GAIN FUNCTION APPROXIMATION IN THE FEEDBACK PARTICLE FILTER

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Abstract. This paper is concerned with numerical algorithms for the problem of gain function approximation in the feedback particle filter. The exact gain function is the solution of a Poisson equation involving a probability-weighted Laplacian. The numerical problem is to approximate this solution using only particles sampled from the probability distribution. A diffusion-map based algorithm is presented for this problem. The algorithm does not require approximation of the probability distribution as an intermediate step. A procedure for carrying out error analysis of the approximation is introduced and certain asymptotic estimates for bias and variance are derived. The paper contains some comparative numerical results for a problem with non-Gaussian distribution. The algorithm is also applied and illustrated for a numerical filtering example.

Key words. Stochastic Processes, Nonlinear filtering, Poisson equation

1. Introduction. This paper is concerned with a numerical solution of a certain partial differential equation (pde) that arises in nonlinear filtering problem in continuous-time settings.

Nonlinear filtering problem: The standard model of the nonlinear filtering problem is given by the following stochastic differential equations (sde):

\begin{align}
\text{(1.1a) State process:} & \quad dX_t = a(X_t) \, dt + dB_t, \quad X_0 \sim p_0 \\
\text{(1.1b) Observation process:} & \quad dZ_t = h(X_t) \, dt + dW_t,
\end{align}

where \( X_t \in \mathbb{R}^d \) is the (hidden) state at time \( t \), \( Z_t \in \mathbb{R} \) is the observation, and \( B_t \), \( W_t \) are two mutually independent standard Wiener processes taking values in \( \mathbb{R}^d \) and \( \mathbb{R} \), respectively. The mappings \( a(\cdot) : \mathbb{R}^d \to \mathbb{R}^d \) and \( h(\cdot) : \mathbb{R}^d \to \mathbb{R} \) are known \( C^1 \) functions, and \( p_0 \) is the density of the prior probability distribution.

The objective of the filtering problem is to compute the posterior distribution of the state \( X_t \) given the time history of observations (filtration) \( Z_t := \sigma(Z_s : 0 \leq s \leq t) \).

The problem is linear Gaussian if \( a(\cdot) \), and \( h(\cdot) \) are linear functions and \( p_0 \) is a Gaussian density. We use \( A \) and \( H \) to denote the matrices that define these linear functions, i.e, \( a(x) = Ax \) and \( h(x) = Hx \). The background on the linear Gaussian problem, along with its solution given by the Kalman-Bucy filter [30], appears in [34].

Feedback particle filter (FPF) is a numerical algorithm to approximate the posterior distribution in nonlinear non-Gaussian settings. Its construction is based on the following two steps:

Step 1: Construct a stochastic process, denoted by \( \tilde{X}_t \in \mathbb{R}^d \), whose posterior distribution (given \( Z_t \)) is equal to the posterior distribution of \( X_t \);

Step 2: Simulate \( N \) stochastic processes, denoted by \( \{X^i_t\}_{i=1}^N \), to empirically approximate the distribution of \( \tilde{X}_t \).
\[
\mathbb{E}[f(X_t) | Z_t] \overset{\text{Step 1}}{=} \mathbb{E}[f(\hat{X}_t) | Z_t] \overset{\text{Step 2}}{=} \frac{1}{N} \sum_{i=1}^{N} f(X_t^i)
\]

The process \(\hat{X}_t\) is referred to as mean-field process and the \(N\) processes \(\{X_t^i\}_{i=1}^{N}\) are referred to as particles. The construction ensures that the filter is exact in the mean-field (\(N = \infty\)) limit.

The details of the two steps are as follows:

**Mean-field process:** In the FPF, the mean-field process \(\hat{X}_t\) evolves according to the sde given by

\[
d\hat{X}_t = a(\hat{X}_t) \, dt + dB_t + K_t(\hat{X}_t) \circ (dZ_t - \frac{h(\hat{X}_t) + \hat{h}_t}{2} \, dt), \quad \hat{X}_0 \sim p_0
\]

where \(B_t\) is a standard Wiener processes independent of \(\hat{X}_0\) and \(\hat{h}_t := \mathbb{E}[h(\hat{X}_t) | Z_t]\). The \(\circ\) indicates that the sde is expressed in its Stratonovich form. The gain function \(K_t(x) := \nabla \phi_t(x)\) where \(\phi_t\) is the solution of the Poisson equation:

\[
\text{(1.3) Poisson equation: } - \frac{1}{p_t(x)} \nabla \cdot (p_t(x) \nabla \phi_t(x)) = -(h(x) - \hat{h}_t) \quad \forall \ x \in \mathbb{R}^d
\]

where \(\nabla\) and \(\nabla \cdot\) denote the gradient and the divergence operators, respectively, and \(p_t\) denotes the conditional density of \(\hat{X}_t\) given \(Z_t\).

**Particles:** The particles \(\{X_t^i\}_{i=1}^{N}\) evolve according to:

\[
dX_t^i = a(X_t^i) \, dt + dB_t^i + K_t^{(N)}(X_t^i) \circ (dZ_t - \frac{h(X_t^i) + \hat{h}_t^{(N)}}{2} \, dt), \quad X_0^i \overset{\text{i.i.d}}{\sim} p_0
\]

for \(i = 1, \ldots, N\), where \(\{B_t^i\}_{i=1}^{N}\) are mutually independent Wiener processes, \(\hat{h}_t^{(N)} := \frac{1}{N} \sum_{i=1}^{N} h(X_t^i)\), and \(K_t^{(N)}\) is the output of an algorithm that approximates the solution to the Poisson equation (1.3)

\[
(1.5) \quad \text{Gain function approximation: } K_t^{(N)} := \text{Algorithm}(\{X_t^i\}_{i=1}^{N}; h)
\]

The notation is suggestive of the fact that algorithm is adapted to the ensemble \(\{X_t^i\}_{i=1}^{N}\) and the function \(h\); the density \(p_t(x)\) is not known in an explicit manner.

Development and error analysis of one such gain function approximation algorithm is the subject of the present paper. Before describing the general case, it is useful to review the filter for the linear Gaussian case where the solution to the Poisson equation is explicitly known.

**FPF for Linear Gaussian setting:** Suppose \(h(x) = Hx\) and \(p_t\) is a Gaussian density with mean \(\tilde{m}_t\) and variance \(\Sigma_t\). Then the solution of the Poisson equation is known in an explicit form [59, Sec. D]. The resulting gain function is constant and equal to the Kalman gain:

\[
K_t(x) \equiv \Sigma_t H^T \quad \forall \ x \in \mathbb{R}^d
\]

Therefore, the mean-field process (1.2) for the linear Gaussian problem is given by:

\[
d\hat{X}_t = A\hat{X}_t \, dt + dB_t + \Sigma_t H^T (dZ_t - \frac{H\hat{X}_t + H\hat{m}_t}{2} \, dt), \quad \hat{X}_0 \sim p_0
\]
Given the explicit form of the gain function (1.6), the empirical approximation of the gain is simply
\[ K_t^{(N)} = \Sigma_t^{(N)} H^\top \] where \( \Sigma_t^{(N)} \) is the empirical covariance of the particles. Therefore, the evolution of the particles is:

\[ dX_t^i = AX_t^i \, dt + dB_t^i + K_t^{(N)} (dZ_t - \frac{HX_t^i + Hm_t^{(N)}}{2} \, dt), \quad X_0^i \overset{i.i.d}{\sim} p_0 \]

for \( i = 1, \ldots, N \), where \( m_t^{(N)} \) is the empirical mean of the particles. The empirical quantities are computed as:

\[ m_t^{(N)} := \frac{1}{N} \sum_{j=1}^{N} X_t^j, \quad \Sigma_t^{(N)} := \frac{1}{N-1} \sum_{j=1}^{N} (X_t^j - m_t^{(N)})(X_t^j - m_t^{(N)})^\top \]

The linear Gaussian FPF (1.7) is identical to the square-root form of the ensemble Kalman filter (EnKF) [8, Eq. 3.3].

One extension of the Kalman gain is the so called constant gain approximation formula whereby the gain \( K_t \) is approximated by its expected value (which represents the best least-squared approximation of the gain by a constant). Remarkably, the expected value admits a closed-form expression which is then readily approximated empirically using the particles:

\[ \text{Const. gain approx:} \quad E[K_t(X_t)|Z_t] = \int_{\mathbb{R}^d} (h(x) - \hat{h}) \, x \, p_t(x) \, dx \approx \frac{1}{N} \sum_{i=1}^{N} (h(X_t^i) - \hat{h}^{(N)}) \, X_t^i \]

The constant gain approximation formula has been used in nonlinear extensions of the EnKF algorithm [19]. The connection to the Poisson equation provides a justification for this formula. The formula is attractive because it provides a consistent (as the number of particles \( N \to \infty \)) approximation of the Kalman gain in the linear Gaussian setting.

Design and analysis of the gain function approximation algorithm (1.5) in the general case is a challenging problem because of two reasons: (i) Apart from the Gaussian case, there are no known closed-form solutions of (2.1); (ii) The density \( p_t(x) \) is not explicitly known. At each time-step, one only has samples \( \{X_t^i\}_{i=1}^{N} \). For the purpose of this paper, these samples are assumed to be i.i.d drawn from \( p_t \). The assumption is justified because in the limit of large \( N \), the particles are approximately i.i.d (by the propagation of chaos); cf., [51].

1.1. Literature survey. Apart from its direct relevance to numerical approximation of the FPF, there are three topics of current research interest that are relevant to the subject of this paper: (i) ensemble Kalman filter; (ii) particle flow algorithms for nonlinear filtering; and (iii) optimal transport. Specifically, the algorithms for gain function approximation described in this paper are also directly applicable to these other topics. These relationships are briefly discussed next:

**Ensemble Kalman filter:** The EnKF algorithm was first developed in the discrete-time setting [23]. In the continuous-time setting, two formulations of the EnKF have been developed: stochastic EnKF, and the more recent deterministic EnKF [9, 44].
As has already been noted, the deterministic EnKF is in fact identical to the FPF algorithm (1.7) in the linear Gaussian setting [9, 52].

The EnKF algorithm provides a consistent approximation in the linear Gaussian setting. Compared to the Kalman filter, the main utility of EnKF is that it does not require propagation of the covariance matrix. This reduces the computational complexity from $O(d^2)$ for the Kalman filter to $O(Nd)$. This is clearly advantageous in high dimensional problems when $N << d$. This property has made EnKF popular in applications such as weather prediction in high dimensional settings [31, 41]. The disadvantage of the EnKF algorithm, of course, is that it does not provide a consistent approximation for nonlinear problems.

FPF represents a the generalization of the EnKF to the nonlinear non-Gaussian setting [52]: With the constant gain approximation, the algorithms are identical. Given this parallel, the problem of improving the EnKF algorithm in more general nonlinear non-Gaussian settings is directly related to the problem of better approximating the gain function in the FPF. In an application software based on EnKF, it is a relatively simple matter to replace the constant gain formula for the gain by more sophisticated approximations described in this paper. Certain empirical evaluations on the performance of FPF in high-dimensional settings are reported in [50, 48, 47, 10].

Error analysis and stability of EnKF is an active area of research; see [37, 35, 21] for linear models and [19, 20, 32] for nonlinear models. The error analysis for the gain function approximation reported in this paper is a step towards error analysis of the FPF along these lines.

**Particle flow algorithms:** The following first-order (and hence an under determined) form of the Poisson equation appears in most types of particle flow algorithms:

\[ \nabla \cdot (p_t(x)K(x)) = (\text{rhs}) \]

where the righthand-side (rhs) is given and $K(x)$ defines a vector field that must be obtained to implement the particle flow. The pde appears in the first interacting particle representation of the continuous-time filtering in [15, 16] and the discrete-time filtering in [17]. Stochastic extensions of these have also recently appeared in [18] where approximate solutions are also described based on Gaussian assumption on the density. The algorithm described here represent an approximation of a particular gradient form solution of the first-order pde.

**Optimal transport:** The mean-field sde (1.2) represents a transport that maps the prior distribution at time 0 to the posterior distribution at an (arbitrary) future time $t > 0$. Synthesis of optimal transport maps for implementing the Bayes formula appears in [43, 13, 22, 54, 28, 12]. The relationship with the Poisson equation is through the ensemble transform filter which relies on a linear programming construction to approximate the optimal transport map [13]. As discussed in [52, Sec. 5.5], the solution of the Poisson equation yields an infinitesimal optimal transport map from the “prior” $p_t(x)$ to an un-normalized “posterior” $p_t(x)\exp(-th(x))$. Another closely related approach is optimal transportation is through the Gibbs flow [28].

Directly related to the FPF, the Galerkin method for the numerical solution of the Poisson equation appeared in original papers [59, 60]. The Galerkin algorithm represents the “direct” pde approach to construct a numerical approximation. The constant gain approximation is a particular example of a Galerkin solution. In general, the main problem with the Galerkin approximation is that it requires a selection of basis functions. This becomes intractable in high dimensions. To mitigate this issue,
a proper orthogonal decomposition (POD)-based procedure to select basis functions is introduced in [11] and a continuation scheme for approximation appears in [38]. Certain probabilistic approaches based on dynamic programming appear in [42].

The diffusion-map based algorithm proposed and analyzed here is inspired by the spectral clustering literature [6, 57]. The particular form of the kernel proposed in our paper was introduced in [14]. Convergence analysis for this operator appears in [27, 46, 14, 24, 26, 58, 7].

1.2. Contributions of this paper. We present a new basis-free diffusion-map based algorithm for approximating the solution of the gain function. The key step is to construct a Markov matrix on a graph defined on the space of particles \( \{X_i^t\}_{i=1}^N \). The value of the function \( \phi \) for the particles, \( \phi(X_i^t) \), is then approximated by solving a fixed-point problem involving the Markov matrix. The fixed-point problem is shown to be a contraction and the method of successive approximation applies to numerically obtain the solution. A procedure for carrying out error analysis of the approximation is introduced in this paper. Certain asymptotic estimates for bias and variance are derived. Comparison with the constant gain approximation formula are provided. These results are illustrated with the aid of some numerical experiments.

The outline of the remainder of this paper is as follows: The mathematical problem of the gain function approximation together with a summary of known results on this topic appears in section 2. The diffusion-map based algorithm is described in a self-contained fashion in section 3. The main theoretical results of this paper including the bias and variance estimates appear in section 4. Some numerical experiments for the same appear in section 5. All the proofs appear in the Appendix.

2. Gain function approximation.

2.1. Problem formulation. This mathematical problem is to numerically approximate the solution of the Poisson’s equation (1.3) introduced in section 1 and also repeated below:

\[
-\Delta \rho \phi = h - \hat{h}
\]

where the weighted Laplacian \( \Delta \rho \phi(x) := \frac{1}{\rho(x)} \nabla \cdot (\rho(x)\nabla \phi(x)) \); \( \rho(x) \) is an everywhere positive probability density on \( \mathbb{R}^d \); \( h(x) \) is a real-valued function defined on \( \mathbb{R}^d \) and \( \hat{h} := \int h(x)\rho(x) \, dx \). The function \( \phi \) is referred to as the solution. Its gradient is referred to as the gain function and denoted as \( K(x) := \nabla \phi(x) \). The pde (2.1) is referred to as the Poisson’s equation.

Assumptions: The following assumptions are made throughout the paper:

(i) **Assumption A1**: The probability density \( \rho \) is of the form \( \rho(x) = e^{-V(x)} \) where the function \( V(x) = \frac{1}{2}(x - m)^\top \Sigma^{-1}(x - m) + w(x) \) for some \( m \in \mathbb{R}^d \), \( \Sigma > 0 \), and \( w \in C_0^\infty(\mathbb{R}^d) \);

(ii) **Assumption A2**: The function \( h(x) = c^\top x + \tilde{w}(x) \) where \( c \in \mathbb{R}^d \) and \( \tilde{w} \in C_0^\infty(\mathbb{R}^d) \).

The numerical approximation problem is as follows:

**Problem statement**: Given \( N \) samples \( \{X^1, \ldots, X^i, \ldots, X^N\} \), drawn i.i.d. from \( \rho \), approximate the gains \( \{K^1, \ldots, K^i, \ldots, K^N\} \), where \( K^i := K(X^i) = \nabla \phi(X^i) \). The density \( \rho \) is not known in an explicit form.

2.2. Mathematical preliminaries.
2.2.1. Notation. \( L^2(\rho) \) is the Hilbert space of square integrable functions on \( \mathbb{R}^d \) equipped with the inner-product, \( \langle \phi, \psi \rangle_{L^2} := \int \phi(x)\psi(x)\rho(x) \, dx \). The associated norm is denoted as \( \| \phi \|_2 := \sqrt{\langle \phi, \phi \rangle} \). The space \( H^1(\rho) \) is the space of square integrable functions \( \phi \) whose derivative (defined in the weak sense) is in \( L^2(\rho) \). For a function \( \phi \in L^2(\rho) \), \( \hat{\phi} := \int \phi(x)\rho(x) \, dx \) denotes the mean. \( L^2_0(\rho) := \{ f \in L^2(\rho) \mid \hat{f} = 0 \} \) and \( H^1_0(\rho) := \{ f \in H^1(\rho) \mid \hat{f} = 0 \} \) denote the co-dimension 1 subspace of functions whose mean is zero. \( L^\infty \) denotes the space of bounded functions on \( \mathbb{R}^d \) with associated norm denoted as \( \| \cdot \|_\infty \). The Borel \( \sigma \)-algebra on \( \mathbb{R}^d \) is denoted by \( \mathcal{B}(\mathbb{R}^d) \). The variance of the random variable \( X \) is denoted as \( \text{Var}(X) \).

2.2.2. Spectral representation. Under Assumption (A1), the weighted Laplacian \( \Delta_\rho \) has a discrete spectrum with an ordered sequence of eigenvalues \( 0 = \lambda_0 < \lambda_1 \leq \lambda_2 \leq \ldots \) and associated eigenfunctions \( \{ e_n \} \) that form a complete orthonormal basis of \( L^2(\rho) \) [5, Cor. 4.10.9]. The trivial eigenfunction \( e_0(x) = 1 \), and for \( f \in L^2_0(\rho) \), the spectral representation yields:

\[
- \Delta_\rho f = \sum_{m=1}^{\infty} \lambda_m \langle e_m, f \rangle e_m
\]

The positivity of the smallest non-trivial eigenvalue (\( \lambda_1 > 0 \)) is referred to as the Poincaré inequality (or the spectral gap condition) [4]. The inequality is equivalently expressed as

\[
\int_{\mathbb{R}^d} (f - \hat{f})^2 \rho \, dx \leq \frac{1}{\lambda_1} \int_{\mathbb{R}^d} |\nabla f|^2 \rho \, dx \quad \forall f \in H^1(\rho)
\]

where \( \hat{f} = \int f \rho \, dx \).

The Poincaré inequality is important to show that the Poisson equation is well-posed and a unique solution exists. The solution to the Poisson equation is defined using the weak formulation.

2.2.3. Weak formulation. A function \( \phi \in H^1_0(\rho) \) is said to be a weak solution of (2.1) if

\[
\int \nabla \phi(x) \cdot \nabla \psi(x) \rho(x) \, dx = \int (h(x) - \hat{h})\psi(x)\rho(x) \, dx \quad \forall \psi \in H^1(\rho)
\]

Equation (2.3) is referred to as the weak-form of the Poisson’s equation. The weak-form is expressed succinctly as \( \langle \nabla \phi, \nabla \psi \rangle = \langle h - \hat{h}, \psi \rangle \) where \( \langle \cdot, \cdot \rangle \) is the inner-product in \( L^2(\rho) \). The existence and uniqueness of the solution to the weak-form of the Poisson equation is stated in the following Proposition.

**Proposition 2.1.** [36, Thm. 2.2.] Suppose \( \rho \) satisfies Assumption (A1) and \( h \) satisfies Assumption (A2). Then there exists a unique function \( \phi \in H^1_0(\rho) \) that satisfies the weak-form of the Poisson equation (2.3). The solution satisfies the bound:

\[
\int |\nabla \phi(x)|^2 \rho(x) \, dx \leq \frac{1}{\lambda_1} \int (h(x) - \hat{h})^2 \rho(x) \, dx
\]

The weak formulation has led to the Galerkin algorithm presented in the original FPF papers [59]. A special case of the Galerkin solution is the constant gain approximation formula (1.8). The formula is obtained as the best least-square approximation.
The kernel algorithm presented in this paper is based on the semigroup formulation of the Poisson equation.

2.2.4. Semigroup. Let \( \{P_t\}_{t \geq 0} \) be the semigroup associated with the weighted Laplacian \( \Delta_\rho \). The semigroup allows for a probabilistic interpretation which is described next. Consider the following reversible Markov process \( \{S_t\}_{t \geq 0} \) evolving in \( \mathbb{R}^d \):

\[
dS_t = -\nabla V(S_t) \, dt + \sqrt{2} \, dB_t
\]

where \( V(x) = -\log(\rho(x)) \) and \( \{B_t\}_{t \geq 0} \) is a standard Weiner process in \( \mathbb{R}^d \). Then

\[
P_t f(x) = \mathbb{E}[f(S_t)|S_0 = x]
\]

It is straightforward to verify that \( P_t : L^2(\rho) \rightarrow L^2(\rho) \) is symmetric, i.e., \( \langle P_t f, g \rangle = \langle f, P_t g \rangle \) for all \( f, g \in L^2(\rho) \) and \( \rho(x) = e^{-V(x)} \) is its invariant density. The semigroup also admits a kernel representation:

\[
P_t f(x) = \sum_{m=1}^{\infty} e^{-t\lambda_m} \langle e_m, f \rangle e_m(x) = \int_{\mathbb{R}^d} \tilde{k}_t(x,y)f(y)\rho(y) \, dy
\]

where \( \tilde{k}_t(x,y) := \sum_{m=0}^{\infty} e^{-t\lambda_m} e_m(x)e_m(y) \).

The spectral gap implies that \( \|P_t\|_{L^2_0(\rho)} = e^{-t\lambda_1} < 1 \). Hence, \( P_t \) is a strict contraction on \( L^2_0(\rho) \). For the special case of Gaussian density \( \rho = \mathcal{N}(m, \Sigma) \), the eigenfunctions are given by the Hermite polynomials. This leads to an explicit formula for the kernel \( \tilde{k}_t(x,y) \) in the Gaussian case, as described in Appendix A.

Consider the heat equation

\[
\frac{\partial u}{\partial t} = \Delta_\rho u + (h - \hat{h}), \quad u(0, x) = f(x)
\]

Its solution is given in terms of the semigroup as follows:

\[
u(t, x) = P_t f(x) + \int_0^t P_{t-s}(h - \hat{h})(x) \, ds
\]

Letting \( f(x) = \phi(x) \) where \( \phi \) solves the Poisson equation (2.1) yields the following fixed-point equation for \( t = \epsilon \):

\[
(2.4) \quad (\text{exact fixed-point equation}) \quad \phi = P_\epsilon \phi + \int_0^\epsilon P_s (h - \hat{h}) \, ds
\]

Equation (2.4) is referred to as the semigroup form of the Poisson equation (2.1).

The following Proposition shows that the weak form (2.3) and the semigroup form (2.4) are equivalent. The proof appears in the Appendix B.

**Proposition 2.2.** Suppose \( \rho \) satisfies Assumption (A1) and \( h \) satisfies Assumption (A2). Then the unique solution \( \phi \in H^1_0(\rho) \) to the weak form (2.3) is also the unique solution to the fixed-point equation (2.4).

The semigroup formulation has led to the diffusion-map based algorithm which is the main focus of the remainder of this paper.
3. Diffusion-map based Algorithm. The diffusion-map based algorithm is based on a numerical approximation of the fixed-point equation (2.4). The main technique is to approximate the semigroup $P_\epsilon$ in the following three steps:

1. **Diffusion-map approximation:** A family of Markov operators $\{T_\epsilon\}_{\epsilon > 0}$ are defined as follows:

\[
T_\epsilon f(x) := \frac{1}{n_\epsilon(x)} \int_{\mathbb{R}^d} k_\epsilon(x, y) f(y) \rho(y) \, dy
\]

where $n_\epsilon(x) := \int k_\epsilon(x, y) \rho(y) \, dy$ is the normalization factor,

\[
k_\epsilon(x, y) := \frac{g_\epsilon(x, y)}{\sqrt{\int g_\epsilon(x, z) \rho(z) \, dz} \sqrt{\int g_\epsilon(y, z) \rho(z) \, dz}}
\]

and $g_\epsilon(x, y) := \exp(-\frac{|x-y|^2}{4\epsilon})$ is the Gaussian kernel in $\mathbb{R}$. For small positive values of $\epsilon$, the Markov operator $T_\epsilon$ is referred to as the diffusion map approximation of the exact semigroup $P_\epsilon$ [14, 27]. The precise statement of this approximation is contained in Proposition 3.2. For the special case of Gaussian density, an explicit formula for the diffusion map appears in the Appendix A.

2. **Empirical approximation:** The operator $T_\epsilon$ is approximated empirically by $\{T^{(N)}_\epsilon\}_{\epsilon > 0, N \in \mathbb{N}}$ defined as follows:

\[
T^{(N)}_\epsilon f(x) := \frac{1}{n^{(N)}_\epsilon(x)} \sum_{j=1}^{N} k^{(N)}_\epsilon(x, X^j) f(X^j)
\]

where $n^{(N)}_\epsilon(x) := \sum_{i=1}^{N} k_\epsilon(x, X^i)$ is the normalization factor and

\[
k^{(N)}_\epsilon(x, y) := \frac{g_\epsilon(x, y)}{\sqrt{\sum_{j=1}^{N} g_\epsilon(x, X^j)} \sqrt{\sum_{j=1}^{N} g_\epsilon(y, X^j)}}
\]

Recall that $X^i \overset{i.i.d.}{\sim} \rho$ for $i = 1, \ldots, N$. So, by law of large numbers (LLN), $T^{(N)}_\epsilon f$ represents an empirical approximation of the diffusion map $T_\epsilon$. The precise statement of the empirical approximation is contained in Proposition 3.3.

3. **Approximation as Markov matrix:** An $N \times N$ Markov matrix $T$ is defined with $(i, j)$-th element given by

\[
T_{ij} = \frac{1}{n^{(N)}_\epsilon(X^i)} k^{(N)}_\epsilon(X^i, X^j)
\]

**Finite-dimensional fixed-point equation:** Using the three steps above, the original infinite-dimensional fixed-point equation (2.4) is approximated as a finite dimensional fixed-point equation

\[
\Phi = T\Phi + \epsilon(h - \pi(h))
\]
where \( h := (h(X^1), \ldots, h(X^N)) \) is a \( N \times 1 \) column vector, and \( \pi(h) = \frac{\sum_{i=1}^{N} \pi_i h(X^i)}{\sum_{i=1}^{N} n_i} \) is the unique stationary distribution of the Markov matrix \( T \). The solution \( \Phi \) is used to define an approximation to the solution of the Poisson equation as follows:

\[
\phi_c^{(N)}(x) := \frac{1}{n^{(N)}(x)} \sum_{j=1}^{N} k^{(N)}_c(x, X^j) \Phi_j + \epsilon(h(x) - \pi(h))
\]

The approximation for the gain function is as follows:

\[
K_c^{(N)}(x) = \nabla \left[ \frac{1}{n^{(N)}(x)} \sum_{j=1}^{N} k^{(N)}_c(x, X^j) (\Phi_j + \epsilon h_j) \right]
\]

Upon evaluating the gradient in closed-form, the following linear formula results for the gain function evaluated at particle locations:

\[
K_i := K_c^{(N)}(X^i) = \sum_{j=1}^{N} s_{ij} X^j
\]

where

\[
s_{ij} := \frac{1}{2\epsilon} \frac{T_{ij} (r_j - \sum_{k=1}^{N} T_{ik} r_k)}{\pi_i} \quad r_j := \Phi_j + \epsilon h_j
\]

The overall algorithm is tabulated in Algorithm 3.1.

**Algorithm 3.1** diffusion-map based algorithm for gain function approximation

**Require:** \( \{X^i\}_{i=1}^{N}, \{h(X^i)\}_{i=1}^{N}, \Phi_{prev}, \epsilon, L \)

**Ensure:** \( \{K_i\}_{i=1}^{N} \)

1. Calculate \( g_{ij} := \exp(-|X^i - X^j|^2/4\epsilon) \) for \( i, j = 1 \) to \( N \)
2. Calculate \( k_{ij} := \frac{g_{ij}}{\sqrt{\sum_i g_{ii}} \sqrt{\sum_j g_{jj}}} \) for \( i, j = 1 \) to \( N \)
3. Calculate \( d_i = \sum_j k_{ij} \) for \( i = 1 \) to \( N \)
4. Calculate \( T_{ij} := \frac{k_{ij}}{d_i} \) for \( i, j = 1 \) to \( N \)
5. Calculate \( \pi_i = \frac{d_i}{\sum_{i=1}^{N} d_i} \) for \( i = 1 \) to \( N \)
6. Calculate \( \hat{h} = \sum_{i=1}^{N} \pi_j h(X^i) \)
7. Initialize \( \Phi = \Phi_{prev} \)
8. for \( t = 1 \) to \( L \) do
   9. \( \Phi_i = \sum_{j=1}^{N} T_{ij} \Phi_j + \epsilon(h - \hat{h}) \) for \( i = 1 \) to \( N \)
10. end for
11. Calculate \( r_i = \Phi_i + \epsilon h_i \) for \( i = 1 \) to \( N \)
12. Calculate \( s_{ij} := \frac{1}{2\epsilon} \frac{T_{ij} (r_j - \sum_{k=1}^{N} T_{ik} r_k)}{\pi_i} \) for \( i, j = 1 \) to \( N \)
13. Calculate \( K_i = \sum_j s_{ij} X^j \) for \( i = 1 \) to \( N \)
Remark 3.1. The computational complexity of the diffusion-map based algorithm is $O(N^2)$ because of the need to assemble the $N \times N$ matrix $T$. The computational complexity may be reduced using the sparsity structure of the matrix $T$ and subsampling techniques. Compared to the Galerkin algorithm with computational complexity of $O(Nd^3)$, the diffusion-map algorithm is advantageous in high-dimensional problems where $d >> N$.

3.1. Approximation results. The notation $G_\epsilon(f)(x) := \int g_\epsilon(x,y)f(y)\,dy$ is used to denote the heat semigroup with a Gaussian kernel $g_\epsilon(x,y)$, and

\begin{align}
U_\epsilon &:= \frac{1}{2} \log(\frac{G_\epsilon(\rho)}{\rho^2}), \quad U := -\frac{1}{2} \log(\rho) \\
W_\epsilon &:= \frac{1}{\epsilon} \log(e^{U_\epsilon}G_\epsilon(e^{-U_\epsilon})), \quad W := |\nabla U|^2 - \Delta U
\end{align}

The proof of the following proposition appears in Appendix E.

**Proposition 3.2.** Consider the family of Markov operators $\{T_\epsilon\}_{\epsilon > 0}$ defined according to (3.1). Let $n \in \mathbb{N}$, $t \in (0, t_0)$ with $t_0 < \infty$, and $\epsilon = \frac{2}{n}$. Then,

(i) The semigroup $P_\epsilon$ and the operator $T_\epsilon^n$ admit the following representations:

\begin{align}
P_\epsilon f(x) &:= e^{U(x)}E[e^{-\int_0^t W(B^\epsilon_s)\,ds}e^{-U(B^\epsilon_t)} f(B^\epsilon_t)] \\
T_\epsilon^n f(x) &:= e^{U(x)}E[e^{-\frac{1}{n} \sum_{i=0}^{n-1} W_\epsilon(B^\epsilon_{s_i})} e^{-U(B^\epsilon_{s_n})} f(B^\epsilon_{s_n})]
\end{align}

for all $x \in \mathbb{R}^d$ where $B^\epsilon_t$ is the Brownian motion with initial condition $B^\epsilon_0 = x$.

(ii) In the asymptotic limit as $\epsilon \to 0$:

\begin{align}
U_\epsilon(x) &:= U(x) + 2\epsilon W(x) + \epsilon \Delta V(x) + \epsilon^2 r^{(1)}(x) \\
W_\epsilon(x) &:= W(x) + \epsilon^2 r^{(2)}(x)
\end{align}

where $|r^{(1)}(x)|$, $|r^{(2)}(x)| = O(|x|^2)$ and $|\nabla r^{(1)}(x)| = O(|x|)$ as $|x| \to \infty$.

(iii) For all functions $f$ such that $f, \nabla f \in L^4(\rho)$:

\begin{align}
\|T^n_\epsilon - P_\epsilon f\|_{L^2(\rho)} \leq \sqrt{\frac{\epsilon}{n}} C(\|f\|_{L^4(\rho)} + \|\nabla f\|_{L^4(\rho)})
\end{align}

where the constant $C$ only depends on $t_0$ and $\rho$.

The proof of the following proposition appears in Appendix H.

**Proposition 3.3.** Consider the diffusion map kernel $\{T_\epsilon\}_{\epsilon > 0}$, and its empirical approximation $\{T_\epsilon^{(N)}\}_{\epsilon > 0, N \in \mathbb{N}}$. Then for any bounded continuous function $f \in C_b(\mathbb{R}^d)$:

(i) (Almost sure convergence) For all $x \in \mathbb{R}^d$

\begin{align}
\lim_{N \to \infty} T_\epsilon^{(N)}f(x) = T_\epsilon f(x) \quad a.s
\end{align}

(ii) (Convergence rate) For any $\delta \in (0, 1)$, in the asymptotic limit as $N \to \infty$,

\begin{align}
\int |T_\epsilon^{(N)}f(x) - T_\epsilon f(x)|^2 \rho(x)\,dx = O(\frac{\log(N)}{N \epsilon^d})
\end{align}

with probability higher than $1 - \delta$. 
Remark 3.4 (Related work). The key idea in the proof of the Proposition 3.2 is the Feynman-Kac representation of the semigroup (3.10). To the best of our knowledge, this representation has not been used before in the analysis of the diffusion map approximation. Most of the existing results concerning the convergence of the diffusion map are based on a Taylor series expansion that would lead to a convergence of the form \( \lim_{\epsilon \to 0} f(x) - T_\epsilon f(x) = \Delta \rho f(x) \) for each \( x \in \mathbb{R}^d \) [27, 14, 24]. Convergence results of the form \( \lim_{n \to \infty} \| T_n f - P_t f \|_2 = 0 \) appear in [14, 56], based on functional analytic arguments. The Taylor series type arguments typically require the distribution to be supported on a compact manifold which not assumed here.

4. Convergence and error analysis. The analysis of the diffusion-map algorithm involves the consideration of the following four fixed point problems:

\[
\begin{align*}
(\text{exact}) & \quad \phi = P_\epsilon \phi + \int_0^\epsilon P_\epsilon (h - \hat{h}) \, ds \\
(\text{diffusion-map approx.}) & \quad \phi_\epsilon = T_\epsilon \phi_\epsilon + \epsilon (h - \hat{h}_\epsilon) \\
(\text{empirical approx.}) & \quad \phi_\epsilon^{(N)} = T_\epsilon^{(N)} \phi_\epsilon^{(N)} + \epsilon (h - \pi(h)) \\
(\text{finite-dim.}) & \quad \Phi = \mathcal{T}\Phi + \epsilon (h - \pi(h))
\end{align*}
\]

where \( \hat{h}_\epsilon := \int h(x) \rho_\epsilon(x) \, dx \) and \( \rho_\epsilon(x) := \frac{n_\epsilon(x) \rho(x)}{\int n_\epsilon(x) \rho(x) \, dx} \) is the density of the invariant probability distribution associated with the Markov operator \( T_\epsilon \).

In practice, the finite-dimensional problem (4.4) is solved. The existence and uniqueness of the solution for this problem is the subject of the following proposition whose proof appears in Appendix D.

Proposition 4.1. Consider the finite-dimensional fixed point equation (4.4). Then almost surely

1. \( T \) is a reversible Markov matrix with a unique stationary distribution

\[
\pi_i := \frac{n_{\epsilon}^{(N)}(X_i)}{\sum_{j=1}^N n_{\epsilon}^{(N)}(X_i)}
\]

for \( i = 1, \ldots, N \).

2. \( T \) is a strict contraction on \( L_2^0(\pi) = \{ v \in \mathbb{R}^N; \sum \pi_i v_i = 0 \} \). Hence the fixed point equation (4.4) has a unique solution \( \Phi \in L_2^0(\pi) \).

3. The (empirical approx.) fixed point equation (4.3) has a unique solution given by (see (3.5))

\[
\phi_\epsilon^{(N)}(x) = \frac{1}{n_{\epsilon}^{(N)}(x)} \sum_{j=1}^N k_\epsilon^{(N)}(x, X^j) \Phi_j + \epsilon (h(x) - \pi(h))
\]

Based on the results in Proposition 2.2 and Proposition 4.1, the exact solution \( \phi \) and the numerical solution \( \phi_\epsilon^{(N)} \) are both well-defined. The remaining task is to show the convergence of \( \phi_\epsilon^{(N)} \to \phi \) as \( N \to \infty \) and \( \epsilon \to 0 \). We break the convergence analysis into two parts, bias and variance:

\[
\phi_\epsilon^{(N)} \xrightarrow{N \uparrow \infty} (\text{variance}) \phi_\epsilon \xrightarrow{\epsilon \downarrow 0} (\text{bias}) \phi
\]

Before describing the general result, it is useful to first introduce an example that helps illustrate the bias-variance trade-off in this problem.
4.1. Example - the scalar case. In the scalar case (where $d = 1$), the Poisson equation is:

$$-rac{1}{\rho(x)} \frac{d}{dx} \left( \rho(x) \frac{d\phi}{dx} (x) \right) = h(x) - \hat{h}$$

Integrating twice yields the solution explicitly

$$K_{\text{exact}}(x) = \frac{d\phi}{dx} (x) = -\frac{1}{\rho(x)} \int_{-\infty}^{x} \rho(z)(h(z) - \hat{h}) \, dz$$

(4.6)

For the choice of $\rho$ as the sum of two Gaussians $\mathcal{N}(-1, \sigma^2)$ and $\mathcal{N}(+1, \sigma^2)$ with $\sigma^2 = 0.2$ and $h(x) = x$, the solution obtained using (4.6) is depicted in Figure 1 (a). Also depicted is the approximate solution obtained using the diffusion-map algorithm with $N = 200$. As $\epsilon \to \infty$ the approximate gain converges to the constant gain approximation. As $\epsilon$ becomes smaller, the approximation becomes more accurate. However, for very small values of $\epsilon$ the approximation is poor due to the variance error.

The bias-variance trade-off while varying the the parameter $\epsilon$ is depicted in Figure 1 (b). The $L^2$ error is computed as a Monte-Carlo average:

$$\text{error} = \frac{1}{M} \sum_{m=1}^{M} \frac{1}{N} \sum_{i=1}^{N} |K^{(m)}(X^i) - K_{\text{exact}}(X^i)|^2$$

(4.7)

Figure 1 (b) depicts the error obtained from averaging over $M = 1000$ simulations as a function of the parameter $\epsilon$. It is observed that for a fixed number of particles $N$, there is an optimal value of $\epsilon$ that minimizes the error.

The vector counterpart of this example appears in subsection 5.1.

4.2. Bias. The analysis of bias has two parts:

1. To show that the (diffusion-map) fixed-point equation (4.2) admits a unique solution $\phi_{\epsilon}$ for all positive choices of $\epsilon$;

2. To show that $\phi_{\epsilon} \to \phi$ as $\epsilon \downarrow 0$. 

Fig. 1. Simulation results for the diffusion-map algorithm for the scalar bimodal example: (a) Approximate gain function for different choices of $\epsilon$ compared to the exact gain function (solid line). The shaded area in the background is the bimodal probability density function $\rho$. The dashed line is the constant gain approximation solution; (b) Gain function approximation error of the diffusion-map algorithm as a function of the parameter $\epsilon$. All the results are with $N = 200$ particles.
For \( n \in \mathbb{N} \), iterate the fixed-point equation (4.2) \( n \) times to obtain:

\[
(4.8) \quad \phi_\epsilon = T_\epsilon^n \phi_\epsilon + \sum_{k=0}^{n-1} \epsilon T_\epsilon^k (h - \hat{h}_\epsilon)
\]

We let \( \epsilon = \frac{t}{n} \) for some \( t > 0 \) and study the solution of this fixed-point equation as \( n \to \infty \). Note that the solution to the iterated fixed-point equation (4.8) is identical to the solution to the fixed-point equation (4.2).

The fixed-point equation (4.8) is the (discrete) Poisson equation that appears in the theory of Markov chain simulation [25, 40] and stochastic control [39, Ch. 9]. Theory presented in these references illustrates how bounds on the solution are obtained under a Foster-Lyapunov drift condition. A similar strategy is adopted here.

In the following proposition, an existence-uniqueness result is described for the fixed-point equation (4.8). The technical step in the proof involves a Foster-Lyapunov condition known as DV(3) [33]. The proof appears in Appendix F.

**Proposition 4.2.** Consider the family of Markov operators \( \{T_\epsilon\}_{\epsilon > 0} \) defined in (3.1). Let \( n \in \mathbb{N} \), \( t \in (0, t_0) \), and \( \epsilon = \frac{t}{n} \), with \( t_0 < \infty \). Then there exists positive constants \( a, b, R, \delta \), a probability measure \( \nu \), and a number \( n_0 \in \mathbb{N} \) such that for all \( n > n_0 \):

\[
\log(e^{-U_\epsilon T_\epsilon^n e^{U_\epsilon}}) \leq -atU_\epsilon + bt \quad \text{(4.9a)}
\]

\[
T_\epsilon^n 1_A(x) \geq \delta \nu(A) \quad \forall |x| \leq R, \forall A \in \mathcal{B}(\mathbb{R}^d) \quad \text{(4.9b)}
\]

Consequently,

(i) The chain with transition kernel \( T_\epsilon^n \) is geometrically ergodic with invariant density

\[
(4.10) \quad \rho_\epsilon(x) := \frac{n_\epsilon(x) \rho(x)}{\int n_\epsilon(x) \rho(x) \, dx}
\]

(ii) \( T_\epsilon^n \) is reversible with respect to the density \( \rho_\epsilon \). It admits a spectral gap as a linear operator \( T_\epsilon^n : L^2_0(\rho_\epsilon) \to L^2_0(\rho_\epsilon) \) that is uniform with respect to \( \epsilon \). The spectral gap is denoted as \( \lambda \).

(iii) There exists a solution to (4.8) with the bound

\[
\|\phi_\epsilon\|_{L^2(\rho_\epsilon)} \leq \frac{t\|h\|_{L^2(\rho_\epsilon)}}{\lambda}
\]

The proof of the following main result appears in Appendix G.

**Theorem 4.3.** Suppose the assumptions (A1)-(A2) hold for the density \( \rho \) and the function \( h \), and \( \phi \) denotes the exact solution of (4.1). Consider the approximation of this problem defined by the (diffusion-map) fixed-point equation (4.2). For the approximate problem:

1. **Existence-Uniqueness:** For each fixed \( \epsilon > 0 \), there exists a unique solution \( \phi_\epsilon \).

2. **Convergence:** In the asymptotic limit as \( \epsilon \to 0 \)

\[
(4.11) \quad \|\phi_\epsilon - \phi\|_{L^2(\rho)} = O(\epsilon)
\]
4.3. Variance. The analysis of the variance concerns the (empirical) fixed-point equation (4.3) whose solution is denoted as $\phi^{(N)}(x)$. The parameter $\epsilon$ is assumed to be positive and fixed and $N$ is assumed to be finite but large.

The existence-uniqueness of $\phi^{(N)}$ has already been shown as part of Prop. 4.1. The convergence has only been shown only for the case where the density has a compact support.

**Assumption A3:** The distribution $\rho$ has compact support given by $\Omega \subset \mathbb{R}^d$.

**Theorem 4.4.** Suppose the assumptions (A2)-(A3) hold for the density $\rho$ and the function $h$, and $\phi_e$ denotes the solution of the (kernel) fixed-point equation (4.2) for a fixed positive parameter $\epsilon$. Consider the approximation of this problem defined by the (empirical) fixed-point equation (4.3). For the approximate problem:

1. **Existence-Uniqueness:** For each finite $N$, there exists (almost surely) a unique solution $\phi^{(N)}(x)$.

2. **Convergence:** The approximate solution $\phi^{(N)}(x)$ converges to the kernel solution $\phi$.

\[
\lim_{N \to \infty} \| \phi^{(N)}(x) - \phi(x) \|_\infty = 0, \text{ a.s.}
\]

**Remark 4.5.** (related work) The proof of the convergence $\phi^{(N)}(x) \to \phi(x)$ is based on similar results in the numerical analysis of integral equations on a grid [1, 2, 3]. A related approach is used in [58] to show the consistency of spectral clustering.

4.4. Relationship to the constant gain approximation. Although the convergence and error analysis pertains to the $\epsilon \downarrow 0$ limit, an important property of the diffusion-map approximation is that the numerical procedure yields a unique solution for arbitrary values of $\epsilon$ (see Proposition 4.1). In fact, more can be said: one recovers the constant gain approximation formula in the $\epsilon \to \infty$ limit.

Before stating the result, it is useful to recall the three formulae for the gain:

(i) **Exact formula:** $K = \nabla \phi$ is defined using the exact solution $\phi(x)$.

(ii) **Kernel formula:** $K_{\epsilon}$ is defined using the solution $\phi_{\epsilon}$ to the (diffusion-map) approximation fixed-point equation:

\[
K_{\epsilon}(x) := \nabla_x \left[ \frac{1}{n_{\epsilon}(x)} \int k_{\epsilon}(x,y)(\phi_{\epsilon}(y) + \epsilon h(y))\rho_{\epsilon}(y) \, dy \right]
\]

(iii) **Empirical formula:** $K_{\epsilon}^{(N)}$ is the empirical version of the kernel formula. It was defined in (3.6) using the solution $\Phi$ of the finite-dimensional fixed-point problem.

The proof of the following Proposition appears in the Appendix J.

**Proposition 4.6.** Consider the fixed-point problems (4.2) and (4.3) in the limit as $\epsilon \to \infty$.

(i) The kernel formula of the gain is given by

\[
\lim_{\epsilon \to \infty} K_{\epsilon} = \int (h(x) - \hat{h})\rho(x) \, dx
\]

(ii) For any finite $N$, the empirical formula of the gain is given by

\[
\lim_{\epsilon \to \infty} K_{\epsilon}^{(N)} = \frac{1}{N} \sum_{i=1}^{N} (h(X^i) - \hat{h}^{(N)})X^i \text{ a.s.}
\]
This result serves to highlight the connection between the FPF and the EnKF: With the diffusion map approximation of the gain, the FPF approaches EnKF in the limit of large $\epsilon$. The parameter $\epsilon$ can then be regarded as the tuning parameter to “improve” the gain. Of course, for any finite value of $N$, this can only be done up to a point – where variance becomes dominant (see Figure 1).

5. Numerics.

5.1. Example - the vector case. A vector generalization of the scalar example in subsection 4.1 is obtained by considering the following form of the probability density function in $d$-dimensions:

$$\rho(x) = \rho_B(x_1) \prod_{n=2}^{d} \rho_G(x_n), \quad \text{for} \quad x = (x_1, x_2, \ldots, x_d) \in \mathbb{R}^d$$

where $\rho_B$ is the bimodal distribution $\frac{1}{2}\mathcal{N}(-1, \sigma^2) + \frac{1}{2}\mathcal{N}(+1, \sigma^2)$ introduced in subsection 4.1, and $\rho_G$ is the Gaussian distribution $\mathcal{N}(0, \sigma^2)$. Also suppose the function $h(x) = x_1$. The simple example is illustrative of realistic application scenarios where the density has non-Gaussian features along certain (not necessarily apriori known) low-dimensional subspace. The directions orthogonal to this subspace are modelled here as Gaussian noise.

For this problem, the exact gain function is easily obtained as

$$K_{\text{exact}}(x) = (K_{\text{exact}}(x_1), 0, \ldots, 0)$$

where the function $K_{\text{exact}}(x_1)$ is given by the formula (4.6) in subsection 4.1. The exact solution is used to compute error properties as dimension increases.

The diffusion-map algorithm (Algorithm 3.1) is simulated to approximate the gain function for this problem. For each particle $X_i = (X_{i1}, \ldots, X_{id})$, the first coordinate $X_{i1} \overset{i.i.d}{\sim} \frac{1}{2}\mathcal{N}(-1, \sigma^2) + \frac{1}{2}\mathcal{N}(+1, \sigma^2)$ and other the coordinates $X_{in} \overset{i.i.d}{\sim} \mathcal{N}(0, \sigma^2)$ for $n = 2, \ldots, d$.

Figure 2 depicts the Monte-Carlo error (4.7) computed from running $M = 100$ simulations. A summary of these results is as follows:

1. Figure 2-(a) depicts the M.C. error as a function of the parameters $\epsilon$ and $d$ for a fixed number of particles $N = 1000$. Also depicted is the error with the constant gain approximation. The constant gain error serves here as baseline. For large values of $\epsilon$, the error asymptotes to the error for the constant-gain approximation. This is because (see Proposition 4.6) the kernel gain approaches the constant gain as $\epsilon \to \infty$.

2. Figure 2-(b) depicts the bias-variance trade-off as a function of number of particles $N$ for the fixed $d = 1$. It is not a surprise that the error gets better, for all choices of $\epsilon$, as the number of particles increase. However, the optimal value of $\epsilon$ – at which the error is the smallest – is relatively insensitive to changes in $N$.

3. Figure 2-(c) depicts the error as function of $N$ for different values of $\epsilon$. The dimension $d = 1$ is fixed. The error goes down as $O(\frac{1}{N})$ and asymptotes to the $O(\epsilon)$ bias. The $O(\frac{1}{N})$ is a LLN type estimate and $O(\epsilon)$ bias error is consistent with the conclusion of the Theorem 4.3.
4. Figure 2-(d) depicts the run time comparison between the diffusion-map algorithm and the constant gain algorithm. The scaling for the diffusion-map algorithm is \(O(N^2)\) which is significantly more expensive than the \(O(N)\) scaling of the constant gain approximation.

5.2. Filtering example. Consider the following filtering problem:

\[
\begin{align*}
dX_t &= 0, \quad X_0 \sim p_0 \\
dZ_t &= h(X_t) \, dt + \sigma_w \, dW_t
\end{align*}
\]

where \(X_t \in \mathbb{R}, Z_t \in \mathbb{R}, \sigma_W > 0\), and \(\{W_t\}\) is standard Brownian motion, independent of \(X_t\). The prior distribution \(p_0\) is Gaussian \(\mathcal{N}(0,1)\) and the observation function \(h(x) = |x|\). For the static filtering problem, the posterior distribution is explicitly given by:

\[
p^*_t(x) = (\text{const.})p_0(x) \exp \left( \frac{1}{\sigma_w^2}(h(x)Z_t - \frac{1}{2}h^2(x)t) \right)
\]

For comparative purposes, the FPF algorithm with the diffusion-map gain approximation and the constant gain approximation are implemented. With the latter approximation, the FPF is an EnKF algorithm. The simulation parameters are as follows: The measurement noise \(\sigma_w = 0.1\). The simulation is carried out for \(T = 500\) time-steps with step-size \(\Delta t = 0.001\). Both the algorithms use \(N = 200\) particles with
identical initialization. For the diffusion-map approximation, the kernel bandwidth $\epsilon = 0.1$.

The numerical results are depicted in Figure 3. The distribution of the particles along with the exact posterior distribution are depicted in Figure 3-(a). It is observed that the FPF algorithm with the diffusion map approximation provides a more accurate approximation of the posterior distribution. In contrast, the constant-gain approximation fails to reproduce the bimodal nature of the posterior distribution.

A quantitative estimate of the performance is provided in terms of a mean squared error (m.s.e.) in estimating the conditional expectation of the function $\psi(x) = x1_{x \leq 0}$. A Monte Carlo estimate of the m.s.e. is depicted in Figure 3-(b) with $M = 100$ runs. At time $t$, it is calculated according to

\[
m.s.e.t = \frac{1}{M} \sum_{m=1}^{M} \left( \frac{1}{N} \sum_{i=1}^{N} \psi(X_{t}^{m,i}) - \int \psi(x)p_{t}^{\star}(x) \, dx \right)^2
\]

At time $t = 0$, the empirical distribution of the particles is an accurate approximation of the prior distribution, because the particles are sampled i.i.d. from the prior distribution. Therefore, the m.s.e at $t = 0$ is small. As time progress, the difference between the empirical distribution and the exact posterior becomes larger because the filter update is not exact. As the time-step $\Delta t$ is small, the main source of the m.s.e. error is due to the error in the gain function approximation. Therefore, the diffusion map FPF with its more accurate approximation of the gain yields better m.s.e., compared to the EnKF using the constant gain approximation.

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for the Gaussian case.

Appendix A. Exact semigroup and and its diffusion map approximation for the Gaussian case. In this section, we provide explicit formulae for the
exact semigroup $P_t$ and its diffusion map approximation $T_\epsilon$, for the special case when the density $\rho$ is a Gaussian $\mathcal{N}(m, \Sigma)$. For the Gaussian case, the semigroup is the Ornstein-Uhlenbeck semigroup [5, Sec. 2.7.1] and its spectral representation is obtained in terms of the Hermite polynomials. For notational ease, after an appropriate change of coordinates, we assume $m = 0$ and $\Sigma = \text{diag}(\sigma_1^2, \ldots, \sigma_d^2)$ where $\sigma_1^2 \geq \sigma_2^2 \geq \ldots \geq \sigma_d^2 > 0$ are ordered eigenvalues of $\Sigma$.

**Definition A.1.** The Hermite polynomials are recursively defined as

$$h_{n+1}(x) = x h_n(x) - h'_n(x), \quad h_0(x) = 1,$$

where the prime $'$ denotes the derivative.

**Proposition A.2.** Suppose the density $\rho$ is Gaussian $\mathcal{N}(0, \Sigma)$ with the variance $\Sigma = \text{diag}(\sigma_1^2, \ldots, \sigma_d^2)$ and $\sigma_1^2 \geq \sigma_2^2 \geq \ldots \geq \sigma_d^2 > 0$. Then

(i) The exact semigroup $P_t$ and the diffusion map $T_\epsilon$ admit the following integral representations:

\begin{align}
(A.1) \quad P_t f(x) &= \int_{\mathbb{R}^d} \prod_{j=1}^d \frac{1}{(2\pi\sigma_j^2)^{1/2}} \exp\left(-\frac{|y_j - e^{-1}\sigma_j^2 x_j|^2}{2\sigma_j^2}\right) f(y) \, dy \\
(A.2) \quad T_\epsilon f(x) &= \int_{\mathbb{R}^d} \prod_{j=1}^d \frac{1}{(4\pi\epsilon(1 - \delta_j))^{1/2}} \exp\left(-\frac{|y_j - (1 - \delta_j)x_j|^2}{4\epsilon(1 - \delta_j)}\right) f(y) \, dy
\end{align}

where $\delta_j := \epsilon \frac{\sigma_j^2 + 4\epsilon}{\sigma_j^2 + 3\epsilon^2 + 4\epsilon}$ for $j = 1, \ldots, d$.

(ii) The operators $P_t$ and $T_\epsilon$ each have a unique invariant Gaussian density given by $\mathcal{N}(0, \Sigma)$ and $\mathcal{N}(0, \Sigma_\epsilon)$, respectively, where $\Sigma_\epsilon = \text{diag}(\sigma_{\epsilon,1}^2, \ldots, \sigma_{\epsilon,d}^2)$ with $\sigma_{\epsilon,j}^2 = \frac{\epsilon(1 - \delta_j)}{\delta_j(2 - \delta_j)}$ for $j = 1, \ldots, d$.

(iii) The eigenvalues and the associated eigenfunctions are as follows:

Spectrum of the semigroup $P_t$: $\lambda_n = \prod_{j=1}^d e^{-n_j \sigma_j^2}, \quad e_n(x) = \prod_{j=1}^d h_{n_j}(\frac{x_j}{\sigma_j})$

Spectrum of the diffusion map $T_\epsilon$: $\lambda_n = \prod_{j=1}^d (1 - \delta_j)^{n_j}, \quad e_n(x) = \prod_{j=1}^d h_{n_j}(\frac{x_j}{\sigma_{\epsilon,j}})$

for $n = (n_1, \ldots, n_d) \in \mathbb{Z}_+^d$.

(iv) The operator norm $\|P_t\|_{L^2(\rho)} = e^{-\sigma_1^2}$ and $\|T_\epsilon\|_{L^2(\rho_\epsilon)} = 1 - \delta_1$.

**Proof.** Omitted. See [55, Prop. 1].

**Appendix B. Proof of Proposition 2.2.**

Based on the use of the spectral representation (2.2), the weak solution of the Poisson equation is readily seen to be

(B.1) $$\phi = \sum_{m=1}^{\infty} \frac{1}{\lambda_m} \langle e_m, h \rangle e_m$$
This solution (B.1) also satisfies the fixed-point equation (2.4) because

\[ P_t \phi + \int_0^t P_s (h - \hat{h}) \, ds = \sum_{m=1}^{\infty} e^{-t \lambda_m} \langle e_m, \phi \rangle e_m + \int_0^t \sum_{m=1}^{\infty} e^{-s \lambda_m} \langle e_m, h \rangle e_m \, ds \]

\[ = \sum_{m=1}^{\infty} e^{-t \lambda_m} \langle e_m, h \rangle e_m + \sum_{m=1}^{\infty} \frac{1 - e^{-t \lambda_m}}{\lambda_m} \langle e_m, h \rangle e_m = \phi \]

The uniqueness of the solution to the fixed-point equation (2.4) follows from the contraction mapping principle because \( \| P_t \|_{L^2(\rho)} = e^{-t \lambda_1} < 1 \).

**Appendix C. Derivation of the linear form of the gain (3.7).** By a direct calculation,

\[ \nabla_x \frac{k_e^{(N)}(x, X^j)}{\sum_{l=1}^N k_e^{(N)}(x, X^l)} = \frac{X^j - x k_e^{(N)}(x, X^j)}{\sum_{l=1}^N k_e^{(N)}(x, X^l)} \frac{\sum_{l=1}^N X^j - x k_e^{(N)}(x, X^l)}{\sum_{l=1}^N k_e^{(N)}(x, X^l)} \frac{k_e^{(N)}(x, X^j)}{\sum_{l=1}^N k_e^{(N)}(x, X^l)} \]

which evaluated at \( x = X^i \) yields

\[ \nabla_x \left( \frac{k_e^{(N)}(x, X^i)}{\sum_{j=1}^N k_e(x, X^j)} \right) \bigg|_{x=X^i} = \frac{1}{2 \epsilon} \left( X^j T_{ij} - \sum_{l=1}^N X^j T_{il} T_{lj} \right) \]

Using the definitions (3.6) for \( K_e^{(N)} \), and (3.8) for \( r \) and \( s \),

\[ K_e^{(N)}(X^i) = \nabla_x \left( \frac{1}{n_e^{(N)}(x)} \sum_{j=1}^N k_e^{(N)}(x, X^j) (\Phi_j + c h_j) \right) \bigg|_{x=X^i} \]

\[ = \nabla_x \left( \frac{\sum_{j=1}^N k_e^{(N)}(x, X^j) r_j}{\sum_{j=1}^N k_e^{(N)}(x, X^j)} \right) \bigg|_{x=X^i} \]

\[ = \frac{1}{2 \epsilon} \left( \sum_{j=1}^N X^j T_{ij} (r_j - \sum_{l=1}^N T_{il} r_l) \right) = \sum_{j=1}^N s_{ij} X^j \]

**Appendix D. Proof of Proposition 4.1.**

1. \( T \) is a Markov matrix because \( T_{ij} = \frac{1}{n_e^{(N)}(X^i)} k_e^{(N)}(X^i, X^j) > 0 \) a.s. and

\[ \sum_{j=1}^N T_{ij} = \frac{1}{n_e^{(N)}(X^i)} \sum_{j=1}^N k_e^{(N)}(X^i, X^j) = \frac{n_e^{(N)}(X^i)}{n_e^{(N)}(X^i)} = 1 \]

The stationary distribution is \( \pi \) because

\[ \sum_{i=1}^N \pi_i T_{ij} = \sum_{i=1}^N \frac{n_e^{(N)}(X^j)}{\sum_{k=1}^N n_e^{(N)}(X^k)} k_e^{(N)}(X^i, X^j) \frac{n_e^{(N)}(X^i)}{n_e^{(N)}(X^i)} \]

\[ = \sum_{i=1}^N k_e^{(N)}(X^i, X^j) \frac{n_e^{(N)}(X^j)}{\sum_{k=1}^N n_e^{(N)}(X^k)} = \frac{n_e^{(N)}(X^j)}{\sum_{k=1}^N n_e^{(N)}(X^k)} = \pi_j \]
All entries of the Markov matrix are positive. Hence the Markov chain is irreducible and aperiodic. Therefore, the stationary distribution is unique. It is reversible because
\[
\pi_i T_{ij} = \frac{n_e^{(N)}(X^i)}{\sum_{k=1}^N n_e^{(N)}(X^k)} \frac{k_e^{(N)}(X^i, X^j)}{\sum_{k=1}^N n_e^{(N)}(X^k)} = \frac{k_e^{(N)}(X^j, X^i)}{\sum_{k=1}^N n_e^{(N)}(X^k)} = \pi_j T_{ji}
\]

2. Denote \( \delta := \min_{ij} T_{ij} \). Then \( \delta > 0 \) a.s. Therefore, \( ||T||_{L^2(\pi)} \leq 1 - \frac{N \delta}{2} < 1 \), and is thus a contraction on \( L^2(\pi) \) \( [49, \text{Ch. 5}] \). It follows, from the contraction mapping principle, that the fixed point equation (3.4) has a unique solution.

3. Evaluating the definition (3.5) at \( x = X^t \) concludes \( \phi_e^{(N)}(X^t) = \Phi_t \) because,

\[
\phi_e^{(N)}(X^i) = \frac{1}{n_e^{(N)}(X^i)} \sum_{j=1}^n k_e^{(N)}(X^i, X^j) \Phi_j + \epsilon(h(X^i) - \pi(h)) = \sum_{j=1}^N T_{ij} \Phi_j + \epsilon(h_i - \pi(h)) = \Phi_t
\]

Therefore \( \phi_e^{(N)} \) solves the fixed-point equation (4.3), because

\[
T_e^{(N)} \phi_e^{(N)}(x) = \frac{1}{\pi_e^{(N)}(x)} \sum_{j=1}^n k_e^{(N)}(x, X^j) \phi_e^{(N)}(X^j) = \frac{1}{n_e^{(N)}(x)} \sum_{j=1}^n k_e^{(N)}(x, X^j) \Phi_j ^{(3.5)} \phi_e^{(N)}(x) - \epsilon(h(x) - \pi(h))
\]

Appendix E. Proof of the Proposition 3.2.

Proof. (i) Let \( U = -\frac{1}{2} \log(\rho) \) and \( W = |\nabla U|^2 - \Delta U \) as defined in (3.9a) and (3.9b). To obtain the representation (3.10) for the semigroup \( P_t \), consider the unitary transformation \( [5, \text{Sec. 1.15.7}] \):

\[
e^{-U} \Delta \rho e^U = \Delta - W
\]

Therefore, for any function \( f \in C_b(\mathbb{R}^d) \),

\[
e^{-U} \int e^U f = \mathbb{E}[e^{-\int_0^t W(B_s^\xi) ds} f(B_t^\xi)]
\]

where the stochastic representation (second equality) follows from the Feynman-Kac formula; \( B_t^\xi \) is a Brownian motion initialized at \( x \). Setting \( f(x) = e^{-U(x)} g(x) \),

\[
P_t g(x) = e^{U(x)} e^{t(\Delta - W)} (e^{-U} g)(x) = e^{U(x)} \mathbb{E}[e^{-\int_0^t W(B_s^\xi) ds} e^{-U(B_s^\xi)} g(B_t^\xi)]
\]

which is the representation (3.10).

Next, the representation (3.11) is obtained. Using the definitions, (3.1) of \( T_e \) and (3.9a) and (3.9b) of \( U_e \) and \( W_e \),

\[
T_e f(x) = \frac{G_e(f e^{-U_e})(x)}{G_e(e^{-U_e})(x)} = e^{U(x) - t W_e(x)} G_e(e^{-U_e} f)(x) = e^{U(x) - t W_e(x) \mathbb{E}[e^{-U_e(B_s^\xi)} f(B_t^\xi)]}
\]
where the final equality follows from using the stochastic representation of the heat semigroup $G_t$. The representation (3.11) is obtained by iterating this formula $n$ times.

(ii) Without loss of generality, upon a change of coordinates, assume $m = 0$ and $\Sigma = \text{diag}(\sigma_1^2, \ldots, \sigma_d^2)$ in Assumption A1. Using the definitions

\[
U_t(x) = U(x) - \frac{1}{2} \log(G_t(x)) + \frac{1}{2} \log(G_t(x))
\]

Now, $\log(G_t(x)) = \log(\rho_y(x; \Sigma) + w(x))$. So, the main calculation is to approximate $\log(G_t(x))$. Using the definition

\[
G_t(x) = \int e^{-\sum_{d=1}^d \frac{|x_n-y_n|^2}{2\sigma_n^2}} e^{-\sum_{d=1}^d \frac{|x_n-y_n|^2}{2\sigma_n^2}} \prod_{n=1}^d (2\pi \sigma_n^2)^{1/2} dy
\]

where $\delta_n = \frac{2\epsilon}{\sigma_n^2 + 2\epsilon}$, $\delta = \text{diag}(\delta_1, \ldots, \delta_d)$ and $G_t^{(\delta)}$ is the semigroup associated with the pde $\frac{\partial}{\partial t} G_t^{(\delta)} f = G_t^{(\delta)} (\text{tr}((I - \delta)Hf))$. 

The Taylor expansion of $G_t^{(\delta)}(e^{-w})$, about $\epsilon = 0$, is expressed as

\[
G_t^{(\delta)}(e^{-w})(x) = e^{-w(x)} + \epsilon \text{Tr}((I - \delta)\nabla^2 e^{-w})(x)
\]

\[
+ \int_0^\epsilon \int_0^\tau \left( \sum_{m,n=1}^d (1 - \delta_m)^2 (1 - \delta_n)^2 G_s^{(\delta)} \partial^2_{m,n} e^{-w}(x) \right) ds d\tau
\]

where $\partial^2_{m,n} := \frac{\partial^2}{\partial x_m^2 \partial x_n^2}$.

Using the property that $G_s^{(\delta)} \partial_n f = \partial_n G_t^{(\delta)} f$, $\|G_t^{(\delta)}(f)\|_\infty \leq \|f\|_\infty$ and the assumption (A1) that $w \in C^\infty_b(\mathbb{R}^d)$, we conclude that $r_\epsilon \in C^\infty_b(\mathbb{R}^d)$. Therefore,

\[
\log(G_t(x)) = \log(\rho_y(x; \Sigma + 2\epsilon I)) - \left( w - \log(1 + \epsilon \text{tr}((I - \delta)\nabla^2 e^{-w} + \epsilon^2 e^{-w}r_\epsilon)) \right) \big|_{(I - \delta)x}
\]

The asymptotic expansion of $w_t^{(1)}(x)$, as $\epsilon \to 0$, is obtained as

\[
w_t^{(1)}(x) = w(x) - 2\epsilon x^\top \Sigma^{-1} \nabla w(x) - \epsilon e^w \Delta e^{-w}(x) + O(\epsilon^2)
\]

where the remainder term has at most linear growth as $|x| \to \infty$. 

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Substituting the asymptotic expression for \( \log(G_\varepsilon \rho(x)) \) in (E.2),

\[
U_\varepsilon(x) = U(x) - \frac{1}{2} \log(\rho_\varepsilon(x; \Sigma)) + \frac{1}{2} w(x) + \frac{1}{2} \log(\rho_\varepsilon(x; \Sigma + 2\varepsilon I)) - \frac{1}{2} w_\varepsilon^{(1)}(x)
\]

\[
= U(x) + \frac{\varepsilon}{2} x^\top \Sigma^{-1}(\Sigma + 2\varepsilon I)^{-1}x - \frac{\varepsilon}{2} \text{Tr}(\Sigma^{-1})
+ \varepsilon x^\top \Sigma^{-1} \nabla w(x) + \frac{\varepsilon}{2} (\|\nabla w(x)\|^2 - \Delta w(x)) + O(\varepsilon^2)
\]

\[
= U(x) + \frac{\varepsilon}{2} [\Sigma^{-1}x + \nabla w(x)]^2 - \frac{\varepsilon}{2} (\text{Tr}(\Sigma^{-1}) + \Delta w(x)) + O(\varepsilon^2)
\]

where the remainder \( O(\varepsilon^2) \) error term has at most quadratic growth as \( |x| \to \infty \). This concludes the proof of approximation (3.12a).

Based on this above calculation, the following estimate for an upper bound of the function \( U \) is obtained (it is used in the proof of Proposition 4.2):

\[
U_\varepsilon(x) \leq \frac{1}{4} x^\top \Sigma^{-1}x + \varepsilon (\|\Sigma^{-1}x\|^2 + \|\nabla w\|_\infty^2 + \|\Delta V\|_\infty) + \varepsilon^2 (C_1 |x|^2 + C_2)
\]

(E.3)

\[
\leq \frac{1}{8\sigma_1^2} |x|^2 + \frac{\sigma_1^2}{8} (\|\nabla w\|_\infty^2 + \|\Delta V\|_\infty + C_2e \sigma_1^2)
\]

where recall \( \sigma_1^2 = \lambda_{\min}(\Sigma) \).

Next, the approximation (3.12b) is derived. Using the definition

\[
\varepsilon W_\varepsilon(x) = U_\varepsilon(x) + \log(G_\varepsilon e^{-U_\varepsilon}(x))
\]

By repeating the steps, just used to approximate \( \log(G_\varepsilon(\rho)) \), it is shown

\[
\log(G_\varepsilon(e^{-U_\varepsilon})) = \log(\rho_\varepsilon(x; 2\Sigma(I + \delta)^{-1} + 2\varepsilon I)) - w_\varepsilon^{(2)}(x)
\]

where

\[
w_\varepsilon^{(2)}(x) = w(x) - \frac{1}{2} w_\varepsilon^{(1)}(x) - \frac{\varepsilon}{2} x^\top \Sigma^{-1} \nabla w(x) - \varepsilon (\frac{1}{4} \|\nabla w(x)\|^2 - \frac{1}{2} \Delta w(x)) + O(\varepsilon^2)
\]

Therefore,

\[
\varepsilon W_\varepsilon(x) = -\log(\rho_\varepsilon(x; 2\Sigma(I + \delta)^{-1})) + \log(\rho_\varepsilon(x; 2\Sigma(I + \delta)^{-1} + 2\varepsilon I))
+ w(x) - \frac{1}{2} w_\varepsilon^{(1)}(x) - w_\varepsilon^{(2)}(x) + O(\varepsilon^2)
\]

\[
= \frac{2\varepsilon}{4} x^\top (I + \delta) \Sigma^{-1}(2\Sigma(I + \delta)^{-1} + 2\varepsilon I)^{-1}x - \frac{\varepsilon}{2} \text{Tr}(\Sigma^{-1})
+ \varepsilon x^\top \Sigma^{-1} \nabla w(x) + \frac{\varepsilon}{2} (\frac{1}{4} \|\nabla w(x)\|^2 - \frac{1}{2} \Delta w(x)) + O(\varepsilon^2)
\]

\[
= \varepsilon (\frac{1}{4} [\Sigma^{-1}x + \nabla w(x)]^2 - \frac{1}{2} (\text{Tr}(\Sigma^{-1}) + \Delta w(x))) + O(\varepsilon^2)
\]

where the error term has at most quadratic growth as \( |x| \to \infty \). This concludes the proof of the approximation (3.12b).
Based on this above calculation, the following estimate for a lower bound of the function $W_\epsilon(x)$ is obtained (it is used in the proof of Proposition 4.2):

$$W_\epsilon(x) = \frac{1}{4}\Sigma^{-1}x + \nabla w(x)^2 - \frac{1}{2}(\text{Tr}(\Sigma^{-1}) + \Delta w(x)) + \epsilon r^{(2)}_\epsilon(x)$$

$$\geq \frac{1}{8}\Sigma^{-1}x^2 - \frac{1}{2}(||\nabla w||^2_\infty + \text{Tr}(\Sigma^{-1}) + ||\Delta w||_\infty) - \epsilon(C_1|x|^2 + C_2)$$

(E.4)

$$\geq \alpha|x|^2 - \beta$$

where $\alpha = \frac{1}{16\sigma_2^2}$, $\beta = \frac{1}{2}(||\nabla w||^2_\infty + \text{Tr}(\Sigma^{-1}) + ||\Delta w||_\infty + \frac{C_4}{8\epsilon})$ and $\epsilon \leq \frac{1}{16C_1\sigma_2^2}$ (where recall $\sigma_2^2 = \lambda_{\text{max}}(\Sigma))$.

(iii) Let $\hat{P}_t$ denote the semigroup for the weighted Laplacian $\Delta_q$ with the density $q(x) = e^{-2U_\epsilon(x)}$. We break the error into two parts:

$$||T^n_\epsilon f - P_t f||_{L^2(\rho)} \leq ||T^n_\epsilon f - \hat{P}_t f||_{L^2(\rho)} + ||\hat{P}_t f - P_t f||_{L^2(\rho)}$$

The bounds for the two terms on the right-hand side are derived in the following two steps:

**Step 1.** Using the stochastic representation (3.10)-(3.11),

$$(T^n_\epsilon - \hat{P}_t)f(x) = e^{U_\epsilon(x)}E[e^{-U_\epsilon(B^\epsilon_{2k_\rho})} f(B^\epsilon_{2k_\rho}) \zeta_t]$$

where $\zeta_t := e^{-\sum_{k=0}^{n-1} W_\epsilon(B^\epsilon_{2k+1})} - e^{-\int_0^t W(B^\epsilon_{2k}) \text{d}s}$. By the Cauchy-Schwartz inequality

$$|(T^n_\epsilon - \hat{P}_t)f(x)| \leq e^{U_\epsilon(x)} E[|f(B^\epsilon_{2k})|^2 e^{-2U_\epsilon(B^\epsilon_{2k})}]^{\frac{1}{2}} E[|\zeta_t|^2]^{\frac{1}{2}}$$

Next we obtain a bound for $\zeta_t$. Upon using the inequality $|e^{-x} - e^{-y}| \leq e^{-\min(x,y)}|x-y|$, (E.5)

$$|\zeta_t| \leq e^{-C} \left| \sum_{k=0}^{n-1} \epsilon(W_\epsilon(B^\epsilon_{2k+1}) - W(B^\epsilon_{2k})) \right| + e^{-C} \int_0^t W(B^\epsilon_{2k}) \text{d}s - \sum_{k=0}^{n-1} \epsilon W(B^\epsilon_{2k+1})$$

where $C = t \min(\min_{x \in \mathbb{R}^d} W(x), \min_{x \in \mathbb{R}^d} W_\epsilon(x))$. Now, $C$ is finite because, as $|x| \to \infty$, $W(x) \to \infty$ (Assumption A1) and $W_\epsilon(x) \to \infty$ (by (3.12b)).

The expectation of the first term on the right-hand side of (E.5) is bounded as follows:

$$E\left[ \left| \sum_{k=0}^{n-1} \epsilon(W_\epsilon(B^\epsilon_{2k+1}) - W(B^\epsilon_{2k})) \right|^2 \right]^{\frac{1}{2}} \leq \sum_{k=0}^{n-1} \epsilon E[|W_\epsilon(B^\epsilon_{2k+1}) - W(B^\epsilon_{2k})|^2]^{\frac{1}{2}}$$

$$\leq \sum_{k=0}^{n-1} \epsilon^2 E[(W_\epsilon(B^\epsilon_{2k+1}) - W(B^\epsilon_{2k}))^2]^{\frac{1}{2}}$$

$$\leq \sum_{k=0}^{n-1} \epsilon^2 \left( 2C_1|x|^2 + 2C_1 E[|B^\epsilon_{2k}|^4]^{\frac{1}{2}} + C_2 \right)$$

$$\leq \epsilon t \left[ 2C_1|x|^2 + 6C_1 t + C_2 \right]$$

where the second inequality follows from the bound $|W_\epsilon(x) - W(x)| = |r^{(2)}_\epsilon(x)| \leq \epsilon(C_1|x|^2 + C_2)$ for some constants $C_1, C_2$ (see (3.12b)).
The expectation of the second term in (E.5) is bounded as follows:

\[
E \left[ \left( \int_0^t W(B_{2s}^x) \, ds - \sum_{k=0}^{n-1} \epsilon W(B_{2k\epsilon}^x) \right)^2 \right]^{\frac{1}{2}} \leq \epsilon (E \left[ \int_0^t |\nabla W(B_{2s}^x)|^2 \, ds \right]^{\frac{1}{2}} + t\|\Delta W\|_{L^\infty})
\]

\[
\leq \epsilon (E \left[ \int_0^t |C_3|x + B_s| + C_4|^2 \, ds \right]^{\frac{1}{2}} + tC_5)
\]

\[
\leq \epsilon t^\frac{1}{2}(C_3|x| + C_5t + C_4) + \epsilon C_5t
\]

where the Taylor expansion of \(W(x)\) is used to obtain the first inequality, and for the second inequality, Assumption (A1) is used to bound \(\|\Delta W\|\) is a constant that only depends on \(\epsilon\) and \(\|\nabla W\|_{L^\infty}\) is used to obtain the first inequality, and for the second inequality, Assumption (A1) is used to bound \(\|\Delta W\|\leq\|\Sigma^{-1}\|\|x| + \|\nabla w\|_{L^\infty} = C_3|x| + C_4\) and \(\|\Delta W\|_{L^\infty} \leq \|\Sigma^{-1}\| + \|\Delta w\|_{L^\infty} = C_5\).

Putting together the two expectation bounds,

\[
|(T^n_{\epsilon_n} - \tilde{P}_t)f(x)| \leq e^{U_t(x)}E[f^2(B_{2t}^x)e^{-2U_t(B_{2t}^x)})^\frac{1}{2} C e t^\frac{1}{2}(x^2 + 1)
\]

where \(C\) is a constant that only depends on \(t_0\). Upon taking the \(L^2(\rho)\) norm

\[
\|T^n_{\epsilon_n} - \tilde{P}_t f\|_{L^2(\rho)}^2
\]

\[
\leq C \epsilon t \int \int f^2(y) (y - x) \rho(y) \, dy \, dx
\]

\[
\leq C \epsilon t \int \int f^2(y) (y - x)^2 |x|^2 + 1 \rho(y) \, dy \, dx
\]

\[
\leq C \epsilon t \int \int f^2(y) (y - x)^2 |x|^4 + 1 \rho(y) \, dy \, dx
\]

\[
\leq C \epsilon t \int \int f^2(y) (y^4 + 2|y|^2 + 1) \rho(y) \, dy \, dx
\]

\[
\leq C \epsilon t \int \int (|y|^4 + 2|y|^2 + 1) e^{8W(x) + o(x)} \rho(y) \, dy \, dx
\]

\[
\leq C \epsilon t \int \int f^4(x) \rho(x) \, dx \, dx
\]

\[
\leq C \epsilon t \|f\|_{L^4(\rho)}^2
\]

**Step 2.** Because \(P_t\) and \(\tilde{P}_t\) are semigroups with generators \(\Delta_\rho\) and \(\Delta_\eta\), respectively, we have the identity: \(P_t f - \tilde{P}_t f = \int_0^t P_{t-s}(\Delta_\rho - \Delta_\eta) \tilde{P}_s f \, ds\). Upon taking the \(L^2(\rho)\) norm of both sides, using the triangle inequality, because \(P_t\) is contraction on \(L^2(\rho)\),

\[
\|P_t f - \tilde{P}_t f\|_{L^2(\rho)} \leq \int_0^t \|(\Delta_\rho - \Delta_\eta) \tilde{P}_s f\|_{L^2(\rho)} \, ds
\]

Now,

\[
\|(\Delta_\rho - \Delta_\eta) \tilde{P}_s f\|_{L^2(\rho)}^2 = 4 \int |(\nabla U(x) - \nabla U_\epsilon(x)) \cdot \nabla (\tilde{P}_s f)(x)|^2 \rho(x) \, dx
\]

\[
\leq 4 \int |(\nabla U(x) - \nabla U_\epsilon(x)|^2 \rho(x) \, dx \left[ \int |\nabla \tilde{P}_s f(x)|^2 \rho(x) \, dx \right] \frac{1}{2}
\]

\[
\leq 4 e^2 \left[ \int |C_1|x + C_2|^4 e^{-2U(x) + 2U_\epsilon(x)} \rho(x) \, dx \right] \frac{1}{2} + \|\nabla f\|_{L^4(\rho)}^2
\]

\[
\leq C \epsilon^2 \|\nabla f\|_{L^4(\rho)}^2
\]

where the identity \(\Delta_\rho f - \Delta_\eta f = 2

\[
\nabla U \cdot \nabla f - 2 \nabla U_\epsilon \cdot \nabla f
\]

is used in the first step, the Cauchy-Schwartz inequality in the second step, and the bounds \(|\nabla U_\epsilon(x) - \nabla U(x)| \leq \epsilon(C_1|x| + C_2)\) and \(|\nabla \tilde{P}_s f|_{L^4(\rho)} \leq \|\nabla f\|_{L^4(\rho)}\) in the third step.
Appendix F. Proof of the Proposition 4.2.

Proof. (i) The Lyapunov condition (4.9a), known as DV(3) of [33], is the necessary and sufficient condition for geometric ergodicity (and in fact the stronger $U$-uniform ergodicity) [40, Thm. 15.0.1]. The distribution $\rho_\epsilon$ is invariant because $\forall f \in C_b(\mathbb{R}^d)$,

$$\int T_\epsilon f(x)\rho_\epsilon(x)\,dx = \int \int \frac{1}{n_\epsilon(x)}k_\epsilon(x,y)f(y)\rho(y)\,dy\frac{n_\epsilon(x)\rho(x)}{\int n_\epsilon(z)\rho(z)\,dz}\,dx$$

$$= \frac{1}{\int n_\epsilon(z)\rho(z)\,dz}\int \int k_\epsilon(x,y)\rho(x)\,dx f(y)\rho(y)\,dy$$

$$= \frac{1}{\int n_\epsilon(z)\rho(z)\,dz}\int f(y)n_\epsilon(y)\rho(y)\,dy = \int f(x)\rho_\epsilon(x)\,dx$$

(ii) The invariant density $\rho_\epsilon$ is reversible because $\forall f, g \in C_b(\mathbb{R}^d)$

$$\int g(x)T_\epsilon f(x)\rho_\epsilon(x)\,dx = \int \int g(x)\frac{k_\epsilon(x,y)}{n_\epsilon(x)}f(y)\rho(y)\frac{n_\epsilon(x)\rho(x)}{\int n_\epsilon(z)\rho(z)\,dz}\,dy\,dx$$

$$= \frac{1}{\int n_\epsilon(z)\rho(z)\,dz}\int T_\epsilon g(y)n_\epsilon(y)f(y)\rho(y)\,dy$$

$$= \int f(y)T_\epsilon g(y)\rho_\epsilon(y)\,dy$$

The spectral gap follows from Lyapunov condition (4.9a) and the fact that the chain is reversible [45, Thm 2.1]. The spectral gap is denoted as $\lambda$.

(iii) The solution $\phi_\epsilon$ satisfies the bound:

$$\|\phi\|_{L^2(\rho_\epsilon)} \leq \frac{\|\sum_{k=0}^{\epsilon-1} T_\epsilon^k (h - \hat{h}_\epsilon)\|_{L^2(\rho_\epsilon)}}{1 - \|T_\epsilon\|_{L^2(\rho_\epsilon)}} \leq \frac{\epsilon n\|h\|_{L^2(\rho_\epsilon)}}{1 - \|T_\epsilon\|_{L^2(\rho_\epsilon)}} \leq \frac{t\|h\|_{L^2(\rho_\epsilon)}}{\lambda}$$

It remains to verify the Lyapunov condition (4.9a): Using (3.11)

$$e^{-U_\epsilon T_\epsilon^n e^{U_\epsilon}(x)} = \mathbb{E}[e^{-\epsilon \sum_{k=0}^{\epsilon-1} W_\epsilon(B_{2n}^k \epsilon)}] \leq \mathbb{E}[e^{-\epsilon \sum_{k=0}^{\epsilon-1} (\alpha |B_{2n}^k \epsilon|^2 - \beta)}]$$

where the second inequality follows from using the lower bound $W_\epsilon(x) \geq \alpha |x|^2 - \beta$ derived in (E.4).

We now claim that

$$\mathbb{E}[e^{-\epsilon \sum_{k=0}^{\epsilon-1} (\alpha |B_{2n}^k \epsilon|^2 - \beta)}] = e^{-\alpha |x|^2 + \beta m}$$

for $m = 1, \ldots, n$ where $\{\alpha_m\}_{m=1}^n$ and $\{\beta_m\}_{m=1}^n$ are defined using the recursions:

$$\alpha_{m+1} = \alpha \epsilon + \frac{\alpha_m}{1 + 4\epsilon \alpha_m}, \quad \alpha_1 = \alpha \epsilon$$

$$\beta_{m+1} = \beta m + \beta \epsilon - \frac{1}{2} \log(1 + 4\epsilon \alpha_m), \quad \beta_1 = \beta \epsilon$$

Assuming for now that the claim is true

$$\log(e^{-\epsilon \sum_{k=0}^{\epsilon-1} (\alpha |B_{2n}^k \epsilon|^2 - \beta)}) \leq \log(\mathbb{E}[e^{-\epsilon \sum_{k=0}^{\epsilon-1} (\alpha |B_{2n}^k \epsilon|^2 - \beta)}]) = -\alpha_n |x|^2 + \beta_n$$

An upper-bound for $\beta_n$ and a lower-bound for $\alpha_n$ are obtained as follows:
1. For the sequence \( \{ \beta_m \}_{m=1}^n \),
\[
\beta_{m+1} \leq \beta_m + \beta \varepsilon, \quad \Rightarrow \quad \beta_n \leq \beta_1 + (n - 1) \beta \varepsilon = \beta t
\]

2. For the sequence \( \{ \alpha_m \}_{m=1}^n \),
\[
\alpha_{m+1} \leq \alpha_m + \alpha \varepsilon, \quad \Rightarrow \quad \alpha_m \leq \alpha_1 + (n - 1) \alpha \varepsilon = \alpha t
\]

Therefore,
\[
\alpha_m + 1 \geq \frac{\alpha_m}{1 + 4 \alpha \varepsilon t} + \alpha \varepsilon, \quad \alpha_1 = \alpha \varepsilon
\]

It then follows
\[
\alpha_n \geq \alpha t e^{-4 \alpha t^2}
\]

Upon using the two bounds
\[
\log(e^{-t U(x)} T^n e^{U(x)}) \leq -\alpha t e^{-4 \alpha t^2} |x|^2 + \beta t \leq -atU(x) + bt
\]

where the second inequality follows from using the upper bound \( U(x) \leq \frac{1}{8\sigma_1} |x|^2 + \frac{8}{3} C \) derived in (E.3). The following estimates are obtained for constants
\[
a = 8\sigma_2^2 \alpha e^{-4\alpha t^2}, \quad b = \beta + C \sigma_1^2 \alpha e^{-4\alpha t^2}
\]

It remains to prove the claim (F.1). The constants \( \alpha_1 \) and \( \beta_1 \) for \( m = 1 \) are easily verified by direct evaluation and for \( m > 1 \),
\[
E[e^{-\sum_{k=0}^m (\alpha |B_{2k}^\varepsilon|)^2 - \beta}]] = E[e^{-\sum_{k=0}^m (\alpha \varepsilon |B_{2k}^\varepsilon|)^2 - \beta - \alpha m}] = e^{-\sum_{k=0}^m (\frac{\alpha \varepsilon}{\varepsilon + \alpha m}) |x|^2 + \beta \varepsilon + \beta \varepsilon m} \leq \frac{1}{4 \varepsilon + \alpha m} \log(1 + 4 \alpha m)
\]

The minorization inequality (4.9b) is obtained next. For \( |x| \leq R \):
\[
T^n A(x) = e^{U(x)} e^{-\sum_{k=0}^{n-1} B_{2k}^\varepsilon(x)} e^{-U(x)} \mathbb{1}_{B_{2n}^\varepsilon \subseteq A} \geq \frac{\min_{|z| \leq R} U(z)}{\max_{|z| \leq R + 10} U(z)} \mathbb{P}(B_{2n}^\varepsilon \subseteq A \cap \{ \sup_{s \in [0,2]} |B_s| \leq 10 \}) \geq \delta \nu(A)
\]

where
\[
\nu(A) = \mathbb{P}(\{ \sup_{s \in [0,2]} |B_s| \leq 10 \})
\]
\[
\delta = \frac{\min_{|z| \leq R \in (0,1)} U(z)}{\max_{|z| \leq R + 10, z \in (0,1)} U(z)} (1 - 2e^{-\frac{50}{\nu}})
\]

because \( \mathbb{P}(\sup_{s \in [0,2]} B_s \geq 10) \leq e^{-\frac{50}{\nu}} \leq e^{-\frac{50}{\nu}}. \)

Appendix G. Proof of Theorem 4.3.

Proof. 
(i) The existence of the solution is proved in Proposition 4.2.
(ii) We break the error into two parts:
\[
\| \phi - \hat{\phi} \|_{L^2(\mu)} \leq \| \phi - \hat{\phi} \|_{L^2(\mu)} + \| \hat{\phi} - \phi \|_{L^2(\mu)}
\]
where $\tilde{\phi}$ is the solution to the fixed point equation $\tilde{\phi} = P_n \tilde{\phi} + \epsilon(h - \hat{h})$ with the exact semigroup $P_n$. The bounds for the two terms on the right-hand side are derived in the following two steps:

**Step 1.** Iterating the formula $\tilde{\phi} = P_n \tilde{\phi} + \epsilon(h - \hat{h})$ for $n = \lceil \frac{1}{\epsilon} \rceil$ times yields,

$$\tilde{\phi} = P_n \tilde{\phi} + \sum_{k=0}^{n-1} \epsilon P^n_k (h - \hat{h})$$

and subtracting this from (4.8) gives

$$\phi_e - \tilde{\phi} = T^n_e (\phi_e - \tilde{\phi}) + (T^n_e - P^n_e) \tilde{\phi} + \sum_{k=0}^{n-1} \epsilon (T^n_k - P^n_k) h + t(h - \hat{h})$$

This forms a (discrete) Poisson equation whose solution exists and is bounded according to Proposition 4.2:

$$\|\phi_e - \tilde{\phi}\|_{L^2(\rho)} \leq \frac{ne}{\lambda} \left( \| T^n_e \|_{L^2(\rho)} + \sum_{k=0}^{n-1} \epsilon (T^n_k - P^n_k) \| h \|_{L^2(\rho)} + ne \| h - \hat{h} \|_{L^2(\rho)} \right)$$

where we used $\| h \|_{L^2(\rho)} \leq C \| h \|_{L^2(\rho)}$ in the second step. This is true because $\rho_e(x) = e^{-U_e(x)} G_s e^{-U_e(x)}(x) = \rho(x) e^{-3\epsilon \Delta V(x) + O(\epsilon^2)} \leq C \rho(x)$ using the formula (3.12a).

It remains to bound the three terms inside the bracket in (G.1):

$$\| T^n_e \|_{L^2(\rho)} = C \sqrt{n \epsilon} \text{ and } \| \nabla \tilde{\phi} \|_{L^2(\rho)}$$

$$\| \sum_{k=0}^{n-1} \epsilon (T^n_k - P^n_k) h \|_{L^2(\rho)} \leq C (n \epsilon) \sqrt{n \epsilon} \| h \|_{L^2(\rho)} + \| \nabla h \|_{L^2(\rho)}$$

$$\| h - \hat{h} \| \leq \int | h(x) | \rho(x) e^{-3\epsilon \Delta V(x) + O(\epsilon^2)} - 1 | \, dx \leq C \| h \|_{L^2(\rho)}$$

by using the error estimates Proposition 3.2-(iii). Therefore,

$$\|\phi_e - \tilde{\phi}\|_{L^2(\rho)} \leq C \| h \|_{L^2(\rho)} + \| \nabla h \|_{L^2(\rho)} + \| \tilde{\phi} \|_{L^2(\rho)} + \| \nabla \tilde{\phi} \|_{L^2(\rho)}$$

**Step 2.** Both $\phi$ and $\tilde{\phi}$ are solutions with the exact semigroup $P_n$. Using the spectral representation (2.2),

$$\phi = \sum_{m=1}^{\infty} \frac{1}{\lambda_m} (h, e_m) e_m, \quad \tilde{\phi} = \sum_{m=1}^{\infty} \frac{\epsilon}{1 - e^{-\epsilon \lambda_m}} (h, e_m) e_m$$

Therefore,

$$\| \tilde{\phi} - \phi \|_{L^2(\rho)}^2 = \epsilon^2 \sum_{m=1}^{\infty} \left( \frac{1}{1 - e^{-\epsilon \lambda_m}} - \frac{1}{\epsilon \lambda_m} \right)^2 | (h, e_m) |^2 \leq \epsilon^2 \| h \|_{L^2(\rho)}^2$$

and thus $\| \tilde{\phi} - \phi \|_{L^2(\rho)} \leq C \| \tilde{\phi} - \phi \|_{L^2(\rho)} \leq \epsilon^2 C \| h \|_{L^2(\rho)}^2$.

Combining the estimates from steps 1 and 2,

$$\|\phi_e - \tilde{\phi}\|_{L^2(\rho)} \leq C \| h \|_{L^2(\rho)} + \| \nabla h \|_{L^2(\rho)} + \| \tilde{\phi} \|_{L^2(\rho)} + \| \nabla \tilde{\phi} \|_{L^2(\rho)}$$

$\square$
Appendix H. Proof of the Proposition 3.3.

Proof. Denote \( \eta_j = (\sqrt{\frac{(g_\epsilon \ast \rho(X^j))}{\sum_{j=1}^{\infty} g_\epsilon(X^j, X^j)} - 1} \) and express:

\[
T_\epsilon^{(N)} f(x) = \int k_\epsilon(x, y) f(y) \rho(y) \, dy + \xi_1^{(N)} + \xi_2^{(N)} - n_\epsilon(x) + \zeta_1^{(N)} + \zeta_2^{(N)}
\]

where

\[
\xi_1^{(N)} = \frac{1}{N} \sum_{j=1}^{N} k_\epsilon(x, X^j) f(X^j) - \mathbb{E}[k_\epsilon(x, X^j) f(X^j)], \quad \zeta_1^{(N)} = \frac{1}{N} \sum_{j=1}^{N} k_\epsilon(x, X^j) f(X^j) \eta_j \\
\xi_2^{(N)} = \frac{1}{N} \sum_{j=1}^{N} k_\epsilon(x, X^j) - \mathbb{E}[k_\epsilon(x, X^j)], \quad \zeta_2^{(N)} = \frac{1}{N} \sum_{j=1}^{N} k_\epsilon(x, X^j) \eta_j
\]

(i) To prove the part-(i) of the Proposition 3.3, the strategy is to show that as \( N \to \infty \) the stochastic terms \( \xi_1^{(N)}, \xi_2^{(N)}, \zeta_1^{(N)}, \zeta_2^{(N)} \) converge to zero almost surely. We do this in two steps below, \( \xi_1^{(N)}, \xi_2^{(N)} \) in step 1, and \( \zeta_1^{(N)}, \zeta_2^{(N)} \) in step 2.

**Step 1:** Convergence of \( \xi_1^{(N)} \) and \( \xi_2^{(N)} \) follows from direct application of the strong law of large numbers (SLLN). The SLLN applies because the summand for \( \xi_1^{(N)} \) and \( \xi_2^{(N)} \) are independent and identically distributed (i.i.d) and moreover have finite variance:

\[
\text{(H.1)} \quad \text{Var}(k_\epsilon(x, X) f(X)) \leq C \frac{\| f \|_{\infty}^2 \rho(x)}{e^{d/2} (g_\epsilon \ast \rho)^2(x)} \\
\text{(H.2)} \quad \text{Var}(k_\epsilon(x, X)) \leq C \frac{\rho(x)}{e^{d/2} (g_\epsilon \ast \rho)^2(x)}
\]

where we used \( g_\epsilon^2(x, y) \leq C e^{-d/2} g_{\epsilon/2}(x, y) \).

**Step 2:** In order to show the almost sure convergence of \( \zeta_1^{(N)} \) and \( \zeta_2^{(N)} \) to zero, we first show that in the limit as \( N \to \infty \),

\[
\text{(H.3)} \quad |\eta_i| \leq C \sqrt{\frac{\log(N/\delta)}{Ne^{d/2} g_\epsilon(X^j)}}, \quad \forall i = 1, \ldots, N
\]

with probability larger than \( 1 - \delta \) for any arbitrary choice of \( \delta \in (0, 1) \). Assuming for now that the claim is true, it then follows

\[
\text{(H.4)} \quad \zeta_1^{(N)} \leq \sqrt{\frac{C \log(N/\delta)}{Ne^{d/2} g_\epsilon(X^j)}} \left( \frac{1}{N} \sum_{j=1}^{N} k_\epsilon(x, X^j) \frac{|f(X^j)|}{\sqrt{g_\epsilon \ast \rho(X^j)}} \right)
\]

with probability larger than \( 1 - \delta \). The term inside the bracket converges almost surely to its limit \( \mathbb{E}[k_\epsilon(x, X) \frac{|f(X)|}{\sqrt{g_\epsilon \ast \rho(X)}}] \), by SLLN, because

\[
\mathbb{E} \left( k_\epsilon(x, X) \frac{|f(X)|}{\sqrt{g_\epsilon \ast \rho(X)}} \right) \leq \frac{C \| f \|_{\infty} \rho(x)}{(g_\epsilon \ast \rho)^{3/2}(x)}
\]

The proof that \( \zeta_1^{(N)} \xrightarrow{a.s.} 0 \) is completed by an application of the Borel-Cantelli lemma. Indeed, choose a sequence \( \{\delta_N\}_{N=1}^{\infty} \) given by \( \delta_N = \frac{1}{N^2} \). Then \( \sum_{N=1}^{\infty} \text{Prob}(\zeta_1^{(N)} > 0) \rightarrow 0 \), completing the proof. 

Therefore, the limit of \( \sum_{N=1}^{\infty} \xi_1^{(N)} + \xi_2^{(N)} - \sum_{N=1}^{\infty} \zeta_1^{(N)} + \zeta_2^{(N)} \) is zero almost surely, which establishes the desired result.
\( \epsilon_N \leq \sum_{N=1}^{\infty} \delta_N < \infty \) where \( \epsilon_N = \sqrt{\frac{C \log(N^3)}{Ne^{d/2}}} \). Because \( \epsilon_N \to 0 \), then \( \zeta_1^{(N)} \to 0 \). The proof of \( \zeta_2^{(N)} \to 0 \) is identical.

It remains to prove the claim (H.3). It follows from the Bernstein inequality. We have for any \( a > 0 \):

\[
\text{Prob} (\eta_i \geq a) = \text{Prob} \left( \frac{1}{N} \sum_{i=1}^{N} g_i (X_i) \geq 1 + a \right) \leq \text{Prob} \left( \frac{1}{N} \sum_{i=1}^{N} g_i (X_j, X_i) \geq 1 + a \right) = \text{Prob} \left( \frac{(g_\epsilon \ast \rho)(X_j)}{g_\epsilon \ast \rho}(X_j) - \frac{1}{N} \sum_{i=1}^{N} g_\epsilon (X_j, X_i) \geq \frac{a}{1 + a} \right)
\]

The random variables \( g_\epsilon (X_i, X_j) \) are i.i.d, bounded by \( (4 \pi \epsilon)^{-\frac{d}{2}} \), and the variance

\[
E \left[ |g_\epsilon (X_i, X_j)|^2 |X_j| \right] \leq \frac{1}{(8 \pi \epsilon)^{d/2}} (g_\epsilon \ast \rho)(X_j)
\]

Therefore by Bernstein inequality,

\[
|\eta_i| \leq C \sqrt{\frac{(g_\epsilon \ast \rho)(X_j) \log(\frac{2}{\delta})}{N(8 \pi \epsilon)^{d/2} (g_\epsilon \ast \rho)(X_j)^2}}
\]

with probability higher than \( 1 - \delta \). The result is obtained by union bound for \( i = 1, \ldots, N \) and \( \|g_\epsilon \ast \rho\|_{\infty} < \infty \).

(ii) Collecting the estimates (H.1), (H.2), and (H.4) and application of the Bernstein inequality yields:

\[
|\xi_1^{(N)}| \leq \sqrt{\frac{C \|f\|_{L_2} \log(\frac{N}{\delta}) \rho(x)}{Ne^{d/2}(g_\epsilon \ast \rho)^2(x)}}, \quad |\xi_2^{(N)}| \leq \sqrt{\frac{C \log(\frac{N}{\delta}) \rho(x)}{Ne^{d/2}(g_\epsilon \ast \rho)^2(x)}}
\]

with probability larger than \( 1 - 4\delta \). Therefore one obtains the bound:

\[
|T_\epsilon^{(N)} f(x) - T_\epsilon f(x)| \leq \sqrt{\frac{C \log(\frac{N}{\delta}) \rho(x)}{Ne^{d/2}(g_\epsilon \ast \rho)^2(x) n(x)}}
\]

with probability larger than \( 1 - 4\delta \). Upon squaring and integrating both sides with respect to \( \rho(x) \) proves the rate:

\[
\|T_\epsilon^{(N)} f - T_\epsilon f\|_2 \leq \sqrt{\frac{C \log(\frac{N}{\delta})}{Ne^{d/2}}} \left( \int \frac{\rho(x)}{(g_\epsilon \ast \rho)^2(x) n(x)} \rho(x) \, dx \right)^{1/2} \leq \sqrt{\frac{C \log(\frac{N}{\delta})}{Ne^{d/2}}} \left( \int e^{-2\epsilon |\nabla V (x)|^2 + \frac{3}{2} (\nabla V (x))^2} \, dx \right)^{1/2} \leq \sqrt{\frac{C \log(\frac{N}{\delta})}{Ne^{d/2}}} \Box
\]
Appendix I. Proof of the Theorem 4.4. In the proof of Theorem 4.4, the function space of interest is $C(\Omega)$, the Banach space of continuous functions on (a compact set) $\Omega \subset \mathbb{R}^d$ equipped with the $\| \cdot \|_\infty$ norm. The space $C_0(\Omega) := \{ f \in C(\Omega) \mid \int f \rho_x = 0 \}$. Consider $T_\epsilon$ and $T_\epsilon^{(N)}$ as linear operators from $C(\Omega)$ to $C(\Omega)$.

Part-(i) has already been proved as part of the Proposition 4.1. The proof of part (ii) relies on the verification of the following three conditions:

(i) The family of operators $\{ T_\epsilon^{(N)} \}_{N=1}^\infty$ is collectively compact, as linear operators on $C(\Omega)$.

(ii) For any function $f \in C(\Omega)$,

\[
\lim_{N \to \infty} \| T_\epsilon^{(N)} f - T_\epsilon f \|_\infty = 0, \quad \text{a.s.}
\]

(iii) The operator $(I - T_\epsilon)^{-1}$ is a bounded operator on $C_0(\Omega)$.

Once these three conditions have been verified, the convergence result (4.12) follows from a standard result in the approximation theory of the numerical solutions of integral equations [29, Thm. 7.6.6].

The proof of the three conditions is as follows:

(i) The collective compactness holds if the set $S = \{ T_\epsilon^{(N)} f ; \forall f \in C(\Omega), \| f \|_\infty \leq 1, N \in \mathbb{N} \}$ is relatively compact. Relative compactness follows from an application of the Arzela-Ascoli theorem. In order to apply Arzela-Ascoli theorem, we need to show that $S$ is uniformly bounded and equicontinuous. The two conditions hold because

\[
\text{(unif. boundedness)} \quad |T_\epsilon^{(N)} f(x)| \leq \| f \|_\infty \sum_{i=1}^N k_{\epsilon i}^{(N)} (x, X^i) \leq 1
\]

\[
\text{(equicontinuous)} \quad |T_\epsilon^{(N)} f(x) - T_\epsilon^{(N)} f(x')| \leq L \frac{\epsilon}{\| x - x' \|} e^{\frac{\epsilon}{2} |x - x'|}
\]

for all $x, x' \in \Omega$ and $f$ such that $\| f \|_\infty \leq 1$. The detailed calculation to obtain the second inequality appears at the end of the proof.

(ii) Fix a function $f \in C(\Omega)$. From Proposition 3.3-(i), we know that $T_\epsilon^{(N)} f(x)$ converges to $T_\epsilon f(x)$ almost surely pointwise for all $x \in \Omega$. Because $\Omega$ is compact and $\{ T_\epsilon^{(N)} f \}$ is equicontinuous, pointwise convergence implies uniform convergence (1.1).

(iii) From parts (i) and (ii) above, it can be concluded that $T_\epsilon$ is a compact operator. Therefore, using the Fredholm alternative theorem, in order to show $(I - T_\epsilon)^{-1}$ is bounded, it is enough to show that $I - T_\epsilon$ is injective. The injectivity property is shown by contradiction. Suppose there exists a function $f \in C_0(\Omega)$ such that $f - T_\epsilon f = 0$. Let $x_0 \in \Omega$ be a point that achieves the maximum of the function $f$. Such a point exists because $f$ is continuous and $\Omega$ is compact. Evaluating $f - T_\epsilon f = 0$ at $x = x_0$ yields

\[
0 = f(x_0) - T_\epsilon f(x_0) = \frac{1}{n_\epsilon(x)} \int k_\epsilon(x_0, y) (f(x_0) - f(y)) \, dy
\]

Because $k_\epsilon(x_0, y) > 0$ and $f(y) \leq f(x_0)$, this implies $f(y) = f(x_0)$ for all $y \in \Omega$. Therefore, the function $f$ is a constant. But the only constant function in $C_0(\Omega)$ is zero. Hence $I - T_\epsilon$ is injective and its inverse $(I - T_\epsilon)^{-1}$ is bounded.
where the last inequality is obtained as follows

\[ |1 - k(x',X')| \leq |1 - g(x',X')| = |1 - e^{-\frac{(x'-x)(x'+x-2X')}{\epsilon}}| \leq \frac{L}{2\epsilon} |x - x'| \frac{1}{\#} |x - x'| \]

where \( L = \max_{x,y \in \Omega} |x - y| \) is the diameter of \( \Omega \).

**Appendix J. Proof of Proposition 4.6.**

1. Consider first the finite-\( N \) case. In the asymptotic limit as \( \epsilon \to \infty \), we have

\[ (2\pi \epsilon)^{d/2} g_{\epsilon}(x,y) = 1 + O(\frac{1}{\epsilon}) \]

Therefore,

\[ k_{\epsilon}^{(N)}(x,y) = \frac{1}{\sqrt{N}} \frac{\sum_{j=1}^{N} g_{\epsilon}(x,X')}{\sqrt{\frac{1}{N} \sum_{j=1}^{N} g_{\epsilon}(y,X')}} = 1 + O(\frac{1}{\epsilon}) \]

and

\[ n_{\epsilon}^{(N)}(x) = \frac{1}{N} \sum_{i=1}^{N} k_{\epsilon}^{(N)}(x,X') = 1 + O(\frac{1}{\epsilon}) \]

and

\[ T_{\epsilon}^{(N)} f(x) = \frac{1}{N} \sum_{j=1}^{N} k_{\epsilon}(x,X') f(X') = \frac{1}{N} \sum_{j=1}^{N} f(X') + O(\frac{1}{\epsilon}) \]

It is also easy to see, e.g., by using a Neumann series solution, that in the asymptotic limit as \( \epsilon \to \infty \), the solution of the fixed-point equation (4.4) is given by

\[ \Phi = \epsilon(h - \frac{1}{N} \sum_{j=1}^{N} h_j) + O(1) \]

Therefore,

\[ r = \Phi + \epsilon h = 2\epsilon h - \epsilon(\frac{1}{N} \sum_{j=1}^{N} h_j) + O(1) \]

\[ s_{ij} = \frac{1}{2\epsilon} T_{ij}(r_{ij} - \sum_{k=1}^{N} T_{ik} r_k) = \frac{1}{N} (h_j - \frac{1}{N} \sum_{l=1}^{N} h_l) + O(\frac{1}{\epsilon}) \]

and using the gain approximation formula (3.7),

\[ K_j = \sum_{j=1}^{N} s_{ij} X^j = \frac{1}{N} \sum_{j=1}^{N} (h_j - \frac{1}{N} \sum_{l=1}^{N} h_l) X^j + O(\frac{1}{\epsilon}) \]
2. The calculations for the kernel formula are entirely analogous. In the asymptotic limit as $\epsilon \to \infty$,

$$T_\epsilon f(x) = \int f(x)\rho(x) \, dx + O\left(\frac{1}{\epsilon}\right)$$

$$\phi_\epsilon(x) = \epsilon(h(x) - \hat{h}) + O(1)$$

and, using $\theta(x) = x$ to denote the coordinate function and $\cdot$ to denote function multiplication, the gain approximation formula (4.13) evaluates to

$$K_\epsilon(x) = \frac{1}{2\epsilon} \left[ T_\epsilon(\theta \cdot \phi_\epsilon + \epsilon(h - \hat{h})) - T_\epsilon(\theta) T_\epsilon(\phi_\epsilon + \epsilon(h - \hat{h})) \right]$$

$$= \frac{1}{2} T_\epsilon(\theta \cdot \frac{\phi_\epsilon}{\epsilon} + h - \hat{h}) - \frac{1}{2} T_\epsilon(\theta) T_\epsilon(\frac{\phi_\epsilon}{\epsilon} + h - \hat{h}) + O\left(\frac{1}{\epsilon}\right)$$

$$= T_\epsilon(\theta \cdot h - \hat{h}) - T_\epsilon(\theta) T_\epsilon(h - \hat{h}) + O\left(\frac{1}{\epsilon}\right)$$

$$= \int x(h(x) - \hat{h}) \rho(x) \, dx + O\left(\frac{1}{\epsilon}\right)$$