x| \leq \sqrt{D}\log N \) or not. In particular, using the analogues of (37),(39) and (40), one gets for \( k = 1, 2 \) and any \( \gamma > 0 \),
\[
\int_{x \in \Omega_0^\delta, y \in \Omega} \left( \log \frac{p_{g,D}(x,y)}{p_{f_0,D}(x,y)} \right)^k p_{f_0,D}(x,y)dx dy
\]
\[
\leq C_{g,f_0}D^{-d/2}(1 + \gamma^{2k}(\log N)^k)N^{-C_{f_0}^+\gamma^2} + C_{g,f_0}N^{C_{f_0}^+\gamma^2} \int_{x \in \Omega_0^\delta} \|p_{g,D}(x,\cdot) - \bar{p}_{g,D}(x,\cdot)\|_{TV} dx,
\]
where the constants are uniform over \( \mathcal{F}' \), \( \| \cdot \|_{TV} \) denotes total variation distance on \( \mathbb{R}^d \), and we implicitly extend \( p_{g,D}(x,\cdot) \) into a probability measure on \( \mathbb{R}^d \) by setting \( p_{g,D}(x,\mathcal{A}) = p_{g,D}(x,\mathcal{A} \cap 0) \) for any Borel set \( \mathcal{A} \) in \( \mathbb{R}^d \). We claim that
\[
\|p_{g,D}(x,\cdot) - \bar{p}_{g,D}(x,\cdot)\|_{TV} \leq 4d \exp\left( -\frac{\delta^2}{20d\|g\|_{\infty}D} \right)
\]
for \( x \in \mathcal{O}_0 \) and any \( g \in \mathcal{F} \) with \( D < D_0(\delta, \|g\|_{C^1}) \) small enough. By (42) the second last display is then bounded by
\[
C_{g,f_0}D^{-d/2}(1 + \gamma^2 k \log N)N^{-C_{g,f_0}^{-1} \gamma^2} + C_{g,f_0}N^{-C_{g,f_0} \gamma^2} \exp \left( -c_{g} \delta D^{-1} \right),
\]
which completes the proof. It thus remains to prove (42). Let \( x \)
then bounded by
\[
x \in \mathcal{O}_0 \text{ and } \bar{r} = \inf \{ t \geq 0, \bar{X}_t \in \partial \mathcal{O} \}
\]
be the hitting time of the boundary \( \partial \mathcal{O} \). For any Borel set \( A \) in \( \mathbb{R}^d \), by the strong Markov property,
\[
p_{g,D}(x,A) = \mathbb{E}_g[1_{\{X_D \in A\}}1_{\{\tau > D\}} | X_0 = x] + \mathbb{E}_g[p_{g,D-\bar{r}}(X_{\bar{r}}, A \cap \emptyset)1_{\{\bar{r} \leq D\}} | X_0 = x]
= \tilde{p}_{g,D}(x,A) - \mathbb{E}_g[1_{\{\bar{X}_D \in A\}}1_{\{\bar{r} \leq D\}} | X_0 = x] + \mathbb{E}_g[p_{g,D-\bar{r}}(X_{\bar{r}}, A \cap \emptyset)1_{\{\bar{r} \leq D\}} | X_0 = x],
\]
since \( X_1 \) and \( \bar{X}_1 \) both started at \( x \in \mathcal{O}_0 \) at \( t = 0 \) coincide until they hit the boundary \( \partial \mathcal{O} \). It follows that
\[
\|p_{g,D}(x, \cdot) - \tilde{p}_{g,D}(x, \cdot)\|_{TV} \leq 2\mathbb{P}g(\bar{r} \leq D | X_0 = x).
\]
We conclude thanks to Lemma 25.

### 6.4. Approximating transition densities for small-time.

This section is devoted to the approximation of small-time transition densities for diffusions in \( \mathbb{R}^d \). We use some Riemannian geometry to derive second-order small-time expansions of the heat kernel, following results that date back to Azencott [4]. Recall that
\[
\tilde{p}_{f,D}, q_{f,D} : \mathbb{R}^d \times \mathbb{R}^d \to [0, \infty)
\]
denote, respectively, (a smooth version of) the transition density of \( (\bar{X}_t)_{t \geq 0} \) defined in (31), and the proxy transition density of an Euler scheme without drift defined in (34). The next result gives an expansion of the log-likelihood ratio of the transition densities, uniformly over the domain \( \mathcal{O} \).

**Lemma 20.** There exist smooth functions: \( \gamma_{f_0,b} : \mathcal{O} \to \mathbb{R}^d \) with
\[
\text{supp}(\gamma_{f_0,b}) \subset \mathcal{O}_0, \quad \| \gamma_{f_0,b} \| \ll \| f - f_0 \|_{C^1},
\]
where the constants in the inequality depend only on an upper bound for \( \| f \|_{C^1}, \| f_0 \|_{C^1} \) and also on \( b \), and such that the following expansion holds:
\[
\log \frac{\tilde{p}_{f_0,D}(x,y)1_{\{x \in \mathcal{O}_0\}}}{\tilde{p}_{f,D}(x,y)} = \log \frac{q_{f_0,D}(x,y)}{q_{f,D}(x,y)} 1_{\{x \in \mathcal{O}_0\}} + \gamma_{f_0,f}(x) \cdot (y - x) + \frac{1}{8D} |y - x|^2 \nabla(f^{-1} - f_0^{-1})(x) \cdot (y - x) 1_{\{x \in \mathcal{O}_0\}} + (\| f - f_0 \|_{C^2} D + \| f - f_0 \|_{C^1} |y - x| D + |y - x|^2 D + \| f - f_0 \|_{C^1} |y - x|^2 + \| f - f_0 \|_{C^1} |y - x| + |y - x|^4) r_{f_0,b}(x,y),
\]
for a remainder term \( r_{f_0,b} : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R} \) satisfying
\[
\sup_{\| f \|_{C^1} + \| f_0 \|_{C^1} \leq r, b \in \mathcal{B}} \| r_{f_0,b} \| \leq \infty
\]
for every \( r > 0 \).

While only local to \( (x,y) \in \mathcal{O} \times \mathcal{O} \), the stability property (43) is sufficient for our purpose: the approximation is only needed for \( (x,y) = (X_{(i-1)D}, X_{iD}) \in \mathcal{O} \times \mathcal{O} \), a property that holds \( \mathbb{P}_{f_0} \)-almost surely. The proof of Lemma 20 is deferred to Appendix 6.4.
We rely on a key second-order estimate of the heat kernel in small time, associated to the metric tensor \( g_{ij}(x) = f(x)^{-1} \delta_{ij} \) induced by the diffusion matrix \( f(x)^{-1} \text{Id} \) on \( \mathbb{R}^d \), viewed as a Riemannian manifold. For \( x, y \in \mathbb{R}^d \), let
\[
\ell_f(x, y) = \inf \left\{ \int_0^1 \frac{|\dot{\gamma}_t|}{f(\gamma_t)^{1/2}} \, dt, \quad \gamma_0 = x, \gamma_1 = y \right\}
\]
denote the Riemannian geodesic distance between \( x \) and \( y \), where the infimum is taken over all smooth paths \( \gamma : [0, 1] \to \mathbb{R}^d \) connecting \( x \) and \( y \) at times 0 and 1, and \( \dot{\gamma}_t \) is the time derivative of \( \gamma_t \).

**Lemma 21.** The following small time expansion holds:
\[
\bar{p}_{f,D}(x, y) = \frac{1}{(4\pi D)^{d/2}} \exp \left( -\frac{1}{4D} \ell_f(x, y)^2 \right) (\alpha_f(x, y) + \beta_f(x, y)D + D^2 \Gamma_{f,D}(x, y)),
\]
where
\[
\tag{44} \| \alpha_f \|_{\infty} + \| \beta_f \|_{\infty} + \sup_{D>0} \| \Gamma_{f,D} \|_{\infty} \lesssim 1,
\]
and the \( \| \cdot \|_{\infty} \)-norm is taken for \( (x, y) \in \mathcal{O} \) and the estimates are uniform over \( f \in \mathcal{C}_N \). Moreover, there exist smooth (at least \( C^4 \)) real-valued functions
\[
\alpha : \mathbb{R} \to \mathbb{R}, \quad \alpha^i : \mathbb{R}^{d \times 1 \times d} \to \mathbb{R}, \alpha^{ij} : \mathbb{R}^{d \times 1 \times d \times d} \to \mathbb{R}, \quad \alpha^{ijk} : \mathbb{R}^{d \times 1 \times d \times d \times d} \to \mathbb{R}
\]
for \( 1 \leq i, j, k \leq d \) and independent of \( f \), such that
\[
\alpha_f(x, y) = \alpha(f(x)) + \sum_{i=1}^d \alpha^i(x, f(x), (\partial_i f(x))_{i'}) (x^i - y^i) \]
\[
+ \sum_{i,j=1}^d \alpha^{ij}(x, f(x), (\partial_i f(x))_{i'}, (\partial_j^2 f(x))_{i'j'})(x^i - y^i)(x^j - y^j) \]
\[
+ \sum_{i,j,k=1}^d \alpha^{ijk}(x, f(x), (\partial_i f(x))_{i'}, (\partial_j^2 f(x))_{i'j'}, (\partial_k^3 f(x))_{i'j'k})(x^i - y^i)(x^j - y^j)(x^k - y^k)
\]
\[
+ |x - y|^4 r_f(x, y),
\]
where \( x = (x^1, \ldots, x^d), y = (y^1, \ldots, y^d) \) and the remainder term satisfies \( \| r_f \|_{\infty} \lesssim 1 \), uniformly in \( f \in \mathcal{C}_N \) with the supremum taken over \( (x, y) \in \mathcal{O} \times \mathcal{O} \). Moreover,
\[
\tag{46} \alpha(f(x)) = f(x)^{-d/2}.
\]
An analogous expansion holds for \( \beta_f \) (except for (46)) with smooth (at least \( C^4 \)) functions
\[
\beta : \mathbb{R}^{d \times 1 \times d \times d} \to \mathbb{R}, \quad \beta^i : \mathbb{R}^{d \times 1 \times d \times d} \to \mathbb{R},
\]
for \( 1 \leq i \leq d \), independent of \( f \) and such that
\[
\beta_f(x, y) = \beta(x, f(x), (\partial_i f(x))_{i'}, (\partial_{i'j'} f(x))_{i'j'})(x^i - y^i) \]
\[
+ \sum_{i=1}^d \beta^i(x, f(x), (\partial_i f(x))_{i'}, (\partial_{i'j'} f(x))_{i'j'}, (\partial_{i'j'k'} f(x))_{i'j'k'})(x^i - y^i) + |x - y|^2 \tilde{r}_f(x, y).
\]
The existence of a small time expansion of the heat kernel in the first part of the lemma is classical, see e.g. [8]. The robust estimates (44) follows from the main result of Azencott [4]. The second part, namely the form of the expansion (45) for the functions $\alpha$ and $\beta$ and how they involve the derivatives of $f$ at $x$ uses the recent result of Bilal [10] that obtains explicit representations by mixing small time and space expansions, a key idea to control the density near the diagonal in small time. We sketch Bilal’s approach and results in the proof below and refer the reader to Section 2 of Bilal’s paper together with his appendix for more details.

**Sketch of proof of Lemma 21.** Consider the Fokker-Planck equation

\begin{equation}
\partial_t \rho_t + \text{div}(b \nabla \rho_t) = \frac{1}{2} \sum_{i,j=1}^d \partial^2_{ij}((\sigma_f \sigma_f^\top)_{ij} \rho_t)
\end{equation}

with initial value $\rho_0(dx)$ as a probability distribution. In our case, $b_{ij}(x) = b(\nabla f(x), x)$ and $(\sigma_f(x)\sigma_f(x)^\top)_{ij} = 2f(x)\delta_{ij}$, yielding

\[
\partial_t \rho_t = \Delta f \rho_t - \text{div}(b \nabla f, \rho_t) =: D f \rho_t,
\]

Whenever existence and uniqueness hold, the solution is given by $\rho_t(y) = \int_0^t \tilde{p}_{f,t}(x, y) \rho_0(dx)$, where $\tilde{p}_{f,t}(x, y)$ is the Markov transition density associated to the process $\tilde{X}$ defined in (31) on the whole space $\mathbb{R}^d$ and that we are looking to expand. Rewriting $\tilde{p}_{f,t}(x, y)$ as $f(x)^{-d/2} K_t^f(x, y)$, this satisfies the Fokker-Planck equation if

\[
\partial_t K_t^f(x, \cdot) = D_f K_t^f(x, \cdot)
\]

with $K_t^f(x, y)dy \to f(x)^d \delta_x(dy)$ weakly as $t \to 0$. Our ansatz for the heat kernel takes the form

\begin{equation}
K_t^f(x, y) \sim K_t^{f,0}(x, y) \sum_{r=0}^{\infty} F_r(x, y) t^r,
\end{equation}

where

\[
K_t^{f,0}(x, y) = \frac{1}{(4\pi t)^{d/2}} \exp \left(-\frac{\ell f(x, y)^2}{4t}\right)
\]

and the notation $u_t = \sum_{r=0}^{k} a_t t^r$ means $a_t = \sum_{r=0}^{k} b_r t^r + O(t^{k+1})$. The existence of such an expansion is provided for instance by Theorem 1.2. in Azencott [4]. It remains to find a formula for the coefficients $F_r(x, y)$ for $r = 0, 1$ that is compatible with the expansion (45) via the representation $\alpha_f(x, y) = f(x)^{-d/2} F_0(x, y)$ and $\beta_f(x, y) = f(x)^{-d/2} F_1(x, y)$, and we can then conclude with Azencott’s result.

In order to do so, we follow Bilal’s approach and sketch the Section 2 of his paper [10]. In that part of the proof and it that part only, we will use Einstein notation for differential operators.\(^1\) By plugging the ansatz (49) into (48) and letting $t \to 0$, one obtains a formula for the functions $F_r$, which reads, for $r = 0$ and $r = 1$ (see in particular equations (2.15) and (2.16) in Section 2 of [10]):

\begin{equation}
2g^{ij} \partial_i \partial_j F_0 = \left(-g^{ij} \partial_i \ell_j^2 + 2d - b^i \partial_i \ell_j \ell_j^2 \right) F_0, \quad F_0(x, x) = 1,
\end{equation}

and

\begin{equation}
(4 + g^{ij} \partial_i \ell_j \ell_j^2 - 2d + b^i \partial_i \ell^2 + 2g^{ij} \partial_i \ell_j \partial_j) F_1 = 0,
\end{equation}

\(^1\)i.e. when an index variable appears twice in a single term and is not otherwise defined it implies summation of that term over all the values of the index.
with \( \partial_i = \frac{\partial}{\partial x^i} \) and where \( g_{ij} = f^{-1} \delta_{ij} \) with inverse \( g^{ij} = f \delta_{ij} \) is the metric tensor induced by the diffusion coefficient \( \sqrt{2f(x)} \delta_{ij} \) and \( b'(x) = b'(\nabla f(x), x) \) in coordinates. We next expand \( \ell_f^2 \) around \( x \) in the \( y \) variable to obtain (see Equation (A.21) in [10]), with \( \epsilon = x - y \):

\[
\ell_f^2(x, y) = g_{ij} \epsilon^i \epsilon^j + \frac{1}{2} \partial_k g_{ij} \epsilon^k \epsilon^j + \left( \frac{1}{2} \partial_i \partial_j g_{kl} - \frac{1}{12} g_{nm} \Gamma^m_{ijk} \right) \epsilon^i \epsilon^j \epsilon^k + O(|\epsilon|^3),
\]

where \( \Gamma^k_{ij} = \frac{1}{2} g^{kl} (\partial_i g_{jl} + \partial_j g_{il} - \partial_l g_{ij}) \) denotes the Christoffel symbol associated with the metric tensor \( g_{ij} \), and this provides with expansions for \( \partial_i \ell_f^2 \) and \( \partial_i \partial_j \ell_f^2 \) around \( x \) in the \( y \) variable (with now \( \partial_i = \frac{\partial}{\partial x^i} \)):

\[
\partial_i \ell_f^2 = 2 g_{ij} \epsilon^i \epsilon^j + \frac{3}{2} \partial_k g_{ij} \epsilon^k \epsilon^j + \left( \frac{3}{2} \partial_i \partial_j g_{kl} - \frac{1}{3} g_{nm} \Gamma^m_{ijk} \right) \epsilon^i \epsilon^j \epsilon^k + O(|\epsilon|^4)
\]

and

\[
\partial_i \partial_j \ell_f^2 = 2 g_{ij} + 3 \partial_k g_{ij} \epsilon^k + \left( 2 \partial_i \partial_j g_{kl} - g_{nm} \Gamma^m_{ijk} \right) \epsilon^k \epsilon^j + O(|\epsilon|^4),
\]

see in particular Equations (A.22) and (A.23) in [10] and where \( a_{(i, \ldots, n)} \) denotes symmetrisation in the indices\(^2\). Next we expand \( F_r(x, y), r = 0, 1 \), around \( x \) in the \( y \) variable, with \( \epsilon = y - x \):

\[
F_r(x, y) = t_r(x) + u_r^i(x) \epsilon^i + v_r^{ij}(x) \epsilon^i \epsilon^j + w_r^{ijk}(x) \epsilon^i \epsilon^j \epsilon^k + O(|\epsilon|^4).
\]

for some functions \( t_r, u_r, v_r \) and \( w_r \) and with \( t_0(x) = 1 \) in particular. Plugging (53) and (54) in (50) and (51) and expanding the solution via the representation (55) in powers of \( \epsilon^i, \epsilon^i \epsilon^j, \epsilon^i \epsilon^j \epsilon^k \) is sufficient to obtain \( t_r, u_r^i, v_r^{ij}, w_r^{ijk} \). For instance, (2.33) in [10] explicitly gives

\[
t_0(x) = 1, \ u_0^i(x) = -\frac{1}{2} a_i(x), \ v_0^{ij}(x) = \frac{1}{8} a_i(x) a_j(x) + \frac{1}{12} R_{ij} - \frac{1}{8} \left( \partial_j a_i(x) + \partial_i a_j(x) \right)
\]

where

\[
a_i(x) = b^i(x) - \partial_j g^{ij}(x) - g^{ij}(x) \partial_j V(x), \ \exp(-2V(x)) = \det(g^{ij}(x)) \quad \text{and} \quad R_{jk} = \partial_j \Gamma^i_{jk} - \partial_j \Gamma^i_{ki} + \Gamma^i_{lm} \Gamma^m_{jk} - \Gamma^i_{jp} \Gamma^j_{ik} + \Gamma^i_{jk} \Gamma^j_{ik} \ 
\]

is the Ricci curvature tensor associated with the metric tensor \( g_{ij} \). In particular,

\[
u_0^i(x) = -\frac{1}{2} a_i(x) = b^i(\nabla f(x), x) - 2 \partial_i f(x) - d \text{ div } f(x).
\]

Also (2.36) in [10] explicitly yields

\[
t_0(x) = \frac{1}{2} g^{ij}(x) R_{ij}(x) = \beta(f(x), (\partial_i f(x))_{ij}, (\partial_i f(x))_{ij}),
\]

\text{i.e.} the scalar Ricci curvature. We can move forward with explicit computations that become increasingly more difficult with the order of approximation and that involve nontrivial geometric quantities. But an inspection of (50) and (51) shows that they involve explicit and rational functions of \( b(\nabla f(x), x) \) and its derivatives, \( f(x), \partial_1 f(x), \partial_2 f(x), \partial_3 f(x) \) and \( \partial_1 \partial_2 f(x) \) with increasing differentiation order for \( F_0 \) while \( F_1 \) involves derivatives of \( f \) of order 2 and higher. The result follows.

\[ \square \]

\textbf{Proof of Lemma 20.} Using Lemma 21, and a first-order Taylor's expansion, write

\[
\log \frac{\tilde{p}_{f_0,D}(x, y)}{p_{f,D}(x, y)} = -\frac{1}{4D}(\ell_{f_0}(x, y)^2 - \ell_f(x, y)^2) + \log \frac{\alpha_{f_0}(x, y)}{\alpha_f(x, y)} \quad \text{where}
\]

\[
\frac{\beta_{f_0}(x, y)}{\alpha_{f_0}(x, y)} - \frac{\beta_f(x, y)}{\alpha_f(x, y)} = D + D^2 \Gamma^l_{f_0,f,D}(x, y),
\]

\[ \text{For instance } a_{(ij)} = \frac{1}{2}(a_{ij} + a_{ji}). \]
where $\sup_{f \in C_N} \sup_{D > 0} \|F'_{f_0, f, D}\|_\infty \lesssim 1$, thanks to (44), (46) and $f(y) \geq f_{\text{min}} > 0$ on $\mathcal{O}$. The linear term in $D$ can be rewritten as

$$\frac{\beta_{f_0}(x, y) - \beta_f(x, y)}{\alpha_{f_0}(x, y)} = \frac{\beta_{f_0}(x, y) - \beta_f(x, y)}{\alpha_{f_0}(x, y)} + (\alpha_f(x, y) - \alpha_{f_0}(x, y)) \frac{\beta_f(x, y)}{\alpha_{f_0}(x, y) \alpha_f(x, y)}.$$ 

Using (45),

$$\alpha_f(x, y) - \alpha_{f_0}(x, y) = \alpha(f(x)) - \alpha(f_0(x))$$

$$+ \sum_{i=1}^d \left( \alpha'(f(x, \partial_i f(x))) - \alpha'(f_0(x, \partial_i f_0(x))) \right) (x^i - y^i)$$

$$+ |x - y|^2 r'_{f_0, f}(x, y),$$

with $\|r'_{f_0, f}\|_\infty \leq C(\|f\|_{C^2}, \|f_0\|_{C^2})$. By (45) and (47) of Lemma 21, we have

$$|\alpha_f(x, y) - \alpha_{f_0}(x, y)| \leq \|f - f_0\|_{C^1} |x - y| + |x - y|^2$$

and

$$|\beta_f(x, y) - \beta_{f_0}(x, y)| \leq \|f - f_0\|_{C^2} + \|f - f_0\|_{C^1} |x - y| + |x - y|^2,$$

with the constant depending only on an upper bound for $\|f\|_{C^1}$ and $\|f_0\|_{C^2}$. Using the expansion for $\alpha_f(x, y)$ in Lemma 21, (46) and that $f \geq f_{\text{min}}$, we have that $\alpha_f(x, y), \alpha_{f_0}(x, y) \geq c > 0$, uniformly over $C_N$. It follows that

$$\left|\frac{\beta_{f_0}(x, y) - \beta_f(x, y)}{\alpha_{f_0}(x, y)}\right| D \leq (\|f - f_0\|_{C^2} D + \|f - f_0\|_{C^1} |x - y| D + |x - y|^2 D) r'_{f_0, f}(x, y),$$

with $\sup_{f \in C_N} \|r''_{f_0, f}\|_\infty \lesssim 1$.

Next, writing $\tilde{\alpha}_f(x, y) = f(y)^{d/2} \alpha_f(x, y)$ and $\tilde{\alpha}_{f_0}(x, y) = f_0(y)^{d/2} \alpha_f(x, y)$,

$$\log \frac{\alpha_{f_0}(x, y)}{\alpha_f(x, y)} = \frac{d}{2} \log \frac{f(y)}{f_0(x)} + \log \tilde{\alpha}_{f_0}(x, y) - \log \tilde{\alpha}_f(x, y).$$

Using the expansion (45),

$$\tilde{\alpha}_f(x, y) = 1 + \sum_{i=1}^d \tilde{\alpha}^i(x, f(x), (\partial_i f(x))_{\partial i})(x^i - y^i)$$

$$+ \sum_{i, j=1}^d \tilde{\alpha}^{ij}(x, f(x), (\partial_i f(x))_{\partial i}, (\partial_j f(x))_{\partial j})(x^i - y^i)(x^j - y^j)$$

$$+ \sum_{i, j, k=1}^d \tilde{\alpha}^{ijk}(x, f(x), (\partial_i f(x))_{\partial i}, (\partial_j f(x))_{\partial j}, (\partial_k f(x))_{\partial k})(x^i - y^i)(x^j - y^j)(x^k - y^k)$$

$$+ |x - y|^4 r_f(x, y)$$

where similarly $\tilde{\alpha}_f^{\lambda}(y) = f(y)^{d/2} \alpha^{\lambda}(y)$ for $\lambda = i, ij, ijk$ and $\alpha^{\lambda}(y)$ are the smooth functions given in (45) that do not depend on $f$ or $f_0$. For notational simplicity, using only a subscript to indicate the dependence on $f$ and setting $z = x - y$, the above expansion can be concisely written as

$$\tilde{\alpha}_f = 1 + \sum_i \tilde{\alpha}_f^i z^i + \sum_{ij} \tilde{\alpha}_f^{ij} z^i z^j + \sum_{ijk} \tilde{\alpha}_f^{ijk} z^i z^j z^k + O(\|z\|^4).$$
Expanding the logarithm around $z = 0$ to order 3,

\[
\log \tilde{\alpha}_f = \sum_i \bar{\alpha}_{ij} z^i + \sum_{ij} \bar{\alpha}_{ij} z^i z^j + \sum_{ijk} \bar{\alpha}_{ijk} z^i z^j z^k + O(|z|^4)
\]

\[
- \frac{1}{2} \left( \sum_i \bar{\alpha}_{ij} z^i + \sum_{ij} \bar{\alpha}_{ij} z^i z^j + \sum_{ijk} \bar{\alpha}_{ijk} z^i z^j z^k + O(|z|^4) \right)^2
\]

\[
+ \frac{1}{3} \left( \sum_i \bar{\alpha}_{ij} z^i + \sum_{ij} \bar{\alpha}_{ij} z^i z^j + \sum_{ijk} \bar{\alpha}_{ijk} z^i z^j z^k + O(|z|^4) \right)^3 + O(|z|^4).
\]

Keeping track of only the leading order terms, the quadratic term in the last display equals

\[
\sum_{ij} (\alpha'_{ij}) z^i z^j + \sum_{ijk} (\alpha''_{ijk}) z^i z^j z^k + O(|z|^4),
\]

with $(\alpha'_{ij}) = \bar{\alpha}_{ij} \bar{\alpha}_{ij}$ and $(\alpha''_{ijk}) = \bar{\alpha}_{ijk} \bar{\alpha}_{ijk}$. Likewise, the cubic term equals $\sum_{ijk} (\alpha''_{ijk}) z^i z^j z^k + O(|z|^4)$ with $(\alpha''_{ijk}) = \bar{\alpha}_{ijk} \bar{\alpha}_{ijk}$.$\bar{\alpha}_{ijk}$. Therefore,

\[
\log \tilde{\alpha}_f = \sum_i \bar{\alpha}_{ij} z^i + \sum_{ij} \bar{\alpha}_{ij} z^i z^j + \sum_{ijk} \bar{\alpha}_{ijk} z^i z^j z^k + O(|z|^4),
\]

with $\bar{\alpha}_{ij} = \bar{\alpha}_{ij}$, $\bar{\alpha}_{ij} = \bar{\alpha}_{ij} - \frac{1}{2} \bar{\alpha}_{ij} \bar{\alpha}_{ij}$ and $\bar{\alpha}_{ijk} = \bar{\alpha}_{ijk} - \frac{1}{2} \bar{\alpha}_{ijk} \bar{\alpha}_{ijk} + \frac{1}{3} \bar{\alpha}_{ijk} \bar{\alpha}_{ijk}$. Set now

\[
\gamma_{f_0,f}(x) = \bar{\alpha}_{ij} (x, f(x), (\partial_i f(x))_{i'}) - \bar{\alpha}_{ij} (x, f_0(x), (\partial_i f_0(x))_{i'}),
\]

\[
\gamma_{f_0,f}(x) = \bar{\alpha}_{ij} (x, f(x), (\partial_i f(x))_{i'}), (\partial_j f(x))_{i'j'} - \bar{\alpha}_{ij} (x, f_0(x), (\partial_i f_0(x))_{i'}), (\partial_j f_0(x))_{i'j'}),
\]

\[
\gamma_{f_0,f}(x) = \bar{\alpha}_{ijk} (x, f(x), (\partial_i f(x))_{i'}, (\partial_j f(x))_{i'j'}, (\partial_k f(x))_{i'j'k'}) - \bar{\alpha}_{ijk} (x, f_0(x), (\partial_i f_0(x))_{i'}, (\partial_j f_0(x))_{i'j'}, (\partial_k f_0(x))_{i'j'k'})
\]

where we recall $\bar{\alpha}_{ij} (y) = f(y)^{d/2} \alpha^j (y)$. This gives the expansion

\[
\log \frac{\tilde{\alpha}_{f_0,f}(x,y)}{\tilde{\alpha}_f(x,y)} = \sum_{i=1}^d \gamma_{f_0,f}(x)(x^i - y^i) + \sum_{i,j=1}^d \gamma_{ij} f_0,f(x)(x^i - y^i)(x^j - y^j)
\]

\[
+ \sum_{i,j,k=1}^d \gamma_{ijk} f_0,f(x)(x^i - y^i)(x^j - y^j)(x^k - y^k) + |x - y|^4 \tilde{\alpha}_{f_0,f}(x,y),
\]

(59)

where $|\tilde{\alpha}_{f_0,f}| \lesssim 1$ is uniform over an upper bound for $\|f\|_{e^4}$ and $\|f_0\|_{e^4}$. By triangle inequality,

$$
\|\gamma_{f_0,f}\| \lesssim \|f\|_{d/2}^d - f_0\|_{d/2}^d + \|f - f_0\|_{e^4},
$$

since $f, f_0 \geq f_{\text{min}}$ and where the constants in the inequality depend only on $f_{\text{min}}$ and an upper bound for $\|f\|_{e^4}$ and $\|f_0\|_{e^4}$. Using similar expressions for $\|\gamma_{f_0,f}\|_{\infty}$ and $\|\gamma_{ij}\|_{\infty}$, we infer

\[
\left| \sum_{i,j=1}^d \gamma_{ij} f_0,f(x)(x^i - y^i)(x^j - y^j) + \sum_{i,j,k=1}^d \gamma_{ijk} f_0,f(x)(x^i - y^i)(x^j - y^j)(x^k - y^k) \right|
\]

\[
\lesssim \|f - f_0\|_{e^2} |x - y|^2 + \|f - f_0\|_{e^3} |x - y|^3,
\]

(60)
Lemma 22. We have

\[
\log \frac{\tilde{p}_{f,D}(x,y)}{p_{f,D}(x,y)} 1_{\{x \in \partial_0^\dagger\}} = \left( -\frac{1}{4D} (\ell_{f_0}(x,y) - \ell_f(x,y))^2 - \frac{d}{2} \log f_0(x) \right) 1_{\{x \in \partial_0^\dagger\}}
\]

\[
+ \gamma_{f_0,f}(x) \cdot (y - x) 1_{\{x \in \partial_0^\dagger\}}
\]

\[
+ \left( |f - f_0|_{|e^2D|} + \|f - f_0\|_{|e^1|} |y - x|D + |y - x|^2 D + \|f - f_0\|_{|e^2|} |y - x|^2
\]

\[
+ \|f - f_0\|_{|e^3|} |y - x|^3 + |y - x|^4 \right) r_{f_0,f}(x,y),
\]

with \( \sup_{f \in \mathcal{E}_N} \|r_{f_0,f}\|_\infty \lesssim 1 \).

With a slight abuse of notation, we may incorporate the term \( 1_{\{x \in \partial_0^\dagger\}} \) into the definition of \( \gamma_{f_0,f}(x) \). The final step is to expand the Riemannian metric \( \ell_f \).

Lemma 22. We have

\[
\ell_f(x,y)^2 = \frac{|x - y|^2}{f(x)} + \frac{1}{2} |x - y|^2 \nabla f^{-1}(x) \cdot (x - y) + |x - y|^4 r_f(x,y),
\]

where \( \sup_{f \in \mathcal{E}_N} \|r_f\|_\infty \lesssim 1 \).

Proof. This is textbook Riemannian geometry, see e.g. Equation (A.21) in Appendix A.3 in [10] displayed in (52) above, with \( \epsilon = x - y \) that gives (Einstein notation)

\[
\ell_f^2(x,y) = g_{ij} \epsilon^i \epsilon^j + \frac{1}{2} \partial_k g_{ij} \epsilon^k \epsilon^j + O(|\epsilon|^4),
\]

for the metric tensor \( g_{ij} = (f(x))^{-1} \delta_{ij} \). This readily gives the result, the uniformity in \( f \in \mathcal{E}_N \) being straightforward.

Combining Lemma 22 with the expansion just derived completes the proof of Lemma 20.

7. Remaining proofs for Theorem 7

7.1 Preliminary estimates. We first gather some technical bounds in the extended Model (28). Although not difficult, the stochastic expansions we need require extra care due to the presence of a boundary. We start with a standard variance estimate.

Lemma 23. For any real-valued function \( \varphi \),

\[
\text{Var}_{f_0} \left( \sum_{i=1}^{N} \varphi(X_{(i-1)^\dagger}) \right) \lesssim ND^{-1} \text{Var}_{f_0}(\varphi(X_0)),
\]

where the constant is uniform over (0, d, \( f_{\text{min}}, r, \delta, \beta \)).

Proof. This is a consequence of the spectral gap property for the Markov chain \( (X_0, X_D, \ldots, X_{ND}) \) that reads \( \|P_{f_0, D} \varphi\|_\infty \lesssim \exp(-\lambda_{f_0} D t) \|\varphi\|_{L^2} \). See e.g. [12] for a probabilistic argument for diffusions with boundaries, but other analytical approaches are obviously possible.

We next need a moment bound for the increments of the diffusion.

Lemma 24. For every \( \tau \geq 0 \) and \( p \geq 1 \), we have

\[
\mathbb{E}_f \left[ \sup_{s \leq t \leq \tau} |X_u - X_s|_p \right] \lesssim 2^{p-1} \left( (2\beta)^p + \|f\|_{|e^1|}^p (t-s)^p + c^p t^\beta \|f\|_\infty^p \right),
\]

where \( c_* \) is a universal constant (arising in the Burkholder-Davis-Gundy inequality) and \( \beta \) quantifies the size of the drift class \( \mathcal{B} \) defined in (29).
The proof is not difficult (see for instance Lions and Sznitman [37]) but requires some extra effort, due to the fact that we need to precisely track constants in \( p \) for later use in Bernstein’s inequalities. It is given in Appendix 10.3. Let
\[
\tau_{i,D} = \inf\{ t \geq 0, \; X_{t+(i-1)D} \in \partial D \}
\]
denote the hitting time of the boundary by the process \( X \).

**Lemma 25.** Let \( f_0 \in \mathcal{F} = \{ f \in \mathcal{F} : \| f \|_{C^\alpha} \leq r \} \) for \( \alpha = \alpha_d \) as in (7). Then
\[
\mathbb{P}_{f_0}(\tau_{i,D} \geq D, A_{i,D}) \lesssim \exp(-cD^{-1}),
\]
where the constants are uniform over \( (r, \delta, b) \).

The proof is given in Appendix 10.4. We will repeatedly use the decomposition
\[
(63) \quad X_{iD} - X_{(i-1)D} = b_{i,D} + \Sigma_{i,D} + L_{i,D},
\]
with
\[
b_{i,D} = \int_{(i-1)D}^{iD} b(\nabla f_0(X_s), X_s)ds, \quad \Sigma_{i,D} = \int_{(i-1)D}^{iD} \sqrt{2f_0(X_s)}dB_s, \quad L_{i,D} = \int_{(i-1)D}^{iD} n(X_s)d\ell|_s,
\]
jointly with the following bounds, for every \( p \geq 1, \)
\[
(64) \quad \|b_{i,D}\| \lesssim D, \quad \mathbb{E}_{f_0}[\|\Sigma_{i,D}\|^p|\mathcal{F}_{(i-1)D}] \lesssim D^{p/2}, \quad \mathbb{E}_{f_0}[\|L_{i,D}\|^p1_{A_{i,D}}] \lesssim D^{p/2}\exp(-cD^{-1}),
\]
which depend only on \( \|f_0\|_{C^1} \) and \( b \). The first bound is obvious, the second one stems from the Burkholder-Davis-Gundy inequality. For the third one, we rely on the following facts: first, writing \( L_{i,D} = (X_{iD} - X_{(i-1)D}) - b_{i,D} - \Sigma_{i,D} \) and using the first two bounds of (64) together with Lemma 24, we have
\[
\mathbb{E}_{f_0}[|L_{i,D}|^p] \lesssim D^{p/2}.
\]
Second, on \( A_{i,D} \cap \{ \tau_{i,D} \geq iD \} \), we have \( L_{i,D} = 0 \). Thus, by Cauchy-Schwarz’s inequality,
\[
\mathbb{E}_{f_0}[|L_{i,D}|^p1_{A_{i,D}}] \lesssim D^{p/2}\mathbb{P}_{f_0}(\tau_{i,D} \geq D, A_{i,D})^{1/2}
\]
and the third estimate in (64) then follows from Lemma 25.

### 7.2. Proofs of Propositions 15 and 17: approximating transition densities in small-time.

**Proof of Proposition 15.** We apply Lemma 20, establishing suitable bounds for the remainder terms.

**Step 1:** Consider first the term \( \sum_{i=1}^{N} \gamma_{f_0,f}(X_{(i-1)D}) \cdot (X_{iD} - X_{(i-1)D}) \) in the remainder of Lemma 20. It splits into three parts thanks to the decomposition (63) and we bound each term separately.

The drift term involving \( b_{i,D} \) is of order \( D \) by (64), hence the property \( \|\gamma_{f_0,f}\|_\infty \lesssim \varepsilon_{1,N} \) yields the crude variance bound \( N^2\varepsilon_{1,N}^2D^2 \) for the first term. For the martingale term, we have
\[
\text{Var}_{f_0}\left( \sum_{i=1}^{N} \gamma_{f_0,f}(X_{(i-1)D}) \cdot \Sigma_{i,D} \right) \leq \sum_{i=1}^{N} \|\gamma_{f_0,f}\|_\infty^2\mathbb{E}_{f_0}[\|\Sigma_{i,D}\|^2] \lesssim N\varepsilon_{1,N}^2D
\]
by the second estimate in (64). For the third term involving \( L_{i,D} \), using that \( \gamma_{f_0,f}(X_{(i-1)D}) \) vanishes on \( (A_{i,D})^c \), we have
\[
\text{Var}_{f_0}\left( \sum_{i=1}^{N} \gamma_{f_0,f}(X_{(i-1)D}) \cdot L_{i,D} \right) \lesssim N\sum_{i=1}^{N} \|\gamma_{f_0,f}\|_\infty^2\mathbb{E}_{f_0}[L_{i,D}^21_{A_{i,D}}] \lesssim N^2\varepsilon_{1,N}^2D\exp(-cD^{-1})
\]
by the third estimate in (64). We have thus established
\[(65)\quad \text{Var}_{f_0}\left(\sum_{i=1}^{N} \gamma_{f_0,f}(X_{(i-1)D}) \cdot (X_{iD} - X_{(i-1)D})\right) \lesssim N^2 \varepsilon_1 \varepsilon_2^2 (D + ND^2 + ND \exp(-cD^{-1})).\]

Step 2: We next consider the term \(\frac{1}{ND} \sum_{i=1}^{N} |X_{iD} - X_{(i-1)D}|^2 \zeta_{f_0,f}(X_{(i-1)D}) \cdot (X_{iD} - X_{(i-1)D}) \mathbf{1}_{A_{i,D}}\), where \(\zeta_{f_0,f} = \nabla(f^{-1} - f_0^{-1})\) satisfies \(\|\zeta_{f_0,f}\|_{\infty} \lesssim \varepsilon_1\) for \(f, f_0 \in \mathcal{F}'\). Using Itô’s formula, it splits into four parts according to the decomposition
\[(66)\quad |X_{iD} - X_{(i-1)D}|^2 = 2d f_0(X_{(i-1)D}) D + \bar{b}_{i,D} + \bar{\Sigma}_{i,D} + \bar{L}_{i,D},\]
with
\[(67)\quad \bar{b}_{i,D} = 2 \int_{(i-1)D}^{iD} (d(f_0(X_s) - f_0(X_{(i-1)D}))) + (X_s - X_{(i-1)D}) \cdot b(\nabla f_0(X_s), X_s) ds,\]
\[(67)\quad \bar{\Sigma}_{i,D} = 2 \int_{(i-1)D}^{iD} \sqrt{2f_0(X_s)}(X_s - X_{(i-1)D}) \cdot dB_s,\]
\[(67)\quad \bar{L}_{i,D} = 2 \int_{(i-1)D}^{iD} (X_s - X_{(i-1)D}) \cdot n(X_s) d\|s\|,\]
appended with the moment estimates
\[(68)\quad \mathbb{E}_{f_0}[|\bar{b}_{i,D}|^p] \lesssim D^{3p/2}, \quad \mathbb{E}_{f_0}[|\bar{\Sigma}_{i,D}|^p|\mathcal{F}_{(i-1)D}] \lesssim D^p, \quad \mathbb{E}_{f_0}[|\bar{L}_{i,D}|^p \mathbf{1}_{A_{i,D}}] \lesssim D^p \exp(-cD^{-1}),\]
as for (64). More precisely,
\[
\mathbb{E}_{f_0}[|\bar{b}_{i,D}|^p] \leq D^{p-1} \int_{(i-1)D}^{iD} \mathbb{E}_{f_0}[|d(f_0(X_s) - f_0(X_{(i-1)D}))) + (X_s - X_{(i-1)D}) \cdot b(\nabla f_0(X_s), X_s)|^p] ds
\leq D^p C_{d,\|f_0\|_t} \mathbb{E}_{f_0} \left(\sup_{(i-1)D \leq s \leq iD} |X_s - X_{(i-1)D}|^p\right)
\leq C_{p,d,\|f_0\|_t} D^{3p/2}
\]
by Jensen’s inequality and Lemma 24, with \(C_{p,\|f_0\|_t} = d\|f_0\|_t + b(1 + \|f_0\|_t + \text{diam}(O))\) and \(C_{p,d,\|f_0\|_t}\) equal to \(C_{p,\|f_0\|_t}\) times the constant in (61). For the martingale part, the Burkholder-Davis-Gundy inequality with constant \(C_p\) yields
\[
\mathbb{E}_{f_0}[|\bar{\Sigma}_{i,D}|^p|\mathcal{F}_{(i-1)D}] \leq C_p 2^{3p/2} \mathbb{E}_{f_0} \left(\int_{(i-1)D}^{iD} 2f_0(X_s)^{3/2} |X_s - X_{(i-1)D}|^2 ds\right)^{p/2} |\mathcal{F}_{(i-1)D}|
\leq C_{p} 2^p \|f_0\|_t^{3p/4} \mathbb{E}_{f_0} \left(\sup_{(i-1)D \leq s \leq iD} |X_s - X_{(i-1)D}|^p\right)
\leq C_p 2^{3p/2} \|f_0\|_t^{3p/4} C_{p,d,\|f_0\|_t} D^p,
\]
where we last used Lemma 24. The last bound in (68) follows exactly the same lines as the last estimate in (64), using now the bounds just established for \(\bar{b}_{i,D}\) and \(\bar{\Sigma}_{i,D}\) instead of those for \(b_{i,D}\) and \(\Sigma_{i,D}\), respectively.

We are now ready to handle the term \(\sum_{i=1}^{N} \frac{d}{dt} f_0(X_{(i-1)D}) \mathbf{1}_{A_{i,D}} \zeta_{f_0,f}(X_{(i-1)D}) \cdot (X_{iD} - X_{(i-1)D})\), exactly as in Step 1, substituting \(\zeta_{f_0,f}(X_{(i-1)D})\) by \(\frac{d}{dt} f_0(X_{(i-1)D}) \zeta_{f_0,f}(X_{(i-1)D}) \mathbf{1}_{A_{i,D}}\). It has the
same variance order as in (65). For the term involving the drift part $b_{i,D}$ we have

$$\text{Var}_{f_0}\left( \frac{1}{8D} \sum_{i=1}^{N} b_{i,D} \zeta_{f_0,f}(X_{(i-1)D}) \cdot (X_{iD} - X_{(i-1)D}) 1_{A_i,D} \right)$$

\[ \lesssim D^{-2} N \sum_{i=1}^{N} \| \zeta_{f_0,f} \|_{\infty}^2 \mathbb{E}_{f_0} \left[ \left| \tilde{b}_{i,D} |X_{iD} - X_{(i-1)D}| \right|^2 \right]. \]

and this yields the order $D^{-2} N^2 \varepsilon_1^2 N D^4 = N \varepsilon_N^2 \left( \frac{\varepsilon_1}{\varepsilon_N} N D^2 \right)$ by Cauchy-Schwarz’s inequality combined with (68) and Lemma 24 for controlling the term within the expectation. For the third term, we use the decomposition

$$\Sigma_{i,D} \zeta_{f_0,f}(X_{(i-1)D}) \cdot (X_{iD} - X_{(i-1)D}) 1_{A_i,D} = I + II + III,$$

with

$$I = \Sigma_{i,D} \zeta_{f_0,f}(X_{(i-1)D}) \cdot b_{i,D} 1_{A_i,D},$$

$$II = \Sigma_{i,D} \zeta_{f_0,f}(X_{(i-1)D}) \cdot \Sigma_{i,D} 1_{A_i,D},$$

$$III = \Sigma_{i,D} \zeta_{f_0,f}(X_{(i-1)D}) \cdot L_{i,D} 1_{A_i,D}.$$

For term $I$,

$$\text{Var}_{f_0}\left( \frac{1}{8D} \sum_{i=1}^{N} \Sigma_{i,D} \zeta_{f_0,f}(X_{(i-1)D}) \cdot b_{i,D} 1_{A_i,D} \right) \lesssim D^{-2} N \sum_{i=1}^{N} \| \zeta_{f_0,f} \|_{\infty}^2 \mathbb{E}_{f_0} \left[ \left| \Sigma_{i,D} \right|^2 |b_{i,D}|^2 \right]$$

and this yields the order $D^{-2} N^2 \varepsilon_1^2 N D^4$ by Cauchy-Schwarz’s inequality combined with (68) and Lemma 24 again. For term $II$, by Itô’s formula,

$$\Sigma_{i,D} \zeta_{f_0,f}(X_{(i-1)D}) \cdot \Sigma_{i,D} = \zeta_{f_0,f}(X_{(i-1)D}) \cdot M_{i,D}$$

\[ + 4 \zeta_{f_0,f}(X_{(i-1)D}) \cdot \int_{(i-1)D}^{iD} (X_s - X_{(i-1)D}) f_0(X_s) ds, \]

where $M_{i,D} = \int_{(i-1)D}^{iD} \sqrt{2f_0(X_s)} (\mathbb{E}_{f_0}[\Sigma_{i,D} |\mathcal{F}_s] + 2 \mathbb{E}_{f_0}[\Sigma_{i,D} |\mathcal{F}_s] \cdot (X_s - X_{(i-1)D})) dB_s$ is a martingale increment such that

$$\mathbb{E}_{f_0} \left[ \left| \zeta_{f_0,f}(X_{(i-1)D}) \cdot M_{i,D} \right|^2 \right] \lesssim \varepsilon_1^2 N D^3,$$

by applying repeatedly Cauchy-Schwarz’s inequality together with (64), (68) and Lemma 24, hence

$$\text{Var}_{f_0}\left( \frac{1}{8D} \sum_{i=1}^{N} \zeta_{f_0,f}(X_{(i-1)D}) \cdot M_{i,D} 1_{A_i,D} \right) = \frac{1}{64D^2} \sum_{i=1}^{N} \mathbb{E}_{f_0} \left[ \left| \zeta_{f_0,f}(X_{(i-1)D}) \cdot M_{i,D} \right|^2 \right] 1_{A_i,D}$$

and this term is of order $D^{-2} N^2 \varepsilon_1^2 N D^3 = N \varepsilon_N^2 \left( \frac{\varepsilon_1}{\varepsilon_N} N D^2 \right)^2 D$. Let $G(x,y) = \zeta_{f_0,f}(x) \cdot (y - x) f_0(y)$. For the second term in (69), by Itô’s formula,

$$\int_{(i-1)D}^{iD} \zeta_{f_0,f}(X_{(i-1)D}) \cdot (X_s - X_{(i-1)D}) f_0(X_s) ds = \tilde{b}_{i,D}(G) + \Sigma_{i,D}(G) + \mathcal{T}_{i,D}(G),$$
with
\[ T_{i,D}(G) = \int_{(i-1)D}^{iD} \int_{(i-1)D}^{s} \mathcal{L}_{f_0} G(X_{(i-1)D}, X_u) du ds, \]
\[ \Sigma_{i,D}(G) = \int_{(i-1)D}^{iD} \int_{(i-1)D}^{s} \nabla G(X_{(i-1)D}, X_u) \sqrt{2f_0(X_u)} \cdot dB_u ds, \]
(70) \[ \bar{T}_{i,D}(G) = \int_{(i-1)D}^{iD} \int_{(i-1)D}^{s} \nabla G(X_{(i-1)D}, X_u) \cdot n(X_u) d|\ell|_u ds. \]

In notation, the differential operators act on \( y \mapsto G(X_{(i-1)D}, y) \) and \( \mathcal{L}_{f_0} = b(\nabla f_0(x), x) \text{div} + f_0(x) \Delta \). The expansion is appended with the moment estimates

\[ E_{f_0}[|\bar{\Sigma}_{i,D}(G)|^p] \lesssim \varepsilon_{1,N}^p D^{2p}, \quad E_{f_0}[|\Sigma_{i,D}(G)|^p|\mathcal{F}_{(i-1)D}] \lesssim \varepsilon_{1,N}^p D^{3p/2}, \]
\[ E_{f_0}[|\bar{T}_{i,D}(G)|^p 1_{A_{i,D}}] \lesssim \varepsilon_{1,N}^p D^{3p/2} \exp(-cD^{-1}), \]

in the same way as before. The variance of \((4D)^{-1} \sum_{i=1}^N \bar{T}_{i,D}(G) 1_{A_{i,D}}\) is of order \( D^{-2} N^2 \varepsilon_{1,N}^2 D^4 \). Also, the \( \Sigma_{i,D}(G) \) are centered \( \mathcal{F}_{i,D} \)-increments hence

\[ \text{Var}_{f_0} \left( \frac{1}{4D} \sum_{i=1}^N \Sigma_{i,D}(G) 1_{A_{i,D}} \right) = \frac{1}{16D^2} \sum_{i=1}^N E_{f_0}[|\Sigma_{i,D}(G)|^2 1_{A_{i,D}}] \lesssim D^{-2} N^2 \varepsilon_{1,N}^2 D^3 \]

and this term is of order \( N \varepsilon_{1,N}^2 \left( \frac{4D}{N} \right)^2 D \). The variance of the term \((4D)^{-1} \sum_{i=1}^N \bar{T}_{i,D}(G) 1_{A_{i,D}}\) is of order \( D^{-2} N^2 \varepsilon_{1,N}^2 D^3 \exp(-cD^{-1}) \), and the term \( II \) is controlled. For the term \( III \), we simply have

\[ \text{Var}_{f_0} \left( \frac{1}{8D} \sum_{i=1}^N \Sigma_{i,D} \zeta_{f_0}(X_{(i-1)D}) \cdot L_{i,D} 1_{A_{i,D}} \right) \lesssim D^{-2} N \sum_{i=1}^N \varepsilon_{1,N}^2 E_{f_0}[|\Sigma_{i,D}|^2 |L_{i,D}|^2 1_{A_{i,D}}] \]

that yields the order \( N^2 \varepsilon_{1,N}^2 D^2 \exp(-cD^{-1}) \). Gathering all these estimates, we obtain that the variance of \( \frac{1}{8D} \sum_{i=1}^N (X_{i,D} - X_{(i-1)D})^2 \zeta_{f_0}(X_{(i-1)D}) \cdot (X_{i,D} - X_{(i-1)D}) 1_{A_{i,D}} \) is no bigger than the order established in (65).

**Step 3:** We finally control the remainder term in the expansion of Lemma 20. Define

\[ R_{f_0}^N = \sum_{i=1}^N \left( \| f - f_0\|_{C^2} D + \| f - f_0\|_{C^3} |X_{i,D} - X_{(i-1)D}| D + |X_{i,D} - X_{(i-1)D}|^2 D \right. \]
\[ + \| f - f_0\|_{C^4} |X_{i,D} - X_{(i-1)D}|^3 + \| f - f_0\|_{C^2} |X_{i,D} - X_{(i-1)D}|^3 \]
\[ + |X_{i,D} - X_{(i-1)D}|^4 \right)^2 r_{f_0,f}(X_{(i-1)D}, X_{i,D}). \]

By Lemma 24, the property \( f \in C_N \) and the fact that \( \| r_{f_0,f} \|_\infty \lesssim 1 \), we readily have

\[ \text{Var}_{f_0}(R_{f_0}^N) \lesssim N^2 (\varepsilon_{2,N}^2 D^2 + \varepsilon_{2,N}^3 D^3 + D^4 + \varepsilon_{2,N}^2 D^2 + \varepsilon_{3,N}^2 D^3 + D^4) \]
\[ \lesssim N \varepsilon_{2,N}^2 (\frac{4D}{N}^2 D^2 + (\frac{4D}{N})^2 N D^3 + N \varepsilon_{N}^{-2} D^4). \]
Step 4: Putting together the estimates established in Steps 1-3, using Lemma 20 and (30), the quantity in Proposition 15 is bounded by a multiple of

$$\text{Var}_{f_0}(\Lambda_{N,D}^N) + \text{Var}_{f_0}\left(\int_{\mathcal{E}_N} \sum_{i=1}^{N} \left[ \log \frac{\widetilde{p}_{f_0,D}(X_i^D)}{p_{f_0,D}(X_i^D)} - \frac{q_{f_0,D}(X_i^D)}{q_{f_0,D}(X_i^D)} \right] 1_{A_{i,D}} \nu(df) \right)$$

$$\lesssim \text{Var}_{f_0}(\Lambda_{N,D}^N) + \sup_{f \in \mathcal{E}_N} \text{Var}_{f_0}\left(\sum_{i=1}^{N} \left[ \log \frac{\widetilde{p}_{f_0,D}(X_i^D)}{p_{f_0,D}(X_i^D)} - \log \frac{q_{f_0,D}(X_i^D)}{q_{f_0,D}(X_i^D)} \right] \right)$$

$$\lesssim \text{Var}_{f_0}(\Lambda_{N,D}^N) + \mathcal{N}^2 \left( \left( \frac{\mathcal{N}}{\mathcal{N}} \right)^2 (D + ND^2) + \left( \frac{\mathcal{N}}{\mathcal{N}} \right)^2 ND^2 + \left( \frac{\mathcal{N}}{\mathcal{N}} \right)^2 ND^3 \right.$$ 

$$+ N \mathcal{N}^2 D^4 + \left( \frac{\mathcal{N}}{\mathcal{N}} \right)^2 ND \exp(-cD^{-1}) \right),$$

as required. □

**Proof of Proposition 17.** The proof follows similar, though easier, lines to that of Proposition 15. We thus provide only a sketch of the main bounds, matching Steps 1-4 for convenience.

Step 1: Consider first the term $\gamma_{f_0,f}(X_0) \cdot (X_D - X_0)$ in the expansion provided by Lemma 20, and where we can insert the term $1_{A_1,D}$ due to the support of $\gamma_{f_0,f}$. In the decomposition (63), the term $\gamma_{f_0,f}(X_0)\Sigma_{0,D}$ has $E_{f_0}$-expectation zero and so does not contribute. It follows that

$$E_{f_0}[\gamma_{f_0,f}(X_0) \cdot (X_D - X_0)] \leq \|\gamma_{f_0,f}\|_\infty (E_{f_0}[\|b_{0,D}\|] + E_{f_0}[L_{0,D}1_{A_1,D}]) \lesssim \mathcal{N} (D + D^{1/2} \exp(-cD^{-1})),$$

where we used the moment bounds (64).

Step 2: Write $\zeta_{f_0,f} = \nabla (f^{-1} - f_0^{-1})$ as before. In a similar way to Step 2 of the proof of Proposition 15, we have the decompositions

$$\frac{1}{8D} |X_D - X_0|^2 1_{A_1,D} = \frac{1}{8D} f_0(X_0) + \frac{1}{8D} \widetilde{b}_{1,D} 1_{A_1,D} + \frac{1}{8D} \Sigma_{1,D} 1_{A_1,D} + \frac{1}{8D} \widetilde{L}_{1,D} 1_{A_1,D}$$

$$\zeta_{f_0,f}(X_0) \cdot (X_D - X_0) = \zeta_{f_0,f}(X_0) \cdot 1_{A_1,D} + \zeta_{f_0,f}(X_0) \cdot \Sigma_{1,D} + \zeta_{f_0,f}(X_0) \cdot L_{1,D},$$

and note the term $E_{f_0}[\frac{1}{8D} |X_D - X_0|^2 \zeta_{f_0,f}(X_0) \cdot (X_D - X_0)]$ is the sum of all expectations of cross terms in the two expansions above. Using the bounds (64) and (68) and the martingale property of $\Sigma_{1,D}$ that ensures $E_{f_0}[\frac{1}{8D} f_0(X_0)\zeta_{f_0,f}(X_0) \cdot \Sigma_{1,D}] = 0$, we see by Cauchy-Schwarz’s inequality for instance that all the expectations of the cross terms are of order at most $(D + D^{1/2} \exp(-cD^{-1}))(\|\zeta_{f_0,f}\|_\infty = \mathcal{N} (D + D^{1/2} \exp(-cD^{-1})))$, except maybe for the term

$$\frac{1}{8D} E_{f_0}[\Sigma_{1,D} \zeta_{f_0,f}(X_0) \cdot \Sigma_{1,D}].$$

By (69), this term exactly equals

$$\frac{1}{4D} E_{f_0}[\zeta_{f_0,f}(X_0) \cdot \int_0^D (X_s - X_0) f_0(X_s) ds] = \frac{1}{4D} E_{f_0}[ \widetilde{b}_{1,D}(G) + \widetilde{L}_{1,D}(G)]$$

according to (70) with $G(x,y) = \zeta_{f_0,f}(x) \cdot (y-x) f_0(y)$, and this term finally has the right order since $E_{f_0}[\widetilde{b}_{1,D}(G)] \lesssim \mathcal{N} D^2$ and $E_{f_0}[\widetilde{L}_{1,D}(G) 1_{A_1,D}] \lesssim \mathcal{N} D^{3/2} \exp(-cD^{-1})$. 

Step 3: With the notation in the proof of Proposition 15, Step 3, it suffices to bound $E_{f_0}[R_{f_0,f}]$. By Lemma 24, the property $f \in \mathcal{E}_N$ and the fact that $\|r_{f_0,f}\|_\infty \lesssim 1$ again, we readily obtain

$$E_{f_0}[R_{f_0,f}^1] \lesssim \mathcal{N} D + \mathcal{N} D^{3/2} + D^2.$$
Step 4: Putting together the above bounds and keeping track of the leading order terms gives

\[
\sup_{f \in \mathcal{E}_N} \mathbb{E}_f \left[ \log \frac{\bar{p}_{f_0,D}(X^D_0)}{p_{f,D}(X^D_0)} 1_{A_{1,D}} \right] \\
\lesssim \sup_{f \in \mathcal{E}_N} \mathbb{E}_f \left[ \log \frac{q_{f_0,D}(X^D_0)}{q_{f,D}(X^D_0)} 1_{A_{1,D}} \right] \\
+ \varepsilon_N^2 \left( \frac{\varepsilon_N}{\varepsilon_N^{1/2}} D + \frac{\varepsilon_N}{\varepsilon_N^{1/2}} D + \frac{\varepsilon_N}{\varepsilon_N^{1/2}} D^{3/2} + \frac{\varepsilon_N}{\varepsilon_N^{1/2}} D^{1/2} \exp(-cD^{-1}) \right),
\]

which completes the proof of Proposition 17. \(\square\)

7.3. Proofs of Propositions 16 and 18: expectation and variance of the log-likelihood with proxy density. Recall that the proxy \(q_{f,D}\) of the transition density \(\bar{p}_{f,D}\) is given by

\[
q_{f,D}(x, y) = \frac{1}{(4\pi D f(x))^{d/2}} \exp \left( -\frac{|y-x|^2}{4D f(x)} \right),
\]

which is the density function of a \(N_d(x, 2D f(x) I_d)\) distribution, formally obtained by taking an Euler scheme without drift. Note that while \(q_{f,D}\) is defined on \(\mathbb{R}^d \times \mathbb{R}^d\), it will be evaluated at \((X_{(i-1),D}, X_{i,D})\), which lies in \(\mathcal{O} \times \mathcal{O}\) almost surely.

**Proof of Proposition 16.** Step 1: We look for a simple expansion of the approximate log-likelihood with the proxy. Write

\[
\log \frac{q_{f,D}(x, y)}{q_{f_0,D}(x, y)} = \frac{d}{2} \log \frac{f_0(x)}{f(x)} - \frac{1}{4D} \left( \frac{1}{f(x)} - \frac{1}{f_0(x)} \right) |y-x|^2 \\
= \frac{d}{2} \left( \log \frac{f_0(x)}{f(x)} - \left( \frac{1}{f_0(x)} - \frac{1}{f(x)} \right) \frac{|y-x|^2}{2D} \right).
\]

Recall the expansion (66) and (67) in the proof of Proposition 15 that takes the form

\[
|X_{i,D} - X_{(i-1),D}|^2 = 2d f_0(X_{(i-1),D})D + b_{i,D} + \bar{\Sigma}_{i,D} + \bar{L}_{i,D}
\]

for appropriate drift, diffusion and boundary remainder terms \(b_{i,D}, \bar{\Sigma}_{i,D}\) and \(\bar{L}_{i,D}\), respectively. Therefore, setting \(\xi_{f_0,f} = \frac{1}{f} - \frac{1}{f_0}\), we obtain

\[
\frac{d}{2} \log \frac{q_{f,D}(X^D_i)}{q_{f_0,D}(X^D_i)} = \frac{d}{2} \log \frac{f_0(X_{(i-1),D})}{f(X_{(i-1),D})} - \left( \frac{f_0(X_{(i-1),D})}{f(X_{(i-1),D})} - 1 \right) \\
+ \frac{1}{2dD} \xi_{f_0,f}(X_{(i-1),D})(b_{i,D} + \bar{\Sigma}_{i,D} + \bar{L}_{i,D}).
\]

Since \(|\log \kappa - (\kappa - 1)| \leq C(\kappa - 1)^2\) in a neighbourhood of \(\kappa = 1\), the property \(\|f - f_0\|_\infty \leq \varepsilon_N\) and \(f \geq f_{\text{min}}\) ensures

\[
\|\log \frac{f_0}{f} - \left( \frac{f_0}{f} - 1 \right)\|_\infty \lesssim \varepsilon_N^2.
\]

By Lemma 23, this entails

\[
\text{Var}_{f_0} \left( \sum_{i=1}^N \left( \log \frac{f_0(X_{(i-1),D})}{f(X_{(i-1),D})} - \left( \frac{f_0(X_{(i-1),D})}{f(X_{(i-1),D})} - 1 \right) \right) 1_{A_{i,D}} \right) \lesssim ND^{-1} \varepsilon_N^2.
\]
Step 2: We next consider the term $\sum_{i=1}^N \frac{1}{2dD} \xi_{f_0}(X_{(i-1)D}) \tilde{b}_{i,D} \mathbf{1}_{A_{i,D}}$ and proceed similarly to Step 2 in the proof of Proposition 15 above. Define $\tilde{G}(x, y) = 2d(f_0(x) - f_0(y)) + 2b(\nabla f_0(y), y) \cdot (x - y)$ so that

$$\tilde{b}_{i,D} = \int_{(i-1)D}^{iD} \tilde{G}(X_{(i-1)D}, X_s)ds = \tilde{b}_{i,D}(\tilde{G}) + \Sigma_{i,D}(\tilde{G}) + \mathcal{I}_{i,D}(\tilde{G}),$$

applying Itô’s formula again, where

$$\begin{align*}
\mathbb{E}_{f_0}[\tilde{b}_{i,D}(\tilde{G})|^p] &\lesssim D^{2p}, \quad \mathbb{E}_{f_0}[|\Sigma_{i,D}(\tilde{G})|^p|\mathcal{F}_{(i-1)D}] \lesssim D^{3p/2}, \\
\mathbb{E}_{f_0}[|\mathcal{I}_{i,D}(\tilde{G})|^p|^p\mathbf{1}_{A_{i,D}}] &\lesssim D^{3p/2} \exp(-cD^{-1})
\end{align*}$$

in the same way as before, uniformly in $b \in B$.

The variance of $\sum_{i=1}^N \frac{1}{2dD} \xi_{f_0}(X_{(i-1)D})(\tilde{b}_{i,D}(\tilde{G}) + r_{i,D}) \mathbf{1}_{A_{i,D}}$ is of order $D^{-2}N^2\varepsilon_N^2D^4$. Also, the $\Sigma_{i,D}(\tilde{G})$ are centered $\mathcal{F}_{i,D}$-increments hence

$$\begin{align*}
\operatorname{Var}_{f_0} \left( \frac{1}{2dD} \sum_{i=1}^N \xi_{f_0}(X_{(i-1)D}) \Sigma_{i,D}(\tilde{G}) \mathbf{1}_{A_{i,D}} \right) &\lesssim \frac{1}{4d^2D^2} \sum_{i=1}^N \mathbb{E}_{f_0}[|\xi_{f_0}(X_{(i-1)D})\Sigma_{i,D}|^2\mathbf{1}_{A_{i,D}}] \\
&\lesssim D^{-2}N\varepsilon_N^2D^3
\end{align*}$$

and this term is of order $N\varepsilon_N^2D$. The variance of $(2dD)^{-1} \sum_{i=1}^N \xi_{f_0}(X_{(i-1)D}) \cdot \mathcal{I}_{i,D}(\tilde{G}) \mathbf{1}_{A_{i,D}}$ is of order $D^{-2}N^2\varepsilon_N^2D^3 \exp(-cD^{-1})$. Gathering all these estimates, we obtain

$$\begin{align*}
\operatorname{Var}_{f_0} \left( \frac{1}{2dD} \sum_{i=1}^N \xi_{f_0}(X_{(i-1)D}) \tilde{b}_{i,D} \mathbf{1}_{A_{i,D}} \right) &\lesssim N\varepsilon_N^2 (ND^2 + D + ND \exp(-cD^{-1})).
\end{align*}$$

Step 3: We now consider the martingale term $\sum_{i=1}^N \frac{1}{2dD} \xi_{f_0}(X_{(i-1)D}) \Sigma_{i,D} \mathbf{1}_{A_{i,D}}$. We have

$$\begin{align*}
\operatorname{Var}_{f_0} \left( \frac{1}{2dD} \sum_{i=1}^N \xi_{f_0}(X_{(i-1)D}) \Sigma_{i,D} \mathbf{1}_{A_{i,D}} \right) &\lesssim \frac{1}{4d^2D} \sum_{i=1}^N \mathbb{E}_{f_0}[|\xi_{f_0}(X_{(i-1)D})\Sigma_{i,D}|^2\mathbf{1}_{A_{i,D}}] \\
&\lesssim D^{-2}N\varepsilon_N^2D^2
\end{align*}$$

and this term has the right order $N\varepsilon_N^2$.

Step 4: We finally consider the remainder term $\sum_{i=1}^N \frac{1}{2dD} \xi_{f_0}(X_{(i-1)D}) \mathcal{I}_{i,D} \mathbf{1}_{A_{i,D}}$ and conclude. We have

$$\begin{align*}
\operatorname{Var}_{f_0} \left( \frac{1}{2dD} \sum_{i=1}^N \xi_{f_0}(X_{(i-1)D}) \mathcal{I}_{i,D} \mathbf{1}_{A_{i,D}} \right) &\lesssim D^{-2}N\sum_{i=1}^N \|\xi_{f_0}\|_{\infty}^2 \mathbb{E}_{f_0}[|\mathcal{I}_{i,D} \mathbf{1}_{A_{i,D}}|^2] \\
&\lesssim N^2\varepsilon_N^2 \exp(-cD^{-1}).
\end{align*}$$

Gathering the estimates from Steps 1-4 completes the proof of Proposition 16. □

Proof of Proposition 18. The proof follows similar, though easier, lines to that of the proof of Proposition 16. We thus provide only a sketch of the main bounds, matching Steps 1-4 for convenience.
Step 1: We again use the expansion (71) that yields
\[
\frac{2}{d} \log \frac{q_{f,D}(X_i^D)}{q_{f_0,D}(X_i^D)} = \log \frac{f_0(X_{i-1,D})}{f(X_{i-1,D})} - \left( \frac{f_0(X_{i-1,D})}{f(X_{i-1,D})} - 1 \right) + \frac{1}{2dD} \xi_{f_0,f}(X_{i-1,D})(\tilde{b}_{i,D} + \tilde{\Sigma}_{i,D} + \tilde{L}_{i,D}).
\]

The main term is bounded above as before:
\[
\| \log \frac{f_0}{f} - \left( \frac{f_0}{f} - 1 \right) \|_\infty \lesssim \varepsilon^2_N,
\]
as follows from \(|\log \kappa - (\kappa - 1)| \leq C(\kappa - 1)^2\) in a neighbourhood of \(\kappa = 1\), together with the properties \(\|f - f_0\|_\infty \leq \varepsilon_N\) and \(f \geq f_{\min}\).

Step 2: By using the refinement of Step 2 in the proof of Proposition 16, we have
\[
\tilde{b}_{i,D} = \tilde{b}_{i,D}(G) + \tilde{\Sigma}_{i,D}(G) + \tilde{T}_{i,D}(G),
\]
where
\[
\mathbb{E}_{f_0}[|\tilde{b}_{i,D}(G)|^\alpha] \lesssim D^{2p}, \quad \mathbb{E}_{f_0}[|\tilde{T}_{i,D}(G)|^\alpha 1_{A_{i,D}}] \lesssim D^{3p/2} \exp(-cD^{-1}),
\]
and \(\tilde{\Sigma}_{i,D}(G)\) is a \(\mathcal{F}_{i,D}\)-martingale increment. Therefore,
\[
\mathbb{E}_{f_0} \left[ \frac{1}{2dD} \xi_{f_0,f}(X_{i-1,D}) \tilde{b}_{i,D} 1_{A_{i,D}} \right] \lesssim \varepsilon_N (D + D^{1/2} \exp(-cD^{-1})).
\]

Step 3: Since \(\tilde{\Sigma}_{i,D}\) is a \(\mathcal{F}_{i,D}\)-increment, we simply have
\[
\mathbb{E}_{f_0} \left[ \frac{1}{2dD} \xi_{f_0,f}(X_{i-1,D}) \tilde{\Sigma}_{i,D} 1_{A_{i,D}} \right] = 0.
\]

Step 4: We finally have
\[
\mathbb{E}_{f_0} \left[ \left| \frac{1}{2dD} \xi_{f_0,f}(X_{i-1,D}) \tilde{L}_{i,D} 1_{A_{i,D}} \right| \right] \lesssim \varepsilon_N D^{1/2} \exp(cD^{-1}).
\]

Gathering the estimates from Steps 1-4 completes the proof of Proposition 18.

\[\blacksquare\]

8. PROOF OF THEOREM 9: AN EXPONENTIAL INEQUALITY FOR A LEAST SQUARES TYPE ESTIMATOR

8.1. Risk decomposition. Recall from (24) that \(P_{f,j}f = 1 + P_j [f - 1]\) for \(f \in \mathcal{F}\), where \(P_j\) is the wavelet projection onto the space \(V_j\) in (22) used to reconstruct functions with support in \(O_0\), such as \(f - 1\) when \(f \in \mathcal{F}\). We will decompose \(\|\tilde{f}_N - P_{f,j}f\|_2\) into martingale, bias and remainder terms that we control on the event
\[
B_N = \{(1 - \kappa) ||g||_2^2 \leq |g|_N^2 \leq (1 + \kappa) ||g||_2^2 \text{ for all } g \in V_j\},
\]
for some fixed \(0 < \kappa < 1\), and where
\[
|g|_N^2 = \frac{1}{N} \sum_{i=1}^N g(X_{i-1,D})^2 1_{A_{i,D}}, \quad A_{i,D} = \{X_{i-1,D} \in O_0^\delta\},
\]
denotes a random empirical semi-norm for every continuous function on the \(\delta/2\)-enlargement \(O_0^\delta\) of \(O_0\). By classical concentration techniques, we prove in Appendix 10.6 the following result.
Lemma 26. Suppose that $2^J \to \infty$ and $2^{Jd} = o(\sqrt{ND})$ as $N \to \infty$. Then for every $0 < \kappa < 1$, as $N \to \infty$,

$$\sup_{f \in \mathcal{F}} \mathbb{P}_f(B_N^f) \to 0.$$ 

By Lemma 26 we have $\sup_{f \in \mathcal{F}} \mathbb{P}_f(B_N^f) \to 0$ as $N \to \infty$ for every $0 < \kappa < 1$ under the theorem hypotheses, so that we may further restrict to working on $B_N$. We have under $P_f$

(73) $$Y_{i,D} = (2d)^{-1}D^{-1}|X_{i,D} - X_{(i-1)D}|^2 = f(X_{(i-1)D}) + R_{i,D},$$

with

(74) $$R_{i,D} = (2d)^{-1}D^{-1}(\bar{b}_{i,D} + \bar{\Sigma}_{i,D} + \bar{L}_{i,D}),$$

where we recall the above decomposition from (66)-(67) but with $f_0$ replaced by $f$. Let

$$\Gamma_N(g) = \frac{1}{N} \sum_{i=1}^{N} (Y_{i,D} - 1 - g(X_{(i-1)D}))^2 1_{A_{i,D}}$$

denote the normalized objective function defining our least squares estimator (25), using in particular that $g(X_{(i-1)D}) = 0$ on $(A_{i,D})^c$ for all $g \in \mathcal{V}_J$. By (73), for any function $g$,

(75) $$\Gamma_N(g) - \Gamma_N(f - 1) = |1 + g - f|_N^2 + \frac{2}{N} \sum_{i=1}^{N} (f - 1 - g(X_{(i-1)D}))R_{i,D} 1_{A_{i,D}}.$$ 

Since $\Gamma_N(\hat{g}_N) = \inf_{g \in \mathcal{V}_J} \Gamma_N(g)$ by construction, we have $\Gamma_N(\hat{g}_N) - \Gamma_N(f - 1) \leq \Gamma_N(P_J[f - 1]) - \Gamma_N(f - 1)$. Substituting (75) into both sides of this inequality with $g = \hat{g}_N$ and $g = P_J[f - 1]$, respectively, then yields (with $\hat{f}_N = \hat{g}_N + 1$)

$$|\hat{f}_N - f|_N^2 + 2N^{-1} \sum_{i=1}^{N} (f - \hat{f}_N)(X_{(i-1)D})R_{i,D} 1_{A_{i,D}}$$

$$\leq |1 + P_J[f - 1] - f|_N^2 + 2N^{-1} \sum_{i=1}^{N} (f - 1 - P_J[f - 1])(X_{(i-1)D})R_{i,D} 1_{A_{i,D}},$$

or equivalently

(76) $$|\hat{f}_N - f|_N^2 \leq |P_J[f - 1] - (f - 1)|_N^2 + 2N^{-1} \sum_{i=1}^{N} (\hat{f}_N - 1 - P_J[f - 1])(X_{(i-1)D})R_{i,D} 1_{A_{i,D}}.$$
Taking we finally obtain the following risk decomposition:

\[
\frac{2}{N} \sum_{i=1}^{N} (\tilde{g}_N - P_j[f - 1])(X_{(i-1)D}) \mathcal{R}_{i,D} \mathbf{1}_{A_i,D} \\
\leq 2\|\tilde{g}_N - P_j[f - 1]\|_2 \sup_{g \in V_J : \|g\|_2 \leq 1} \frac{1}{N} \sum_{i=1}^{N} g(X_{(i-1)D}) \mathcal{R}_{i,D} \mathbf{1}_{A_i,D} \\
\leq \rho\|\tilde{g}_N - P_j[f - 1]\|_2^2 + \rho^{-1} \left( \sup_{g \in V_J : \|g\|_2 \leq 1} \frac{1}{N} \sum_{i=1}^{N} g(X_{(i-1)D}) \mathcal{R}_{i,D} \mathbf{1}_{A_i,D} \right)^2 \\
\leq (1 - \kappa)^{-1} \rho\|\tilde{g}_N - P_j[f - 1]\|_N^2 + \rho^{-1} \left( \sup_{g \in V_J : \|g\|_2 \leq 1} \frac{1}{N} \sum_{i=1}^{N} g(X_{(i-1)D}) \mathcal{R}_{i,D} \mathbf{1}_{A_i,D} \right)^2.
\]

Substituting this last display into (76) then gives

\[
|\tilde{f}_N - f|_N^2 \leq |P_j[f - 1] - (f - 1)|_N^2 + (1 - \kappa)^{-1} \rho|\tilde{g}_N - P_j[f - 1]|_N^2 \\
+ \rho^{-1} \left( \sup_{g \in V_J : \|g\|_2 \leq 1} \frac{1}{N} \sum_{i=1}^{N} g(X_{(i-1)D}) \mathcal{R}_{i,D} \mathbf{1}_{A_i,D} \right)^2.
\]

Using that \(\sqrt{a + b} \leq \sqrt{a} + \sqrt{b}\) for \(a, b > 0\), this implies

\[
|\tilde{f}_N - P_j[f - 1]|_N \leq |\tilde{f}_N - f|_N + |f - 1 - P_j[f - 1]|_N \\
\leq 2|f - 1 - P_j[f - 1]|_N + (1 - \kappa)^{-1/2} \rho^{1/2} |\tilde{f}_N - 1 - P_j[f - 1]|_N \\
+ \rho^{-1/2} \left( \sup_{g \in V_J : \|g\|_2 \leq 1} \frac{1}{N} \sum_{i=1}^{N} g(X_{(i-1)D}) \mathcal{R}_{i,D} \mathbf{1}_{A_i,D} \right).
\]

Collecting the \(|\tilde{f}_N - 1 - P_j[f - 1]|_N\) terms on the left-hand side thus yields the risk decomposition

\[
\left(1 - \sqrt{\frac{\rho}{1 - \kappa}}\right) |\tilde{f}_N - 1 - P_j[f - 1]|_N \\
\leq 2|f - 1 - P_j[f - 1]|_N + \rho^{-1/2} \left( \sup_{g \in V_J : \|g\|_2 \leq 1} \frac{1}{N} \sum_{i=1}^{N} g(X_{(i-1)D}) \mathcal{R}_{i,D} \mathbf{1}_{A_i,D} \right).
\]

Taking \(\rho > 0\) small enough that \(\rho / (1 - \kappa) < 1\) and using that \(|\tilde{f}_N - 1 - P_j[f - 1]|_N \geq \sqrt{1 - \kappa} |\tilde{f}_N - 1 - P_j[f - 1]|_2\) on \(\mathcal{B}_N\), we then obtain that on \(\mathcal{B}_N\),

\[
C^{-1} |\tilde{f}_N - 1 - P_j[f - 1]|_2 \leq 2|f - 1 - P_j[f - 1]|_N + \rho^{-1/2} \left( \sup_{g \in V_J : \|g\|_2 \leq 1} \frac{1}{N} \sum_{i=1}^{N} g(X_{(i-1)D}) \mathcal{R}_{i,D} \mathbf{1}_{A_i,D} \right),
\]

where \(C^{-1} = \sqrt{1 - \kappa} (1 - \sqrt{\rho / (1 - \kappa)}) = \sqrt{1 - \kappa} - \sqrt{\rho} > 0\). Recalling that \(P_J f = 1 + P_J[f - 1]\), we finally obtain the following risk decomposition:

\[
P_f (\|\tilde{f}_N - P_J f\|_2 \geq K\xi_N, \mathcal{B}_N) \leq P_f (|f - 1 - P_j[f - 1]|_N \geq K_1\xi_N, \mathcal{B}_N) \\
+ P_f \left( \sup_{g \in V_J : \|g\|_2 \leq 1} \sum_{i=1}^{N} g(X_{(i-1)D}) \mathcal{R}_{i,D} \mathbf{1}_{A_i,D} \geq K_2 N\xi_N, \mathcal{B}_N \right)
\]

(77)
where the constants $K_i = C_i K$ for constants $C_i$ depending only on $\kappa$ and $\rho_i$ which are henceforth considered fixed. It therefore suffices to prove that each term on the right-hand side of (77) is bounded by a multiple of $e^{-L N \epsilon_N^2}$ for arbitrary fixed $L > 0$ and large enough $K = K(L)$.

8.2. **Bias term.** We consider here the first term in (77), which is a bias term with the randomness only entering from the design in the random empirical semi-norm $|\cdot|_N$. Write $g_J = f - 1 - P_J[f - 1]$ and

$$Z_N(g_J) = |g_J|^2_N - \|g_J\|^2_F = \frac{1}{N} \sum_{i=1}^N \left( g_J(X_{i-1}D)^2 - E[f](X_{i-1}D)^2 \right),$$

since $E[f](g_J(X_{i-1}D)^2) = \|g_J\|^2_F$. The variance satisfies

$$\text{Var}[g_J(X_{i-1}D)^2] \leq E[f](g_J(X_{i-1}D)^4) = \|g_J\|^4_L,$$

while $|g_J(x)^2 - E[f](g_J(X_{i-1}D)^2)| \leq 2\|g_J\|^2_{\infty}$. Since $(X_0, X_D, \ldots, X_{ND})$ is a stationary reversible Markov chain whose spectral gap is lower bounded by $rD$ by (9), Theorem 3.3 of [44] (cf. (3.21)) yields the following Bernstein-type inequality:

$$P_f(|Z_N(g_J)| \geq t) \leq 2 \exp \left( -\frac{rDt^2}{4N\|g_J\|^4_L + 20\|g_J\|^2_{\infty}t} \right)$$

for all $t > 0$. Setting $t = MN\epsilon_N^2$ then gives

$$P_f(|Z_N(g_J)| \geq M\epsilon_N^2) \leq 2 \exp \left( -\frac{rDM^2N\epsilon_N^4}{4\|g_J\|^4_L + 20M\|g_J\|^2_{\infty}\epsilon_N^2} \right).$$

By $L^p$ interpolation, $\|g_J\|_L^4 \leq \|g_J\|^4_L^2 \|g_J\|^2_{\infty}$, Using this and rearranging, one gets that the right-hand side is smaller than $2e^{-L N \epsilon_N^2}$ if

$$4L\|g_J\|^2_L \|g_J\|^2_{\infty} \epsilon_N^2 + 20LM\|g_J\|^2_{\infty} \epsilon_N^2 \epsilon_N^2 \leq rDM^2\epsilon_N^4.$$

But for any $f \in \mathcal{F}_N$ contained in the set defined in the theorem statement, the left side above is bounded by a multiple of $R_0^2\epsilon_N^2 \epsilon_N^2 = O(D\epsilon_N^2)$ under the assumed hypothesis $R_0^2\epsilon_N^2 \leq D\epsilon_N^2$. Since also $r = r(f_{\min}, 0)$ by (9), this verifies the condition in the last display. In summary, we have shown that for any $L > 0$, there exists $M = M(L, r) > 0$ large enough such that

$$\sup_{f \in \mathcal{F}_N} P_f(|f - 1 - P_J[f - 1]|_N^2 \geq \|f - 1 - P_J[f - 1]\|^2 + M\epsilon_N^2) \leq 2e^{-L N \epsilon_N^2},$$

under the theorem hypotheses.

8.3. **Deviation of the remainder term.** We now consider the second term in (77) involving $\mathcal{R}_{i,D}$. By a union bound, up to a modification of the constants, it suffices to prove the deviation for each term in the decomposition (74).

**Step 1:** We postpone the term involving the drift $\tilde{b}_{i,D}$ to Step 3 and rather first control the term involving $\Sigma_{i,D}$ in (74). We will prove

$$P_f \left( \sup_{g \in \mathcal{F}_N, \|g\| \leq 1} |\overline{Z}_N(g)| \geq MN\epsilon_N, B_N \right) \leq e^{-L N \epsilon_N^2},$$

for sufficiently large $M$, where

$$\overline{Z}_N(g) = D^{-1} \sum_{i=1}^N g(X_{i-1}D)\Sigma_{i,D}1_{A_{i,D}}.$$
Define
\[ \mathbb{P}_{B_N,f} = \mathbb{P}_f(\cdot | \mathbb{B}_N) = \mathbb{P}_f(\mathbb{B}_N)^{-1}\mathbb{P}_f(\cdot \cap \mathbb{B}_N). \]
Since \( \mathbb{P}_f(\mathbb{B}_N) \to 1 \) uniformly in \( f \) by Lemma 26, we have \( \mathbb{P}_f(\cdot \cap \mathbb{B}_N) \leq \mathbb{P}_{B_N,f} \) for \( N \) large enough. It thus suffices to establish (78) with \( \mathbb{P}_{B_N,f} \) instead of \( \mathbb{P}_f \). We prove a Bernstein inequality for the increments of the process \( (\bar{Z}_N(g) : g \in V_f) \) and conclude using a chaining argument under \( \mathbb{P}_{B_N,f} \). To that end, we need the following Bernstein inequality, see e.g. [45, 21].

**Lemma 27.** Let \((M_n)_{n \geq 0} \) be a \((\mathcal{G}_n)_{n \geq 0}\)-martingale with \( M_0 = 0 \) and let \((M)_n = \sum_{i=1}^n \mathbb{E}[|M_i - M_{i-1}|^2 \mid \mathcal{G}_{i-1}] \) denotes its predictable quadratic variation. If for some \( c > 0 \),
\[ \sum_{i=1}^n \mathbb{E}[|M_i - M_{i-1}|^p \mid \mathcal{G}_{i-1}] \leq \frac{c^{p-2}p!}{2} (M)_n \quad \text{for every } p \geq 2, \]
then for every \( t, y > 0 \),
\[ \mathbb{P}(M_n \geq t, (M)_n \leq y) \leq \exp\left( -\frac{t^2}{2(y + ct)} \right). \]

We will apply Lemma 27 to the \( \mathcal{G}_n \)-martingale \( M_n = \bar{Z}_N(g) = D^{-1} \sum_{i=1}^n g(X_{(i-1)D}) \bar{\Sigma}_i D \mathbf{1}_{A_{i,D}}, \)
with \( \bar{\Sigma}_i = \sigma(X_{iD} : 0 \leq i \leq n) \). First, applying the Burkholder-Davis-Gundy inequality with best constant \( c^{p/2}p^{p/2} \) (see e.g. [6]), we have for all \( p \geq 1 \):
\[ \mathbb{E}_f \left[ |D^{-1}\bar{\Sigma}_i D \mathbf{1}_{A_{i,D}}|^p \mid \mathcal{F}_{(i-1)D} \right] \]
\[ = D^{-p} \mathbb{E}_f \left[ \int_{(i-1)D}^{iD} \sqrt{2} f(X_s)(X_s - X_{(i-1)D}) \cdot dB_s \mid \mathcal{F}_{(i-1)D} \right] \mathbf{1}_{A_{i,D}} \]
\[ \leq D^{-p} (2\|f\|_\infty c_{*,p})^{p/2} \mathbb{E}_f \left[ \int_{(i-1)D}^{iD} |X_s - X_{(i-1)D}|^2 |dB_s|^p \mid \mathcal{F}_{(i-1)D} \right] \]
\[ \leq (D^{-1}2\|f\|_\infty c_{*,p})^{p/2} \max_{1 \leq i \leq d} \mathbb{E}_f \left[ \sup_{(i-1)D \leq s \leq iD} |X_s - X_{(i-1)D}|^p \mid \mathcal{F}_{(i-1)D} \right] \]
\[ \leq (2\|f\|_\infty c_{*,p})^{p/2} 2^{p-1} (\|f\|_p)^p D^{p/2} + (c_{*,p})^{p/2} \|f\|_\infty^p \]
\[ \leq (C\|f\|_{\ell^2}^{3/2})^{p/2} p!, \]
for some \( C > 0 \) that only depends on \( d \), since \( D \to 0 \) and where we used Lemma 24 to obtain the second last inequality together with \( p^p \leq (C')^{p}p! \) for some universal constant \( C' \geq 1 \). Next, we claim that the following lower bound holds
\[ \mathbb{E}_f \left[ (D^{-1}\bar{\Sigma}_i D)^2 \mathbf{1}_{A_{i,D}} \mid \mathcal{F}_{(i-1)D} \right] \geq d_{\min}^2 - O(D^{1/2}). \]
Assuming for now that (79) is true, for \( D \to 0 \) small enough,
\[ \sum_{i=1}^n |g(X_{(i-1)D})|^p \leq \|g\|_{\ell^\infty}^p \sum_{i=1}^n |g(X_{(i-1)D})|^2 \frac{2}{d_{\min}} \mathbb{E}_f \left[ (D^{-1}\bar{\Sigma}_i D)^2 \mathbf{1}_{A_{i,D}} \mid \mathcal{F}_{(i-1)D} \right] \]
\[ = \frac{2}{d_{\min}} \|g\|_{\ell^\infty}^{p-2} (M)_n. \]
Applying Lemma 27 at $n$ for any $\varepsilon$ Setting $u$ Moreover, recalling that Using that upon taking $M \geq m$ We may therefore apply the generic chaining bound in Lemma 32 in Section 10.5 below with $D$ for small enough $D$. The condition of Lemma 27 therefore holds with 

$$c = C_{\|f\|_{C^1}} \max (1, 4C^2 \|f\|_{C^1}^2 dB^{-1} f_{\text{min}}^{-2}) C \|f\|_{C^1}^{3/2} \|g\|_\infty.$$ 

Moreover, recalling that $g \in V_J$ in (77) and using the bound (68), on the event $B_N$,

$$\langle M \rangle_N = \frac{1}{D^2} \sum_{i=1}^{N} g(X(i-1)_D)^2 E_f[\tilde{S}^2_{i,D}|\mathcal{F}(i-1)_D][A_{i,D} \leq C_{\|f\|_{C^1}} N |g|_N^2 \leq C_{\|f\|_{C^1}} (1 + \kappa)N \|g\|_2^2.$$ 

Applying Lemma 27 at $n = N$ with $y = C_{\|f\|_{C^1}} (1 + \kappa)N \|g\|_2^2$, we finally obtain for all $t > 0$,

$$\mathbb{P}_{B_N,f}(\{ \bar{Z}_N(g) \geq t \}) \leq 2\mathbb{P}_{f}(\{ |M_N| \geq t, B_N \}) \leq 2\mathbb{P}_{f}(\{ |M_N| \geq t, \langle M \rangle_N \leq C_{\|f\|_{C^1}} N \|g|_N^2 \}) \leq 4 \exp \left( -\frac{t^2}{2(C_{\|f\|_{C^1}} N \|g|_N^2 + C_{\|f\|_{C^1}} f_{\text{min}} \|g\|_\infty t) \right).$$

Using that $\|g\|_\infty \leq C2^{Jd/2}\|g\|_2$ for $g \in V_J$, we have that for all $g, g' \in V_J$ and $t > 0$,

$$\mathbb{P}_{B_N,f}(\{ \bar{Z}_N(g) - \bar{Z}_N(g') \geq t \}) \leq 4 \exp \left( -\frac{Ct^2}{N \|g - g'|_2^2 + 2^{Jd/2} \|g - g'|_2^4} \right).$$

We may therefore apply the generic chaining bound in Lemma 32 in Section 10.5 below with $m = \dim(V_J) = O(2^{Jd})$, $\|g\|_2 = \sup_{g, h \in V_J} \|g - h\|_2 \leq 2$, $\alpha^2 = N$, $\beta = 2^{Jd/2}$ to obtain that for all $u \geq 1$,

$$\mathbb{P}_{B_N,f}(\sup_{g \in V_J: \|g\|_2 \leq 1} \bar{Z}_N(g) \geq C_{\|f\|_{C^1}, f_{\text{min}}}(2^{3Jd/2} + 2^{Jd/2}N^{1/2} + 2^{Jd/2}u + N^{1/2} \sqrt{u}) \leq e^{-u}.$$ 

Setting $u = LN\varepsilon_N^2$ with $L > 0$ then gives

$$\mathbb{P}_{B_N,f}(\sup_{g \in V_J: \|g\|_2 \leq 1} \bar{Z}_N(g) \geq MN\xi_N) \leq e^{-LN\varepsilon_N^2}$$

for any $\varepsilon_N, \xi_N, 2^J$ satisfying

(80) \hspace{1cm} 2^{3Jd/2}N^{-1} + 2^{Jd/2}N^{-1/2} + 2^{Jd/2}\varepsilon_N^2 + \varepsilon_N \lesssim \xi_N

upon taking $M = M(L, \|f\|_{C^1}, f_{\text{min}})$ large enough. This establishes (78), so that we have the required exponential inequality in (77) for the term $(dD)^{-1}\tilde{S}_{i,D}$ in $\mathcal{R}_{i,D}$. 
It remains to prove (79). By Itô’s isometry,
\[
\mathbb{E}_f \left[ (D^{-1} \sum_{i=1}^D)^2 1_{A_{i,D}} \middle| \mathcal{F}_{(i-1)D} \right] = \frac{8}{D^2} \mathbb{E}_f \left[ \int_{(i-1)D}^{iD} |X_s - X_{(i-1)D}|^2 f(X_s) ds \middle| \mathcal{F}_{(i-1)D} \right] 1_{A_{i,D}} \\
\geq \frac{8}{D^2} \mathbb{E}_f \left[ \int_{(i-1)D}^{iD} |X_s - X_{(i-1)D}|^2 ds \middle| \mathcal{F}_{(i-1)D} \right] 1_{A_{i,D}},
\]
where \( \tau_{i,D} \) defined in (62) is the hitting time of the boundary \( \partial \Omega \) by the process \( X \) started at time \((i-1)D \). Furthermore,
\[
\mathbb{E}_f \left[ \int_{(i-1)D}^{iD} |X_s - X_{(i-1)D}|^2 ds \middle| \mathcal{F}_{(i-1)D} \right] = \mathbb{E}_f \left[ \int_{(i-1)D}^{iD} df(X_u) du \middle| \mathcal{F}_{(i-1)D} \right] \\
+ 2 \mathbb{E}_f \left[ \int_{(i-1)D}^{iD} (X_s - X_{(i-1)D}) \cdot \nabla f(X_u) du \middle| \mathcal{F}_{(i-1)D} \right].
\]
Lemma 24 applied to the second term of the right-hand side of (81) yields
\[
\left| 2 \mathbb{E}_f \left[ \int_{(i-1)D}^{iD} (X_s - X_{(i-1)D}) \cdot \nabla f(X_u) du \middle| \mathcal{F}_{(i-1)D} \right] \right| \lesssim D^{2+1/2}
\]
up to a (deterministic) constant that depends only on \( \|f\|_{C^1} \), while the first term of the right-hand side of (81) times \( 1_{A_{i,D}} \) can bounded below by \( d_{\min} \) times
\[
\mathbb{E}_f \left[ (\tau_{i,D} \wedge D)^2 1_{\{\tau_{i,D} \geq D\}} \middle| \mathcal{F}_{(i-1)D} \right] 1_{A_{i,D}} = \mathbb{D}^2 \mathbb{P}_f (\tau_{i,D} \geq D \middle| \mathcal{F}_{(i-1)D}) 1_{A_{i,D}} \\
\geq D^2 (1 - C \exp(-cD^{-1})) 1_{A_{i,D}}
\]
thanks to Lemma 25. We thus have
\[
\mathbb{E}_f \left[ \int_{(i-1)D}^{iD} |X_s - X_{(i-1)D}|^2 ds \middle| \mathcal{F}_{(i-1)D} \right] \geq dD^2 f_{\min} - O(D^{5/2})
\]
and (79) readily follows.

**Step 2:** We next turn to the boundary term in (74). Set \( \bar{L}_N(g) = D^{-1} \sum_{i=1}^N g(X_{(i-1)D}) \bar{\tilde{L}}_{i,D} 1_{A_{i,D}} \).
Since \( \sup_{g \in V_J \|g\|_2 \leq 1} |g|_{H_N}^2 \leq (1 + \kappa) \) on \( B_N \), by Cauchy-Schwarz’s inequality,
\[
\mathbb{P}_f \left( \sup_{g \in V_J \|g\|_2 \leq 1} |\bar{L}_N(g)| \geq CN \xi_N, B_N \right) \leq \mathbb{P}_f \left( |(1 + \kappa) D^{-2} N^{-1} \sum_{i=1}^N \bar{\tilde{L}}_{i,D}^2 1_{A_{i,D}} \geq C \xi_N^2 \right) \\
\leq \sum_{i=1}^N \mathbb{P}_f (\tau_{i,D} \geq D, A_{i,D}) \lesssim N \exp(-cD^{-1})
\]
using that \( \bar{L}_{i,D} \) vanishes on \( \{\tau_{i,D} < D\} \cap A_{i,D} \) and Lemma 25.

**Step 3:** We finally consider the drift term in (74). Setting \( \bar{b}_N(g) = D^{-1} \sum_{i=1}^N g(X_{(i-1)D}) \bar{\bar{b}}_{i,D} 1_{A_{i,D}} \), we will prove
\[
\mathbb{P}_f \left( \sup_{g \in V_J \|g\|_2 \leq 1} |\bar{b}_N(g)| \geq MN \xi_N, B_N \right) \leq C \exp(-LN \xi_N^2)
\]

for arbitrary fixed $L > 0$ and $M = M(L)$ large enough, under the assumption $ND^2 \to 0$. By Itô’s formula, with $H(x, y) = d(f(y) - f(x)) + (y - x) \cdot \nabla f(y)$, similarly to (70) in Step 2 of the proof of Proposition 15, we can decompose

$$\tilde{b}_{i,D} = \int_{(i-1)D}^{iD} H(X_{(i-1)D}, X_s)ds = \tilde{b}_{i,D}(H) + \tilde{\Sigma}_{i,D}(H) + \tilde{T}_{i,D}(H),$$

with

$$\tilde{b}_{i,D}(H) = \int_{(i-1)D}^{iD} \int_{(i-1)D}^s \mathcal{L}_f H(X_{(i-1)D}, X_u)du
ds$$

$$\tilde{\Sigma}_{i,D}(H) = \int_{(i-1)D}^{iD} \int_{(i-1)D}^s \nabla H(X_{(i-1)D}, X_u) \sqrt{2f(X_u)} \cdot dB_u
ds$$

$$\tilde{T}_{i,D}(H) = \int_{(i-1)D}^{iD} \int_{(i-1)D}^s \nabla H(X_{(i-1)D}, X_u) \cdot n(X_u)dBds.$$

We bound the deviation probability of each contribution in the expansion of $\tilde{b}_N(g)$ via a union bound. Using Cauchy-Schwarz’s inequality and the bound

$$\left| \int_{(i-1)D}^{iD} \int_{(i-1)D}^s \mathcal{L}_f H(X_{(i-1)D}, X_u)du
ds \right| \leq \frac{1}{2} D^2 \|\mathcal{L}_f H\|_\infty \leq C_0 \|f\|_{\mathcal{C}_3} D^2,$$

where the supremum is taken over $(x, y) \in \mathcal{O} \times \mathcal{O}$, we derive

$$\mathbb{P} \left( \sup_{g \in V_{\mathcal{O}}, \|g\|_{\mathcal{C}_2} \leq 1} D^{-1} \sum_{i=1}^N g(X_{(i-1)D})\tilde{b}_{i,D}(H)1_{A_{i,D}} \geq C N \xi_N, \mathcal{B}_N \right) \leq \mathbb{P} \left( N^{-1} \sum_{i=1}^N (\tilde{b}_{i,D}(H))^2 \geq C^2 D^2 \xi_N^2 \right) \leq N1 \left\{ C_2^{2} \|f\|_{\mathcal{C}_3} D^2 \geq C \xi_N \right\}$$

where we used that $\sup_{g \in V_{\mathcal{O}}, \|g\|_{\mathcal{C}_2} \leq 1} |g|_{\mathcal{C}_2}^2 \leq (1 + \kappa)$ on $\mathcal{B}_N$. The assumptions $ND^2 \to 0$ and $N\xi_N^2 \to \infty$ together imply that for sufficiently large $N$, we necessarily have $C_0 \|f\|_{\mathcal{C}_3} D^2 < C \xi_N^2$ and the above probability is thus zero. For the martingale term associated to $\tilde{\Sigma}_{i,D}(H)$, we proceed exactly as in Step 1: define

$$\mathcal{M}_n = D^{-n} \sum_{i=1}^n g(X_{(i-1)D})\tilde{\Sigma}_{i,D}(H)1_{A_{i,D}}.$$
with $C_{\|f\|_{\infty}^3} \geq C' \max(1, (2\varepsilon_+ \|f\|_{\infty})^{1/2} \|\nabla H\|_{\infty})$ and $C'$ a universal constant such that $p^p \leq C' p!$.

It follows that
\[
\sum_{i=1}^{n} \mathbb{E}[|M_i - M_{i-1}|^p \mid \mathcal{F}_{(i-1)D}] = \sum_{i=1}^{n} g(X_{i(i-1)})^p \mathbb{E} \left[ |D^{-1} \Sigma_{i,D}(H) \mathbf{1}_{A_{i,D}}|^p \mid \mathcal{F}_{(i-1)D} \right]
\leq (D^{1/2} C_{\|f\|_{\infty}^3} \|g\|_{\infty})^{p-2} p! \mathbb{E}(M)_{n},
\]
so that the condition of Lemma 27 holds with $c = D^{1/2} C_{\|f\|_{\infty}^3} \|g\|_{\infty}$ for instance. Moreover,
\[
\mathbb{E}(M)_{N} = \sum_{i=1}^{n} g(X_{i(i-1)D})^2 \mathbb{E} \left[ |D^{-1} \Sigma_{i,D}(H) \mathbf{1}_{A_{i,D}}|^2 \mid \mathcal{F}_{(i-1)D} \right] \leq CN \|g\|_{2}^2 D \leq C(1+\kappa) \|g\|_{2}^2 ND
\]
on the event $\mathcal{B}_{N}$, so that applying Lemma 27 with $n = N$ and $y = (1+\kappa) \|g\|_{2}^2 ND$ yields
\[
\mathbb{P}_{\mathcal{B}_{N}}(\overline{D}^{-1} \sum_{i=1}^{n} g(X_{i(i-1)D}) \Sigma_{i,D}(H) \mathbf{1}_{A_{i,D}} \geq t) \leq C \mathbb{P}_{\mathcal{B}_{N}}(\overline{M} \geq t, \overline{M} \leq (1+\kappa) \|g\|_{2}^2 ND)
\leq 2C \exp \left( -C \frac{t^2}{ND \|g\|_{2}^2 + D^1/2 \|g\|_{\infty}} \right)
\]
for all $t > 0$. Setting $\overline{Z}_N(g) = D^{-1} \sum_{i=1}^{n} g(X_{i(i-1)D}) \Sigma_{i,D}(H) \mathbf{1}_{A_{i,D}}$, the process $\overline{Z}_N = (\overline{Z}_N(g) : g \in \{V_j : \|g\|_{2} \leq 1\})$ therefore satisfies the conditions of Lemma 32 with $m = \dim(V_j) = O(2^{jD})$, $\|g\|_{2} \leq 2$, $\alpha^2 = ND$, $\beta = D^{1/2} 2^{jD/2}$, where we have also used the linearity of $g \mapsto \overline{Z}_N(g)$ and that $\|g\|_{\infty} \leq C \|g\|_{2}$ for $g \in V_j$. Lemma 32 thus implies that for all $u \geq 1$,
\[
\mathbb{P}_{\mathcal{B}_{N}} \left( \sup_{g \in V_j, \|g\|_{2} \leq 1} |\overline{Z}_N(g)| \geq CD^{1/2} (2^{3jD/2} + 2^{jD/2} N^{1/2} + \sqrt{\alpha} N^{1/2} + u 2^{jD/2}) \right) \leq e^{-u}.
\]
Returning to (82), we want a bound of the form
\[
\mathbb{P}_{\mathcal{B}_{N}} \left( \sup_{g \in V_j, \|g\|_{2} \leq 1} |\overline{Z}_N(g)| \geq CN \varepsilon_N \right) \leq e^{-L N \varepsilon_N^2}.
\]
Setting $u = LN \varepsilon_N^2$ in the second last display, this follows as soon as
\[
D^{1/2} (2^{3jD/2} N^{-1} + 2^{jD/2} N^{-1/2} + \varepsilon_N + 2^{jD/2} \varepsilon_N^2) \lesssim \varepsilon_N.
\]
But this is exactly condition (80) above with the left-side multiplied by the superoptimal factor $D^{1/2}$, and hence this condition is implied by (80). For the boundary term associated to $\overline{L}_{i,D}(H)$, we proceed exactly as in Step 2, replacing $\overline{L}_{i,D}$ by $\overline{L}_{i,D}$. The conclusion is the same.

9. PROOFS OF POSTERIOR CONTRACTION RESULTS

9.1. Proof of Theorem 12: a general contraction theorem. The proof follows the general testing approach of [25] and the idea of using plug-in tests based on frequentist estimators satisfying concentration inequalities [26], adapted to the present high-frequency multidimensional diffusion setting. The next result follows by combining the proof of Theorem 8.9 in [25] for the i.i.d. case with our evidence lower bound in Theorem 7.

Lemma 28. Suppose $f_0 \in \mathcal{F}_0$ and let $\Pi = \Pi_N$ be a sequence of prior distributions supported on $\mathcal{F}$ in (13). Further let $0 < \varepsilon_N \leq \varepsilon_{1,N} \leq \varepsilon_{2,N} \leq \varepsilon_{3,N} \rightarrow 0$, $\xi_N \rightarrow 0$ be positive sequences such that $N \varepsilon_N^2 \rightarrow \infty$, let $E_N$ and $V_N$ be the corresponding quantities defined in (17), and let $r > 0$ be fixed. Set
\[
\varepsilon_{N} = \left\{ f \in \mathcal{F} : \|f\|_{\infty} \leq r, \|f - f_0\|_{\infty} \leq \varepsilon_N, \|f - f_0\|_{\infty} \leq \varepsilon_{k,N} \text{ for } k = 1, 2, 3 \right\}
\]
to be the set defined in (16) and $C_0 > 0$ to be the fixed constant in Theorem 7, which depends only on $f_0, r, d, 0, \delta, f_{\text{min}}$. Suppose that for some $K_0 > 0$,

$$E_N \leq K_0 \varepsilon_N^2, \quad V_N/(N^2 \varepsilon_N^2) \to 0,$$

as $N \to \infty$. Further suppose that for some $C, L, M > 0$, the prior $\Pi$ satisfies $\Pi(\mathcal{C}_N) \geq e^{-CN\varepsilon_N}$, and there exist sets $\mathcal{F}_N \subseteq \mathcal{T}$ satisfying $\Pi(\mathcal{F}_N) \leq L e^{-(C_0K_0 + 2)N\varepsilon_N}$, events $B_N$ satisfying $\mathbb{P}_{f_0}(B_N) \to 1$ and a sequence of test functions $\Psi_N = \Psi_N(X_0, X_D, \ldots, X_N)$ such that

$$\mathbb{E}_{f_0}[\Psi_N 1_{B_N}] \to 0,$$

$$\sup_{f \in \mathcal{F}_N: \|f - f_0\|_2 \geq M\varepsilon_N} \mathbb{E}_f[(1 - \Psi_N)1_{B_N}] \leq Le^{-(C_0K_0 + 2)N\varepsilon_N}.$$

Then as $N \to \infty$,

$$\mathbb{E}_{f_0} \Pi(f : \|f - f_0\|_2 \geq M\varepsilon_N | X_0, X_D, \ldots, X_N) \to 0.$$

**Proof.** Writing $A_N = \{f : \|f - f_0\|_2 \geq M\varepsilon_N\}$ and $X^N = (X_0, X_D, \ldots, X_N)$, we have

$$\mathbb{E}_{f_0} \Pi(A_N | X^N) \leq \mathbb{E}_{f_0} \Pi(A_N | X^N)(1 - \Psi_N)1_{B_N} + \mathbb{E}_{f_0} [\Psi_N 1_{B_N}] + \mathbb{P}_{f_0}(B_N^c).$$

Since the last two terms tend to zero by assumption, it remains to control the first term. We thus need only prove convergence in $\mathbb{P}_{f_0}$-probability to zero of

$$\Pi(A_N | X^N)(1 - \Psi_N)1_{B_N} = \frac{\int_{A_N} \prod_{i=1}^N \frac{p_{f_0,D}(X_i)}{p_{f_0,D}(X_i)} \pi_i(f)}{\int_{\mathcal{F}_N} \prod_{i=1}^N \frac{p_{f_0,D}(X_i)}{p_{f_0,D}(X_i)} \pi_i(f)}(1 - \Psi_N)1_{B_N}.$$

By Theorem 7, we have for any $c > 0$ and any probability measure $\nu$ supported on $\mathcal{C}_N$,

$$\mathbb{P}_{f_0} \left( \int_{\mathcal{C}_N} \prod_{i=1}^N \frac{p_{f_0,D}(X_i)}{p_{f_0,D}(X_i)} \nu(df) \leq e^{-cN\varepsilon_N - c_0 N E_N} \right) \leq \frac{V_N}{c^2 N^2 \varepsilon_N^2}.$$

Let $\nu = \Pi(\cdot \cap \mathcal{C}_N)/\Pi(\mathcal{C}_N)$ be the prior distribution conditioned to the set $\mathcal{C}_N$, and define the events

$$\Omega_N = \left\{ \int_{\mathcal{C}_N} \prod_{i=1}^N \frac{p_{f_0,D}(X_i)}{p_{f_0,D}(X_i)} \pi_i(f) \geq \Pi(\mathcal{C}_N e^{-(C_0K_0 + 1)N\varepsilon_N}) e^{-(C_0K_0 + 1)N\varepsilon_N} \geq e^{-(C_0K_0 + 1)N\varepsilon_N} \right\},$$

where we used $\Pi(\mathcal{C}_N) \geq e^{-CN\varepsilon_N}$ in the last inequality. Setting $c = 1$ and since $E_N \leq K_0 \varepsilon_N^2$ by assumption, the second last display implies $\mathbb{P}_{f_0}(\Omega_N) \leq V_N/(N^2 \varepsilon_N^2) \to 0$ as $N \to \infty$. Thus for any $\eta > 0$,

$$\mathbb{P}_{f_0}(\Pi(A_N | X^N)(1 - \Psi_N)1_{B_N} > \eta) \leq \mathbb{P}_{f_0} \left( e^{(C_0K_0 + 1)N\varepsilon_N} \int_{A_N} \prod_{i=1}^N \frac{p_{f_0,D}(X_i)}{p_{f_0,D}(X_i)} \pi_i(f)(1 - \Psi_N)1_{B_N} > \eta \right) + \mathbb{P}_{f_0}(\Omega_N).$$

By Fubini’s theorem and since $0 \leq 1 - \Psi_N \leq 1$,

$$\mathbb{E}_{f_0} \int_{A_N} \prod_{i=1}^N \frac{p_{f_0,D}(X_i)}{p_{f_0,D}(X_i)} \pi_i(f)(1 - \Psi_N)1_{B_N}$$

$$= \int_{A_N} \mathbb{E}_f[(1 - \Psi_N)1_{B_N}] \pi_i(f)$$

$$\leq \Pi(\mathcal{F}_N^c) + \sup_{f \in \mathcal{F}_N: \|f - f_0\|_2 \geq M\varepsilon_N} \mathbb{E}_f[(1 - \Psi_N)1_{B_N}] \leq 2Le^{-(C_0K_0 + 2)N\varepsilon_N}.$$
using the assumptions on the tests $\Psi_N$ and on $\mathcal{F}_N$. Combining the last two displays and using Markov’s inequality gives for any $\eta > 0$,

$$
\mathbb{P}_{f_0}(\Pi(A_N|X_N^N)(1 - \Psi_N)1_{B_N} > \eta) \leq 2\eta^{-1}Le^{-N\varepsilon_N^2} + \mathbb{P}_{f_0}(\Omega_N) \to 0
$$

since $N\varepsilon_N^2 \to \infty$ as $N \to \infty$. \hfill \Box

It therefore remains to show that the required tests in Lemma 28 exist under the conditions of Theorem 12. Setting $\hat{f}_N$ to be the projection estimator in (26), consider tests of the form

$$
\Psi = \Psi_N(X_0, X_D, \ldots, X_N) = \{||\hat{f}_N - f_0||_2 \geq \bar{M}\xi_N\},
$$

where $\bar{M} > 0$ is a large enough constant. The required properties then follow from Theorem 9.

**Lemma 29.** Let $\varepsilon_N, \xi_N \to 0$, $2^J = 2^J_N \to \infty$ and $R_J$ satisfy the conditions of Theorem 9 and define the sets

$$
\mathcal{F}_N^\prime = \{f \in \mathcal{F}: ||f||_{C^1} \leq R, ||f - \bar{P}_Jf||_2 \leq C\xi_N, ||f - \bar{P}_Jf||_\infty \leq R_J\},
$$

where $C, R > 0$ and $\bar{P}_J$ denotes the projection (24). Assume the true $f_0 \in \mathcal{F}_0$ satisfies the same conditions as $\mathcal{F}_N^\prime$, possibly up to different constants (e.g. $||f_0 - \bar{P}_Jf_0||_2 \leq M_0\xi_N$ for some $M_0 > 0$). Then for any $R > 0$, one can take $M, \bar{M} > 0$ large enough (depending also on $R$) such that the tests $\Psi_N$ in (83) satisfy

$$
\mathbb{E}_{f_0}[\Psi_N 1_{B_N}] \to 0, \sup_{f \in \mathcal{F}_N: ||f - f_0||_2 \geq M\xi_N} \mathbb{E}_f[(1 - \Psi_N)1_{B_N}] \leq C'e^{-JN\varepsilon_N^2},
$$

where the event $B_N$ satisfies $\sup_{f \in \mathcal{F}} \mathbb{P}_{f}(B_N^c) \to 0$ as $N \to \infty$.

**Proof.** Consider the event $B_N$ in (72) and used in Theorem 9, which by Lemma 26 satisfies $\mathbb{P}_{f_0}(B_N) \to 1$ as $N \to \infty$ since $f_0 \in \mathcal{F}_0 \subset \mathcal{F}$. Using the definition (83) of the test $\Psi_N$, that $||f_0 - \bar{P}_Jf_0||_2 \leq M_0\xi_N$ and the triangle inequality,

$$
\mathbb{E}_{f_0}[\Psi_N 1_{B_N}] \leq \mathbb{P}_{f_0}(||\hat{f}_N - \bar{P}_Jf_0||_2 \geq (\bar{M} - M_0)\xi_N, B_N).
$$

Since the conditions of Theorem 9 are satisfied, applying that theorem with $\bar{M} > 0$ large enough bounds the right-hand side by $C'e^{-JN\varepsilon_N^2} \to 0$, giving the first part of the lemma.

For the type-II errors, let $f \in \mathcal{F}_N$ satisfy $||f - f_0||_2 \geq M\xi_N$ for some $M > 0$ to be specified below. Then, since $||f - \bar{P}_Jf||_2 \leq C\xi_N$,

$$
\mathbb{E}_f[(1 - \Psi_N)1_{B_N}] = \mathbb{P}_f(||\hat{f}_N - f_0||_2 \leq \bar{M}\xi_N, B_N)
\leq \mathbb{P}_f(||f_0 - f||_2 - ||\hat{f}_N - \bar{P}_Jf||_2 - ||f - \bar{P}_Jf||_2 \leq \bar{M}\xi_N, B_N)
\leq \mathbb{P}_f((M - \bar{M} - C)\xi_N \leq ||\hat{f}_N - \bar{P}_Jf||_2, B_N) \leq C'e^{-JN\varepsilon_N^2},
$$

uniformly over such $f$, where the last inequality follows from Theorem 9 upon taking $M = M(R, \bar{M}, C) > 0$ large enough. \hfill \Box

Theorem 12 then follows from using the tests in Lemma 29 together with Lemma 28.
9.2. Proof of Theorem 2: contraction rates for Gaussian priors. Let \( \| \cdot \|_{H^r} \) denote the RKHS of \( W \). Then \( \chi W \) in (12) is a mean-zero Gaussian process with RKHS \( H_{\chi W} = \{ \chi w : w \in H^r \} \) and whose RKHS norm satisfies that for every \( w \in H^r \), there exists some \( w^* \in H^r \) such that \( \chi w = \chi w^* \) and

\[
\| \chi w \|_{H^r} = \| w^* \|_{H^r}
\]

(Exercise 2.6.5 of [27]). Furthermore, we have that \( H^r = H^r \) with RKHS norm \( \| \cdot \|_{H^r} = \sqrt{N} \varepsilon_N \).

We require the following Lemma about the concentration of Gaussian measures on suitable sieve sets. The proof is similar to Theorem 2.2.2 of [39] (see also Lemma 5.2(i) in [29]) and is hence omitted.

**Lemma 30.** For \( s, M > 0 \) and the sequence \( \varepsilon_N = N^{-\frac{s}{2d+r}} \), define the sets

\[
W_N = \{ W = W_1 + W_2 : \| W_1 \|_\infty \leq \varepsilon_N, \; \| W_2 \|_{H^r} \leq M, \; \| W \|_{H^r} \leq M \}.
\]

Let \( W = V/(\sqrt{N} \varepsilon_N) \) for \( V \sim \Pi_V \) a mean-zero Gaussian process satisfying Condition 1. Then for every \( K > 0 \), there exists \( M > 0 \) large enough such that \( \Pi_W (W_N) \leq e^{-K N \varepsilon_N^K} \).

**Proof of Theorem 2.** We verify the assumptions of Theorem 12 with \( \varepsilon_N = N^{-\frac{s}{2d+r}} \), \( \varepsilon_k, N = N^{-\frac{s}{2d+r}} \), \( k = 1, 2, 3 \), and \( 2j \approx N^{-\frac{s}{2d+r}} \) as in Remark 8, so that \( E_N \leq K_0 \varepsilon_N^2 \) and \( V_N/(N^{2} \varepsilon_N^2) \to 0 \).

**Small-ball probability:** consider the “small-ball condition” (ii) in Theorem 12. Recall that under the prior \( \Pi \) in (12), \( f = \Phi(\chi W) \) with \( W = V/(\sqrt{N} \varepsilon_N) \) for \( V \) a mean-zero Gaussian process and \( \Phi(x) = f_{\min} + (1 - f_{\min}) e^x \).

We first state some useful inequalities regarding the smoothness of functions when composed with \( \Phi \) and \( \Phi^{-1} \). When composed with a uniformly bounded function \( g : \Theta \to \mathbb{R} \) satisfying \( \| g \|_\infty \leq M \), we may restrict the domain of \( \Phi \) to \( [-M, M] \). Since \( \Phi(k) = (1 - f_{\min}) e^x \) satisfies \( \| \Phi(k) \|_{L^\infty[-M,M]} \leq e^M \) for \( k = 1, 2, \ldots \), we deduce that \( \| \Phi \|_{C^k[-M,M]} \leq (C_k d e M)^{< \infty} \) for \( k = 1, 2, \ldots \). By Theorem 4.3(ii)(3) in [20], we thus have that for any \( r \geq 1 \),

\[
\| \Phi(g) \|_{C^r} \leq C_{r,d} \| \Phi \|_{C^r[-M,M]} (1 + \| g \|_{C^r}) \leq C_{r,d,M} (1 + \| g \|_{C^r}) \quad \forall g : \| g \|_\infty \leq M.
\]

Using the multivariate version of Faà di Bruno’s formula [15], one can show that for any \( g_1, g_2 \in C^k \) with \( \| g_1 \|_\infty \leq M \) and integer \( k \geq 1 \),

\[
\Phi(g_1) - \Phi(g_2) \leq C_{k,d,M} \left( 1 + \| g_1 \|_{C^k} + \| g_2 \|_{C^k} \right) \| g_1 - g_2 \|_{C^k} \quad \forall g_1, g_2 : \| g_1 \|_\infty, \| g_2 \|_\infty \leq M
\]

(see e.g. Lemma 2 in [50] for the proof of a similar argument). Turning to \( \Phi^{-1}(y) = \log \frac{y - f_{\min}}{y - f_{\min}} \), we have \( \| \Phi^{-1}(-1) \|_{L^\infty[2f_{\min}, \infty)} \leq (k - 1) e^{f_{\min}} < \infty \) for \( k = 1, 2, \ldots \), so that \( \| \Phi^{-1} \|_{L^\infty(\Theta)} \leq (k - 1) e^{f_{\min}} \) for \( k = 1, 2, \ldots \). Similarly, since \( f_0 \in F_0 \cap C^\alpha \) satisfies \( f_0 \geq 2f_{\min} \), arguing as (85) implies that \( u_0 = \Phi^{-1}(f_0) \in C^\alpha \). Similarly, since \( f_0 \in F_0 \subseteq C^\alpha (O) \) for \( \alpha = 4 \sqrt{2} [d/4 + 1/2] \) in (7), we may find \( r > 0 \) large enough that \( \| u_0 \|_{C^\alpha} \leq r/2 \).

Let \( g : O \to \mathbb{R} \) satisfy \( \| g \|_{C^\alpha} \leq r \). By (85), \( \| \Phi(g) \|_{C^\alpha} \leq C_{a,d,r} \), while by (86), we have \( \| \Phi(g) - \Phi(w_0) \|_{C^\alpha} \leq C_{k,d,r} \| g - w_0 \|_{C^\alpha} \) for \( k = 1, 2, 3 \) and \( \alpha \geq 4 \). Similarly, \( \| \Phi(g) - \Phi(w_0) \|_{C^\alpha} \leq C_{r} |g - w_0|_{\infty} \) using that the exponential function is Lipschitz on a bounded interval. Setting \( g = \chi w \), we thus have

\[
\{ w \in C^1(\Theta) : \| \chi w \|_{C^\alpha} \leq r, \| \chi w - w_0 \|_{\infty} \leq \varepsilon_N, \| \chi w - w_0 \|_{C^\alpha} \leq \varepsilon_k,N \text{ for } k = 1, 2, 3 \}
\]

\[
\subset \{ w \in C^1(\Theta) : \| \Phi(\chi w) \|_{C^\alpha} \leq C, \| \Phi(\chi w) - f_0 \|_{\infty} \leq \varepsilon_N, \| \Phi(\chi w) - f_0 \|_{C^\alpha} \leq \varepsilon_k,N \text{ for } k = 1, 2, 3 \},
\]
where the \( \preceq \) above depend only on \( d, \alpha, r \). Writing \( \Pi_W \) and \( \Pi \) for the prior laws of \( W \) and \( f = \Phi(\chi W) \), respectively, the prior probability \( \Pi(\mathcal{C}_N) \) equals the \( \Pi_W \)-probability of the last set in above display. We thus conclude that

\[
\Pi(\mathcal{C}_N) \geq \Pi_W(W \in \mathcal{C}^1(\emptyset)) : \| \chi W \|_{e^{\alpha}} \leq r, \| \chi W - w_0 \|_{\infty} \preceq \varepsilon_N, \| \chi W - w_0 \|_{e^k} \preceq \varepsilon_{k,N} \text{ for } k = 1, 2, 3),
\]

where the \( \preceq \) above depend only on \( \Phi, d, \alpha \). Under the theorem hypotheses, the last probability is lower bounded by

\[
\Pi_W(W \in \mathcal{C}^1(\emptyset)) : \| \chi W - \chi v_{0,N} \|_{e^{\alpha}} \leq 2r, \| \chi W - \chi v_{0,N} \|_{\infty} \preceq \varepsilon_N, \| \chi W \|_{e^k} \preceq \varepsilon_{k,N} \text{ for } k = 1, 2, 3),
\]

possibly after replacing \( r > 0 \) by a larger constant and then \( \varepsilon_{k,N} \) by a multiple of itself. Since \( \chi W \) is a mean-zero Gaussian process under the prior, and \( \chi v_{0,N} \in \mathbb{H}_W \) is in its RKHS, Lemma 1.27 of [25] lower bounds the last display by

\[
e^{-\frac{1}{2} \| \chi v_{0,N} \|_{\mathbb{H}_W}^2} \Pi_W(W \in \mathcal{C}^1(\emptyset)) : \| \chi W \|_{e^{\alpha}} \leq 2r, \| \chi W \|_{\infty} \preceq \varepsilon_N, \| \chi W \|_{e^k} \preceq \varepsilon_{k,N} \text{ for } k = 1, 2, 3).
\]

Note that \( \| \chi v_{0,N} \|_{\mathbb{H}_W}^2 \leq N \varepsilon_N^2 \| v_{0,N} \|_{\mathbb{H}_V}^2 = O(N \varepsilon_N^2) \) using Exercise 2.6.5 of [27] and the assumption on \( v_{0,N} \). Using the last display, that \( \chi \in \mathcal{C}^\infty, W = V/\sqrt{N} \varepsilon_N \) and the Gaussian correlation inequality [53] (see Lemma A.2 in [29] for the exact formulation we use), we have

\[
\Pi(\mathcal{C}_N) \geq e^{-CN\varepsilon_N^3} \Pi_V(V \in \mathcal{C}^1(\emptyset)) : \| V \|_{e^{\alpha}} \leq 2r\sqrt{N} \varepsilon_N
\]

(87)

for some \( C > 0 \) and where above we have written \( \varepsilon_{0,N} = \varepsilon_N \). It therefore suffices to lower bound each of the prior probabilities in (87).

Let \( \overline{N}(A, \| \cdot \|, \tau) \) denote the covering number of a set \( A \) by \( \| \cdot \| \)-balls of radius \( \tau \). For \( \mathbb{H}_{V,1} \) and \( \mathbb{H}_{V} \) the unit balls of the RKHS \( \mathbb{H}_{V} \) and \( \mathbb{H}' \), respectively, we have under Condition 1 that for integer \( k \geq 0 \),

\[
\log \overline{N}(\mathbb{H}_{V,1}, \| \cdot \|_{e^k}, \tau) \leq \log \overline{N}(c \mathbb{H}_V^k, \| \cdot \|_{e^k}, \tau) \preceq \tau^{-\frac{2d}{(s-k)-d}},
\]

where the last inequality follows by arguing as in the proof of Theorem 4.3.36 in [27] as soon as \( s - k > d/2 \). Applying the small ball estimate in Theorem 1.2 of [35] (in particular, (1.3) in [35] with exponents \( \alpha = \frac{2d}{2(s-k)-d} \) and \( \beta = 0 \), we have for \( s - k > d/2 \),

\[
\Pi_V(\| V \|_{e^k} \leq \eta) \geq \exp \left( -c \eta^{-\frac{2d}{(s-k)-d}} \right) \quad \text{as } \eta \to 0.
\]

Using the last display with \( \eta_N = 1/(\log N) \) and \( k = \alpha \) shows that the first prior probability in (87) is greater than or equal to \( e^{-c(\log N)^{\alpha}} \geq e^{-CN\varepsilon_N^3} \) for \( s > \alpha + d/2 \) and some \( k > 0 \). In particular, it can be checked that the minimal smoothness \( s_{d,a}^* \), defined in (14) assumed in the present theorem satisfies \( s_{d,a}^* \geq \alpha + d/2 \) for any dimension \( d \in \mathbb{N} \), and hence this last condition is satisfied. For the choice \( \varepsilon_{k,N} = N^{-\frac{2d}{(s-k)-d}}, \) we have \( \sqrt{N} \varepsilon_{0,N} \varepsilon_{k,N} = N^{-\frac{2(k-d)}{2(s-k)-d}} \to 0 \) for \( s > k + d/2 \). Using the last display with \( \eta = \eta_{k,N} = c\sqrt{N} \varepsilon_{0,N} \varepsilon_{k,N} \) then yields

\[
\prod_{k=0}^3 \Pi_V(\| V \|_{e^k} \leq \sqrt{N} \varepsilon_{N} \varepsilon_{k,N}) \geq \prod_{k=0}^3 \exp \left( -c \eta_{k,N}^{-\frac{2d}{(s-k)-d}} \right) \geq \exp \left( -c N \varepsilon_N^3 \right).
\]
using that \((\sqrt{N}\varepsilon_{0,N}\varepsilon_{N,K})^{-\frac{2d}{N-\frac{d}{2}}} = N^{-\frac{2d}{N-\frac{d}{2}}} = N^{-\frac{2}{d}}\). Together with (87), this gives the required lower bound \(\Pi(\varepsilon_N) \geq e^{-C_N\varepsilon_N^2}\) for any fixed \(r > 1\) and \(s > k + d/2\), which verifies the small-ball condition (ii) in Theorem 12.

**Sieve sets:** consider the condition (i) in Theorem 12. For \(s\) as in this theorem and \(M > 0\), let \(\mathcal{W}_N\) be the set defined in (84). For any \(K > 0\), we can find \(M = M(K) > 0\) sufficiently large that \(\Pi_{\mathcal{W}}(\mathcal{W}_N) \leq e^{-KN^2}\) by Lemma 30. In particular, let \(K > C + C_0K_0 + 2\) for \(C\) the constant in Theorem 12 coming from the small-ball condition (ii) just proved. Define

\[ \mathcal{F}_N = \{ f = \Phi(\chi w) : w \in \mathcal{W}_N \}, \]

so that \(\Pi(\mathcal{F}_N) \leq e^{-KN^2}\), as required. Since \(w \in \mathcal{W}_N\) satisfies \(\|w\|_{\varepsilon_1} \leq M\), we have \(\|\Phi(\chi w)\|_{\varepsilon_1} \leq C_{d,M}(1 + \|\chi\|_{\varepsilon_1}\|w\|_{\varepsilon_1}) \leq C_{d,M}\chi(1 + M)\) using (85). To verify the bias conditions, we invoke Lemma 31 below with \(p = 2, \infty\) to get that for all \(f \in \mathcal{F}_N\),

\[ \|f - \overline{P}_J f\|_p \lesssim \varepsilon_N + 2^{-J(s-d/2+d/p)} \lesssim 2^{-J(s-d/2+d/p)}. \]

Therefore, since \(2^{-J_s} \approx \varepsilon_N, \mathcal{F}_N\) satisfies

\[ \mathcal{F}_N \subseteq \{ f \in \mathcal{F} : \|f\|_{\varepsilon_1} \leq 1, \|f - \overline{P}_J f\|_2 \lesssim \varepsilon_N, \|f - \overline{P}_J f\|_{\infty} \lesssim R_J \} \]

for \(R_J \approx 2^{-J(s-d/2)} \approx N^{-\frac{2d}{d+2}},\) i.e. condition (i) in Theorem 12.

We last verify the numeric constraints on the sequence choices with also \(D = N^{-a}, a \in (1/2, 1)\). Since \(f_0 \in \mathcal{F}_0 \cap \mathcal{C}(0)\), we have by similar arguments to the above that \(\|f_0 - \overline{P}_J f_0\|_2 \leq \varepsilon_N\) and \(\|f_0 - \overline{P}_J f_0\|_{\infty} \lesssim R_J\). The condition \(2^{Jd} \approx N^{-\frac{2d}{2-d}} = o\left(\sqrt{N}\right) = o(N^{1-a/2}) \) is equivalent to \(\frac{2d(1+a)}{d+2} < s\). Turning to the quantitative conditions (27), for our sequence choices these reduce to

\[ \frac{R_J^2}{\varepsilon_N^2} \lesssim D\xi_N \quad \Longleftrightarrow \quad N^{\frac{2}{d+2} - \frac{2d}{d+2}} \lesssim \xi_N \]

\[ 2^{3Jd/2} N^{-1} + 2^{Jd/2} N^{-1/2} + 2^{-Jd/2} N^{-1} + \varepsilon_N \lesssim \xi_N \quad \Longleftrightarrow \quad N^{-\frac{2d}{d+2}} + N^{-\frac{2d}{d+2}} \lesssim \xi_N \]

Since \(s > d/2\) by assumption, we finally get rate \(\xi_N \approx N^{-\frac{2d}{d+2}} + N^{-\frac{2d}{d+2}},\) i.e. the largest of the two conditions above. One can check that \(N^{-\frac{2d}{d+2}}\) is the largest term for \(s > \frac{d(1+a)}{2(1-a)}\) in \((1/2, 1)\). \(\square \)

**Lemma 31.** For \(s > d/2 \land 0 < \varepsilon_N \leq M\), let \(\mathcal{W}_N\) be the set (84). Let \(\Phi(x) = f_{\min} + (1 - f_{\min})e^x\) be the link function, \(\chi \in \mathcal{C}(0)\) a smooth cutoff function such that \(\chi \equiv 1\) on \(K\) and \(\chi \equiv 0\) outside \(O_0, w \in \mathcal{W}_N\) and \(\overline{P}_J\) be the projection operator (24). Then for \(p \in [2, \infty]\) and \(w \in \mathcal{W}_N\),

\[ \|\Phi(\chi w) - \overline{P}_J(\Phi(\chi w))\|_p \leq C(\varepsilon_N + 2^{-J(s-d/2+d/p)}), \]

where \(C\) depends only on \(\Phi, \chi, p, M, s, d, \text{vol}(\mathcal{O})\) and the wavelet basis.

**Proof.** Let \(w \in \mathcal{W}_N\) and write \(w = w_1 + w_2\) as in (84). Then for any \(x \in \mathcal{O},\)

\[ |\Phi(\chi w)(x) - 1 - P_J[\Phi(\chi w) - 1](x)| \leq |\Phi(\chi w_1 + \chi w_2)(x) - \Phi(\chi w_2)(x)| + |\Phi(\chi w_2)(x) - 1 - P_J[\Phi(\chi w_2) - 1](x)| + |P_J[\Phi(\chi w_2) - 1](x) - P_J[\Phi(\chi w_1 + \chi w_2) - 1](x)|. \]

By the mean-value theorem, the first term in (88) is bounded by \(\varepsilon\|\chi\|_{\infty}(\|w_1\|_{\infty} + \|w_2\|_{\infty})\|\chi\|_{\infty}\|w_1\|_{\infty} \lesssim \|w_1\|_{\infty} \|w_2\|_{\infty} \|w_2\|_{\infty} \lesssim M\) by the Sobolev embedding theorem.

Let \(K_j(x, y) = 2^{jd} \sum_{k \in \mathbb{Z}} \phi(2^j x - k)\phi(2^j y - k)\) denote the wavelet projection kernel on all of \(\mathbb{R}^d\), where \(\phi\) is the Daubechies father wavelet. By the localization property of wavelets, \(\int_{\mathbb{R}^d} |K_j(x, y)| dy \lesssim \)
1 for all $x \in \mathbb{R}^d$. Since the full $L^2$-projection operator $\bar{P}_J : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ onto $\{\psi_{l,r} : l \leq J, r \in \mathbb{Z}^d\}$ satisfies $P_J[g](x) = \int_{\mathbb{R}^d} K_J(x,y) g(y) dy$ and $P_J$ and $\bar{P}_J$ coincide for functions whose support is contained in $O_0$, the third term in (88) can be expanded as

$$|P_J[\Phi \circ (\chi w_2) - 1](x) - P_J[\Phi \circ (\chi w_1 + \chi w_2) - 1](x)|$$

$$= \left| \int_{\mathbb{R}^d} K_J(x,y) \left( \Phi(\chi(y)w_2(y)) - \Phi(\chi(y)w_1(y) + \chi(y)w_2(y)) \right) dy \right|$$

$$\leq C_{M,\chi} \|\chi\|_\infty \|w_1\|_\infty \int_{\mathbb{R}^d} |K_J(x,y)| dy \lesssim \|w_1\|_\infty,$$

where we applied the mean-value theorem as above for the first inequality. Combining the bounds for (88), taking $p^{th}$-powers of everything and integrating over the bounded domain $\Omega$ then yields

$$\|\Phi \circ (\chi w) - 1 - P_J[\Phi \circ (\chi w) - 1]\|_p \lesssim \|w_1\|_{L^p} + \|\Phi \circ (\chi w_2) - 1 - P_J[\Phi \circ (\chi w_2) - 1]\|_p.$$

Since $\text{supp}(\Phi \circ (\chi w_2) - 1) \subseteq O_0$, we may replace the $L^p(\Omega)$ norm in the last term by $L^p(\mathbb{R}^d)$ and the projection operator $P_J$ by $\bar{P}_J$. Applying Corollary 3.3.1 of [13], we then get

$$\|\Phi \circ (\chi w_2) - 1 - \bar{P}_J[\Phi \circ (\chi w_2) - 1]\|_{L^p(\mathbb{R}^d)} \lesssim 2^{-Jf}\|\Phi \circ (\chi w_2) - 1\|_{B^p_{pq}}$$

for any $1 \leq q \leq \infty$. Using the embedding $H^s(\mathbb{R}^d) = B^s_{22}(\mathbb{R}^d) \hookrightarrow B^{s-d/2+d/p}_{pq}$ for any $p \geq 2$ ([27], Proposition 4.3.10), we may set $t = s - d/2 + d/p$ and $q = 2$ in the last display and replace the $B^t_{pq}$-norm by an $H^s$-norm. Since $\|\chi w_2\|_s \leq C_{\chi,s,d} M$ by the Sobolev embedding theorem, we may also replace $\Phi$ in the last composition by some smooth function $\Phi^M$ that coincides with $\Phi$ on $[-CM,CM]$, but is bounded and all of whose derivatives are uniformly continuous (depending on $M$). Since $s > d/2 \vee 1$, Theorem 4(i) of [57] yields $\|\Phi^M \circ (\chi w_2) - 1\|_{H^s} \lesssim \|w_2\|_{H^s} + \|w_2\|_{H^s}^s$, where the constant depends on $\chi, p, M, s, d, \text{vol}(\Omega)$. Substituting in the bounds for $w_1$ and $w_2$ coming from the definition (84) of $W_N$ then gives the result. 

9.3. Proof of Corollaries 3 and 4: examples of Gaussian process priors.

Proof of Corollary 3. The Matérn process on all of $\mathbb{R}^d$ has RKHS norm equal to $\| \cdot \|_{H^s} = \| \cdot \|_{H^s(\mathbb{R}^d)}$ ([25], Chapter 11), and hence its restriction to $\Omega$ has RKHS norm equal to $H^s(\Omega)$ by Exercise 2.6.5 of [27]. Moreover, by Proposition 1.4 of [25], $V$ has a version who sample paths are in $\mathcal{C}^\infty(\Omega)$ II-almost surely for any $r < s - d/2$. In particular, $\mathcal{C}^\infty(\Omega)$ is a separable linear subspace of $\mathcal{C}^4(\Omega)$ for any $r > 4$, a suitable choice of which exists as soon as $s > d/2 + 4$. The Matérn process thus satisfies Condition 1 for $s > d/2 + 4$ since its RKHS norm equals the $H^s(\Omega)$-norm.

We may therefore apply Theorem 2 to the Matérn process when $f_0 \in \mathcal{C}^\infty(\Omega)$. Indeed, since $w_0 = \Phi^{-1}(f_0) \in \mathcal{C}^\infty(\Omega)$ by (85) (which applies also to $\Phi^{-1}$) and $\text{supp}(w_0) \subseteq K$, we may take the constant sequence $v_{0,N} = w_0 \in H^s(\Omega) = \mathbb{V}_V$, which trivially satisfies the conditions (i)-(iii) in Theorem 2. 

Proof of Corollary 4. The Gaussian wavelet series prior (15) has RKHS equal to

$$\mathbb{V}_V = \left\{ h = \sum_{l=J_0}^J \sum_{r \in R_l} h_{l,r} \psi_{l,r} : \|h\|^2_{\mathbb{V}_V} = \sum_{l=J_0}^J \sum_{r \in R_l} 2^{2l}s h_{l,r}^2 < \infty \right\},$$
with \( \|h\|_{W^s_V} = \infty \) if \( h \) is not a truncated sum up to level \( J \). Hence \( \mathbb{H}_V \hookrightarrow H^s(\Omega) \) by the wavelet characterization of \( L^2 \)-Sobolev norms. Draws from the prior \((15)\) are finite sums of wavelets \((\psi_r)\), hence \( V \) will almost surely have the same Hölder smoothness as \((\psi_r)\). Thus taking a smooth enough wavelet basis, we have that \( V \) is supported on a separable linear subspace of \( \mathcal{C}^s(\Omega) \), thereby satisfying Condition \( 1 \).

We may therefore apply Theorem \( 2 \). For \( f_0 \in \mathcal{C}^s(\Omega) \), \( w_0 = \Phi^{-1}(f_0) \in \mathcal{C}^s(\Omega) \) by \((85)\) (which applies also to \( \Phi^{-1} \) and \( \text{supp}(w_0) \subseteq K \subseteq 0_0 \)). Set

\[
\psi_{0,N}(x) = \sum_{l=J_0}^J \sum_{r \in R_l} \langle w_0, \psi_{rJ} \rangle_{2} \psi_{rJ}(x),
\]

the wavelet projection at resolution level \( J \). In particular, \( \|\psi_{0,N}\|_{W^s_V} \approx \|\psi_{0,N}\|_{H^s} \leq \|w_0\|_{H^s} < \infty \). Moreover, using that \( w_0 = \chi w_0 \) and the standard Besov space embeddings \( B_{\infty \infty}^{r} \hookrightarrow \ell^r \hookrightarrow B_r^{\infty} \) for all \( r \geq 0 \), we have

\[
\|w_0 - \chi_{\psi_{0,N}}\|_{C^k} \lesssim \|w_0 - \chi_{\psi_{0,N}}\|_{C^k} \leq \sum_{l=J+1}^{\infty} 2^{l(k+d/2)} \max_{r \in R_l} |\langle w_0, \psi_{rJ} \rangle_{2}| \lesssim \|w_0\|_{B_{\infty \infty}^{r}} \sum_{j=J+1}^{\infty} 2^{-l(s-k)} \lesssim \|w_0\|_{C^s} 2^{-J(s-k)} \lesssim N^{-\frac{k}{d+s}}
\]

since \( 2^J \approx N^{\frac{d}{d+s}} \). Together these verify conditions (i)-(iii) of Theorem \( 2 \), thereby giving the desired result. \( \square \)

10. Appendix

10.1. Proof of Theorem \( 6 \): minimax lower bound. We go along a classical scheme via the usual Assouad cube technique, see for instance Tsybakov [62].

Step 1: Pick a cube \([c_1, c_2]^d \subset \mathcal{K}\) and a smooth wavelet \( \psi \) with compact support on \( \mathbb{R} \). Set \( \psi_{J,k} = 2^{J/2}(2^{J/2} - k) \) and denote by \( K \) a maximal set of indices \( k \) such that \( \text{supp}(\psi_{J,k}) \subset [c_1, c_2] \) for all \( k \in K \), and \( \text{supp}(\psi_{J,k}) \cap \text{supp}(\psi_{J,k'}) = \emptyset \) for every \( k, k' \in K \) with \( k \neq k' \). For \( \ell = (\ell_1, \ldots, \ell_d) \in (K_J)^d \), set

\[
\psi_{J,\ell}(x) = \prod_{i=1}^d \psi_{J,\ell_i}(x^i), \quad x = (x^1, \ldots, x^d) \in \mathbb{O},
\]

so that \( \text{supp}(\psi_{J,\ell}) \subset [c_1, c_2]^d \) and \( \text{supp}(\psi_{J,\ell}) \cap \text{supp}(\psi_{J,\ell'}) = \emptyset \) for \( \ell \neq \ell' \) in \( (K_J)^d \). For \( \varepsilon = (\varepsilon_{(\ell_1, \ldots, \ell_d)} : \ell_1, \ldots, \ell_d \in K_J) \in \{-1, 1\}^{K_J^d} \), we set

\[
f_{\varepsilon}(x) = 1 + \gamma \sum_{(\ell_1, \ldots, \ell_d) \in (K_J)^d} \varepsilon_{(\ell_1, \ldots, \ell_d)} \psi_{J,\ell_1}(\ell_1, \ldots, \ell_d), \quad \varepsilon_{(\ell_1, \ldots, \ell_d)} \in \{-1, 1\}.
\]

Taking \( \gamma \approx N^{-1/2} \) and \( 2^J \approx N^{1/(2s+d)} \), we have \( f_{\varepsilon} \in \mathcal{C}_0 \cap \{f : \|f\|_{C^s} \leq M\} \) by choosing prefactors sufficiently small to accomodate constants.
Step 2: For an arbitrary estimator \( \hat{f}_N \), we repeat the classical argument to bound the maximal \( L^2 \) risk. We have

\[
\sup_{f \in \mathcal{F}_0 \cap \{ f \| f \|_{e^*} \leq M \}} \mathbb{E}_f [||\hat{f}_N - f||_2^2] \geq \max_{\varepsilon \in \{-1,1\}^{|K_j|^d}} \mathbb{E}_{f_{x}} [||\hat{f}_N - f_{x}\|_2^2]
\]

\[
\geq \frac{1}{2|K_j|^d} \sum_{(\ell_1, \ldots, \ell_d) \in (K_j)^d} \sum_{\varepsilon \in \{-1,1\}^{|K_j|^d}} \int_{\sup(\psi_{\ell_1, \ldots, \ell_d})} \mathbb{E}_{f_{x}} [||\hat{f}_N - f_{x}\|_2^2] dx.
\]

For a given configuration \((\ell_1, \ldots, \ell_d)\), we write \( \varepsilon = (\varepsilon_{(\ell_1, \ldots, \ell_d)}, \varepsilon_{(\ell_1, \ldots, \ell_d)}) \in \{-1,1\}^{|K_j|^d} \) with \( \varepsilon_{(\ell_1, \ldots, \ell_d)} \in \{-1,1\} \), possibly after reordering. It follows that

\[
\sum_{\varepsilon \in \{-1,1\}^{|K_j|^d-1}} \int_{\sup(\psi_{\ell_1, \ldots, \ell_d})} \mathbb{E}_{f_{x}} [||\hat{f}_N - f_{x}\|_2^2] dx
\]

\[
= \sum_{\varepsilon \in \{-1,1\}^{|K_j|^d-1}} \int_{\sup(\psi_{\ell_1, \ldots, \ell_d})} \left( \mathbb{E}_{f_{(\ell_1, \ldots, \ell_d),1}} [||\hat{f}_N - f_{(\ell_1, \ldots, \ell_d),1}\|_2^2] + \mathbb{E}_{f_{(\ell_1, \ldots, \ell_d),-1}} [||\hat{f}_N - f_{(\ell_1, \ldots, \ell_d),-1}\|_2^2] \right) dx
\]

\[
\geq \frac{1}{2} \sum_{\varepsilon \in \{-1,1\}^{|K_j|^d-1}} \int_{\sup(\psi_{\ell_1, \ldots, \ell_d})} \left[ f_{(\ell_1, \ldots, \ell_d),1}(x) - f_{(\ell_1, \ldots, \ell_d),-1}(x) \right]^2 dx
\]

\[
\times e^{-\rho} \left( 1 - (1 - e^{-\rho})^{-1} \|f_{(\ell_1, \ldots, \ell_d),1} - f_{(\ell_1, \ldots, \ell_d),-1}\|_{TV} \right)
\]

for any \( \rho > 0 \), as follows by triangle inequality and classical information bounds, see e.g. [30] Section 5. From

\[
\int_{\sup(\psi_{\ell_1, \ldots, \ell_d})} \left[ f_{(\ell_1, \ldots, \ell_d),1}(x) - f_{(\ell_1, \ldots, \ell_d),-1}(x) \right]^2 dx = 4\gamma^2 \|\psi_{(\ell_1, \ldots, \ell_d)}\|_{L^2}^2 \simeq \gamma^2,
\]

we infer

\[
\sup_{f \in \mathcal{F}_0 \cap \{ f \| f \|_{e^*} \leq M \}} \mathbb{E}_f [||\hat{f}_N - f\|_2^2] \gtrsim 2^d \gamma^2 \simeq N^{-2s/(2s+d)}
\]

by taking \( \rho \) sufficiently large and using \( |K_j| \simeq 2^d \), provided the total variation is bounded away from 1 uniformly in \( \varepsilon \).

Step 3: Write \( g_\varepsilon = f_{(\ell_1, \ldots, \ell_d),1} \) and \( h_\varepsilon = f_{(\ell_1, \ldots, \ell_d),-1} \). It remains to bound

\[
\|P_{g_\varepsilon} - P_{h_\varepsilon}\|_{TV} \leq 2E_{g_\varepsilon} \left[ \log \frac{dP_{g_\varepsilon}}{dP_{h_\varepsilon}} \right] = 2NE_{g_\varepsilon} \left[ \log \frac{dP_{g_\varepsilon}(X_0, X_D)}{P_{h_\varepsilon}(X_0, X_D)} \right]
\]

by Pinsker’s inequality and the fact that the diffusion is stationary for the last equality. We plan to apply a slight modification of Theorem 7 having \( \varepsilon_N = N^{-1/2} \) for subsets \( \mathcal{E}_N \) of the form \( \|f - f_0\|_2 \leq \varepsilon_N \) and \( \|f - f_0\|_\infty \to 0 \), the rest being unchanged. This is simply done by revisiting Step 1 in the proof of Proposition 18. Indeed, it suffices to notice that

\[
E_{f_0} \left[ \log \frac{f_0(X_{(i-1)}D)}{f(X_{(i-1)}D)} - \left( \frac{f_0(X_{(i-1)}D)}{f(X_{(i-1)}D)} - 1 \right) \right] \lesssim \|f_0 - f\|_2^2
\]

for \( \|f - f_0\|_\infty \) sufficiently small, as follows from \( |\log \kappa - (\kappa - 1)| \leq C(\kappa - 1)^2 \) in a neighbourhood of \( \kappa = 1 \), together with the property \( f \geq f_{\text{min}} \). Here, we used the fact that since \( X_0 \) is distributed according to the invariant measure of the process, which is uniform over , the process is stationary
and $X_{(i-1)D}$ is uniformly distributed over $\emptyset$ as well. We apply the result to $f_0 = g_\varepsilon$ and $f = h_\varepsilon$ and check that under the sampling assumption $D = N^{-a}$ with $1/2 < a < 1$, we have $E_N \lesssim N^{-1}$.

The result follows.

10.2. Proof of Theorem 10. If $f \in \mathcal{F}_0$ and $\|f\|_{C^1} \leq M$, we have $0 \leq f(x) \leq M$ for every $x \in \emptyset$. By construction, we also have $0 \leq \bar{f}_N(x) \leq M$ for every $x \in \emptyset$. It follows that

$$\mathbb{E}_f[\|\bar{f}_N - f\|_2^2] \leq \mathbb{E}_f[\|\bar{f}_N - f\|_2^2 1_{B_N}] + 2M^2 \mathbb{P}_f(B_N),$$

where $B_N$ is the event in (72). A glance at the proof of Lemma 26 shows that we in fact have the rate

$$\sup_{f \in \mathcal{F}} \mathbb{P}_f(B_N^c) \lesssim e^{-2jd} \lesssim N^{-1},$$

hence the second term has a negligible order. Next, $|\bar{f}_N(x) - f(x)| = |\min(\bar{f}_N(x), M) - f(x)| \leq |\bar{f}_N(x) - f(x)|$ since $0 \leq f(x) \leq M$. Therefore,

$$\mathbb{E}_f[\|\bar{f}_N - f\|_2^2 1_{B_N}] \leq \mathbb{E}_f[\|\bar{f}_N - f\|_2^2 1_{B_N}] \lesssim \|f - \overline{P}_J f\|_2^2 + \mathbb{E}_f[\|\bar{f}_N - \overline{P}_J f\|_2^2 1_{B_N}],$$

where $\overline{P}_J f$ denotes the projection (24). The first term is of order $2^{-2Js} \approx N^{-2s/(2s + d)}$ by wavelet approximation since the Daubechies wavelet has at least $|s| - 1$ vanishing moments, and thus has the right order. The second term also has the right order as a direct consequence of Theorem 9.

10.3. Proof of Lemma 24. Set

$$Y_t = X_0 + \int_0^t b(\nabla f(X_s), X_s) ds + \int_0^t \sqrt{2f(X_s)} dB_s.$$

Then $(X, \ell)$ is solution of the Skorokhod problem for $(\emptyset, n, Y)$ since

$$X_t = Y_t + \int_0^t n(X_s) d\ell_s,$$

and the Skorokhod mapping: $\Gamma : Y \mapsto X = \Gamma Y$ is uniquely defined see e.g. Lions and Sznitman [37]. Moreover, we have $\Omega_\delta(\Gamma Y) \leq \Omega_\delta(Y)$, where

$$\Omega_\delta(\psi) = \sup_{0 \leq s, t \leq T; |t - s| \leq \delta} |\psi(t) - \psi(s)|$$

denotes the modulus of continuity of $\psi : [0, T] \rightarrow \mathbb{R}^d$, so that it suffices to prove (61) for $Y$ instead of $X$. We bound the first term by

$$\sup_{s \leq u \leq t} \left| \int_s^u \nabla f(X_v) dv \right|^p \leq C_\psi^p (1 + \|f\|_{C^1})^p (t - s)^p$$

uniformly over $b \in \mathcal{B}$. For the second term, we apply the Burkholder-Davis-Gundy inequality to obtain

$$\mathbb{E}_f \left[ \sup_{s \leq u \leq t} \left| \int_s^u \sqrt{2f(X_v)} dB_v \right|^p \middle| \mathcal{F}_s \right] \leq c_p^p t^{p/2} p^{p/2} \mathbb{E}_f \left[ \int_s^t f(X_u) du \right]^{p/2} \left| \mathcal{F}_s \right|$$

$$\leq c_p^p t^{p/2} p^{p/2} \|f\|_{C^1}^p (t - s)^{p/2}.$$
10.4. Proof of Lemma 25. Consider the process \((\tilde{X}_t)_{t \geq 0}\) defined in (31). On \(A_{i,D}\), the two paths \((X_t - X_{(i-1)D})_{t \geq (i-1)D}\) and \((\tilde{X}_t - X_{(i-1)D})_{t \geq (i-1)D}\) coincide for \(t - (i-1)D \leq \tau_{i,D}\). Using that \(\text{dist}(O^0, \partial O) \geq \delta/2\), it follows that
\[
P_{f_0}(\tau_{i,D} \geq D, A_{i,D}) \leq P_{f_0}\left( \sup_{0 \leq t \leq D} |\tilde{X}_{(i-1)D+t} - X_{(i-1)D}|^2 > \frac{\delta}{4}, X_{(i-1)D} \in O^0_\delta \right)
\leq \sup_{x \in O^0_\delta} P_{f_0}\left( \sup_{0 \leq t \leq D} |\tilde{X}_t - x|^2 > \frac{\delta}{4} \mid X_0 = x \right),
\]
by the Markov property. By Itô’s formula, we further have
\[
\sup_{0 \leq t \leq D} |\tilde{X}_t - x|^2 \leq 2b^2(1 + \text{diam}(O) + \|f_0\|_{c^1})^2 D^2 + 2 \sup_{0 \leq t \leq D} \int_0^t (2f_0(\tilde{X}_s))^{1/2} dB_s^2,
\]
and hence
\[
P_{f_0}\left( \sup_{0 \leq t \leq D} |\tilde{X}_t - x|^2 \geq \frac{1}{4} \delta^2 \mid X_0 = x \right) \leq P_{f_0}\left( \sup_{0 \leq t \leq D} |M_t(g)|^2 \geq \frac{1}{2} \delta^2 - C_{f_0} D^2 \mid X_0 = x \right)
\leq P_{f_0}\left( \sup_{0 \leq t \leq D} |M_t(f_0)|^2 \geq \frac{1}{8} \delta^2 \mid X_0 = x \right)
\]
for small enough \(D\), where \(M_t(f_0) = \int_0^t (2f_0(\tilde{X}_s))^{1/2} dB_s\) is a \(d\)-dimensional martingale with predictable bracket \(\langle M_t^i, f_t^j \rangle_t = 2 \int_0^t f_0(\tilde{X}_s) dB_s^i dB_s^j \leq 2\|f_0\|_{c^2} \delta \). It follows that for any \(x \in O^0_\delta:\)
\[
P_{f_0}\left( \sup_{0 \leq t \leq D} M_t \geq x, \langle M \rangle_t \leq y \right) \leq e^{-x^2/(2y)}
\]
(see e.g. [52] p.154).

10.5. A generic chaining inequality and the event \(B_N\). In several places, we require the following concentration inequality, which is based on a chaining argument for stochastic processes with mixed tails, see Theorem 2.2.28 in [60] or Theorem 3.5 in [22].

Lemma 32. Let \(S \subset L^2(O)\) be a finite-dimensional linear space with dimension \(\dim(S) = m < \infty\). Let \(Z = (Z(g) : g \in \mathcal{G})\) be a stochastic process with index set \(\mathcal{G} \subset S\) satisfying \(\|\mathcal{G}\|_2 = \sup_{g,h \in \mathcal{G}} \|g - h\|_2 < \infty\). Suppose that \(Z\) satisfies for all \(g, h \in \mathcal{G}\) and \(t \geq 0\),
\[
P \left( \|Z(g) - Z(h)\| \geq t \right) \leq C \exp \left( -\frac{ct^2}{\alpha^2 \|g - h\|_2^2 + \beta \|g - h\|_2 t} \right),
\]
where \(C, c, \alpha, \beta > 0\). Then for any \(g_0 \in \mathcal{G}\) and all \(u \geq 1\),
\[
P \left( \sup_{g \in \mathcal{G}} |Z(g) - Z(g_0)| \geq K \left( m\beta + \sqrt{m\alpha} + \beta u + \alpha \sqrt{u} \right) \right) \leq e^{-u},
\]
where \(K\) depends only on \(C\) and \(c\).
Proof. Let \((e_k : 1 \leq k \leq m)\) be an \(L^2\)-orthonormal basis for \(S\). After rearranging, the Bernstein inequality implies that for \(C_1, C_2 > 0\) large enough, depending only on \(C\) and \(c\),

\[
P \left( \|Z(g) - Z(h)\| \geq C_1 \beta u \|g - h\|_2 + C_2 \alpha \sqrt{u} \|g - h\|_2 \right) \leq 2 e^{-u}
\]

holds for all \(u \geq 0\). The process \(Z\) therefore has a \textit{mixed tail} as in (3.8) of Dirksen \cite{22} with respect to the metrics

\[
d_1(g, h) = C_1 \beta \|g - h\|_2 = C_1 \beta \langle g - h, e_k \rangle_2 \|e_k\|_2, \\
d_2(g, h) = C_2 \alpha \|g - h\|_2 = C_2 \alpha \|g - h, e_k \rangle_2 \|e_k\|_2,
\]

where the last equalities follow from Parseval’s theorem and \(\| \cdot \|_m\) is the Euclidean norm on \(\mathbb{R}^m\). The \(d_1\) and \(d_2\)-diameters of \(\mathcal{G}\) are therefore bounded by \(\Delta_{d_1}(\mathcal{G}) \leq C_1 \beta \|\mathcal{G}\|_2\) and \(\Delta_{d_2}(\mathcal{G}) \leq C_2 \alpha \|\mathcal{G}\|_2\), respectively. Theorem 3.5 of [22] thus yields that for absolute constants \(C', c' > 0\) and any \(u \geq 1\),

\[
P \left( \sup_{g \in \mathcal{G}} |Z(g) - Z(g_0)| \geq C' \gamma_1(\mathcal{G}, d_1) + C' \gamma_2(\mathcal{G}, d_2) + c' C_1 \beta \|\mathcal{G}\|_2 u + c' C_2 \alpha \|\mathcal{G}\|_2 \sqrt{u} \right) \leq e^{-u},
\]

where \(\gamma_1, \gamma_2\) are the ‘generic chaining functionals’ defined in [22]. In particular, (2.3) of [22] gives the estimate \(\gamma_1(\mathcal{G}, d_1) \leq C(\alpha) \int_0^\infty (\log \mathcal{N}(\mathcal{G}, d_1, \varepsilon))^{1/\alpha} d\varepsilon\), where \(\mathcal{N}(\mathcal{G}, d_1, \varepsilon)\) denotes the covering number of the set \(\mathcal{G}\), i.e. the smallest number of \(d_1\)-balls of radius \(\varepsilon\) needed to cover \(\mathcal{G}\). Since \(\mathcal{G} \subset \mathcal{S}\) and \(\mathcal{S}\) is a finite-dimensional linear space, the second-last display implies that

\[
\mathcal{N}(\mathcal{G}, d_1, \varepsilon) \leq \mathcal{N}(\{ x \in \mathbb{R}^m : \|x\|_2 \leq \|\mathcal{G}\|_2 \}, C_1 \beta \|\mathcal{G}\|_2 \varepsilon),
\]

and likewise for \(d_2\). Using for instance Proposition 4.3.34 in the textbook [27] to bound the log-covering number of a ball in finite-dimensional Euclidean space,

\[
\gamma_1(\mathcal{G}, d_1) \lesssim \int_0^\infty \log \mathcal{N}(\{ x \in \mathbb{R}^m : \|x\|_2 \leq \|\mathcal{G}\|_2 \}, C_1 \beta \|\mathcal{G}\|_2 \varepsilon) d\varepsilon \\
\quad \leq \int_0^{\Delta_{d_1}(\mathcal{G})} m \log \left( \frac{3 \Delta_{d_1}(\mathcal{G})}{\varepsilon} \right) d\varepsilon = m \Delta_{d_1}(\mathcal{G}) \int_0^1 \log(3/\alpha) d\alpha \lesssim m C_1 \beta \|\mathcal{G}\|_2.
\]

Similarly,

\[
\gamma_2(\mathcal{G}, d_2) \lesssim \int_0^{\Delta_{d_2}(\mathcal{G})} \sqrt{m \log \left( \frac{3 \Delta_{d_2}(\mathcal{G})}{\varepsilon} \right)} d\varepsilon = \sqrt{m} \Delta_{d_2}(\mathcal{G}) \int_0^1 \sqrt{\log(3/\alpha) d\alpha} \lesssim \sqrt{m} C_2 \alpha \|\mathcal{G}\|_2.
\]

Substituting these bounds into the exponential inequality derived above then gives the result. \(\square\)

10.6. Proof of Lemma 26. We have

\[
\begin{align*}
P_f(\mathcal{B}_N') &\leq P_f(\exists g \in V_J : (1 - \kappa) \|g\|_2^2 > |g(N)^2|) + P_f(\exists g \in V_J : |g|^2 > (1 + \kappa) \|g\|_2^2) \\
&= P_f(\exists g \in V_J : \|g\|_2 = 1, 1 - \kappa > |g(N)^2|) + P_f(\exists g \in V_J : \|g\|_2 = 1, |g|^2 > 1 + \kappa) \\
&= 2 \sup_{g \in V_J, \|g\|_2 = 1} \left| |g(N)^2| - 1 \right| > \kappa \\
&= 2 \sup_{g \in V_J, \|g\|_2 = 1} \left| \sum_{i=1}^N (g(X_iD)^2 - \mathbb{E}_f[g(X_iD)^2]) \right| > \kappa N.
\end{align*}
\]
since $\mathbb{E}_f[g(X_{1D})^2] = \int_0^1 g(x)^2 dx = 1$ by stationarity. Write $\mathcal{G}_f = \{g \in V_f : \|g\|_2 = 1\}$ and define the process $Z_N = (Z_N(g) : g \in \mathcal{G}_f)$ by

$$Z_N(g) = \sum_{i=1}^{N} (g(X_{iD})^2 - \mathbb{E}_f[g(X_{iD})^2]).$$

For $g, h \in \mathcal{G}_f$, we have $\mathbb{E}_f[g(X_{iD})^2 - h(X_{iD})^2] = 0$ and $\text{Var}_f(g(X_{iD})^2 - h(X_{iD})^2) = \|g^2 - h^2\|^2_2$. Since $(X_0, X_D, \ldots, X_{ND})$ is a stationary reversible Markov chain whose spectral gap is lower bounded by $rD$ by (9), Theorem 3.3 of [44] (cf. (3.21)) yields

$$\mathbb{P}_f(\|Z_N(g) - Z_N(h)\| \geq t) = \mathbb{P}_f \left( \left| \sum_{i=1}^{N} (g(X_{iD})^2 - h(X_{iD})^2) \right| \geq t \right)$$

$$\leq 2 \exp \left( -\frac{\lambda_f D t^2}{4N\|g^2 - h^2\|_2^2 + 10\|g - h\|_\infty t} \right)$$

$$\leq 2 \exp \left( -\frac{\lambda_f D t^2}{4N\|g + h\|_\infty^2 \|g - h\|_2^2 + 10\|g + h\|_\infty \|g - h\|_\infty t} \right)$$

$$\leq 2 \exp \left( -\frac{Ct^2}{N2^{fD}D^{-1}\|g - h\|_2^2 + 2^{fD}D^{-1}\|g - h\|_2t} \right)$$

using that $\|g\|_\infty \leq C2^{fD/2}\|g\|_2 = C2^{fD/2}$ for $g \in \mathcal{G}_f$, and where $C$ depends on $r$, and hence $f_{\min}$ and $\mathcal{O}$ by (9). Applying Lemma 32 with $m = \dim(V_f) = O(2^{fD})$, $\|g\|_2 = \sup_{g,h \in \mathcal{G}_f} \|g - h\|_2 \leq 2$, $\alpha = N2^{fD}D^{-1}$, $\beta = 2^{fD}D^{-1}$ and $u = 2^{fD}$ thus gives

$$\mathbb{P}_f \left( \sup_{g \in \mathcal{G}_f} \|Z_N(g)\| \geq C \left( 2^{fD}D^{-1} + 2^{fD}N^{1/2}D^{-1/2} \right) \right) \leq e^{-2^{fD}} \to 0$$

since $2^f \to \infty$ as $N \to \infty$. Since $2^{fD}$ is by assumption, the right-hand side within the last probability is $o(N)$ as $N \to \infty$. Together with (89) this gives the result.

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