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ABSTRACT

Score-based density ratio estimation is essential for measuring discrepancies between probability distributions, yet existing methods often suffer from high computational costs, **requiring many function evaluations to maintain accuracy**. We propose One-Step Score-Based Density Ratio Estimation (OS-DRE), an analytic and efficient framework that eliminates the need for numerical solvers. Our approach is based on a spatiotemporal decomposition of the time score function, where its temporal component is represented with an RBF-based (radial basis function) analytic frame. This transforms the intractable temporal integral into a closed-form weighted sum, enabling OS-DRE to estimate density ratios with only one function evaluation while preserving high accuracy. Theoretical analysis provides a rigorous truncation error bounds, ensuring provable accuracy with finite bases. Empirical results show that OS-DRE achieves competitive performance while completing density ratio estimation in a single step, effectively resolving the long-standing accuracy-efficiency trade-off in score-based methods.

1 INTRODUCTION

Density ratio estimation (DRE) is a fundamental task in machine learning and statistics, used to quantify the discrepancies between two probability distributions (Sugiyama et al., 2012). It plays a central role in a variety of applications, including continual learning (Zhang et al., 2023), mutual information estimation (Letizia et al., 2024; Chen et al., 2025), Large Language Models (LLMs) alignment (Higuchi & Suzuki, 2025; Xiao et al., 2025), and causal inference (Wang et al., 2025). However, classical DRE faces a significant challenge known as the density-chasm problem, where non-overlapping (Srivastava et al., 2023; Chen et al., 2025) or high-discrepancy distributions (Rhodes et al., 2020; Wang et al., 2025) lead to unstable and inaccurate estimates.

A significant advance has been the emergence of continuous, score-based methods (Choi et al., 2022; Yu et al., 2025; Chen et al., 2025), which reframe the log-density ratio as the path integral of a time-dependent score function along a smooth interpolation between the two distributions (see Fig. 5 for illustration). This continuous formulation transforms the DRE between p_0 and p_1 , i.e., $r(\mathbf{x}) = p_1(\mathbf{x})/p_0(\mathbf{x})$, into solving the integral $\log r(\mathbf{x}) = \int_0^1 \partial_t \log p_t(\mathbf{x}) dt$, with $\partial_t \log p_t(\mathbf{x})$ being the *time score*. While this mitigates the density-chasm problem, existing score-based methods still rely on computationally expensive numerical integration techniques, including ODE solvers (Choi et al., 2022) and fine-grained quadratures (Norcliffe & Deisenroth, 2023). **Achieving reliable estimates requires many repeated score evaluations, which results in a high number of function evaluations (NFE) and substantial computational overhead.**

In this work, we introduce **One-Step Score-Based Density Ratio Estimation (OS-DRE)**, a novel framework that is *solver-free* and computes the density ratio integral in a single step. Our key

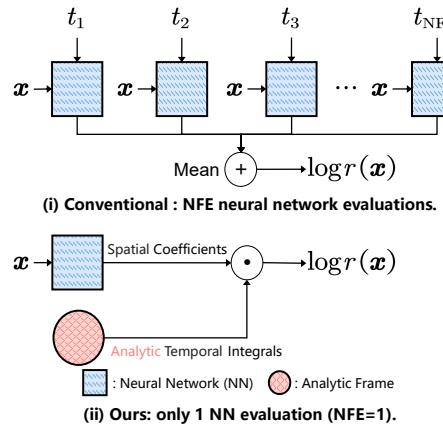


Figure 1: Illustrative comparison of conventional (i) and proposed (ii) score-based DRE methods. The NFE of conventional methods depends on the chosen numerical solver.

innovation is to replace numerical integration with an analytic solution. We achieve this by proposing a spatiotemporal decomposition of the time score, where we represent its temporal component using an *analytic frame*, which is a mathematical frame whose elements $\{g_k\}_{k=1}^{\infty}$ possess closed-form temporal integrals. This allows us to re-express the integral as a simple weighted sum:

$$\log r(\mathbf{x}) = \int_0^1 \partial_t \log p_t(\mathbf{x}) dt = \sum_{k=1}^{\infty} h_k(\mathbf{x}) \int_0^1 g_k(t) dt \approx \langle \mathbf{h}^{(K)}(\mathbf{x}), \bar{\mathbf{g}}^{(K)} \rangle, \quad (1)$$

where $\mathbf{h}^{(K)}(\mathbf{x}) = [h_1^{(K)}(\mathbf{x}), h_2^{(K)}(\mathbf{x}), \dots, h_K^{(K)}(\mathbf{x})]$ and $\bar{\mathbf{g}}^{(K)} = [\bar{g}_1, \bar{g}_2, \dots, \bar{g}_K]$ are two K -dimensional vectors with $\bar{g}_k = \int_0^1 g_k(t) dt$. As illustrated in Fig. 1, our method employs a neural network (blue squares) to predict the spatial coefficients $\mathbf{h}^{(K)}(\mathbf{x})$ in a single forward pass, which then weight the pre-computed, analytic integrals of our frame elements (red circles). This approach reduces the NFE to just **one**, drastically improving computational efficiency.

Our framework is grounded in rigorous approximation theory. We construct our analytic frames using radial basis functions (RBFs) and prove that this construction yields a temporal basis that is both *complete* in the infinite limit (guaranteeing convergence) and *stable* for any finite number of basis functions (ensuring numerical robustness). Furthermore, we provide a theoretical truncation error bound, which guarantees that the approximation accuracy can be systematically controlled. The main contributions of this work are:

- We propose OS-DRE, the first **path-integral-based**, score-based DRE method that analytically estimates the density ratio in a single step, eliminating the need for numerical solvers **while preserving the flexibility of the continuous formulation**.
- We introduce the concept of an analytic frame, a temporal basis with closed-form integrals, which enables the direct, analytic computation of the density ratio integral.
- We provide a complete theoretical framework for our method, including proofs for the completeness of our RBF-based construction, and a formal analysis of the truncation error.
- We validate OS-DRE through extensive experiments, demonstrating that it achieves competitive performance on several benchmark datasets with unparalleled computational efficiency.

2 RELATED WORKS AND PROBLEM STATEMENT

Related Works. Density Ratio Estimation (DRE) is a cornerstone task in machine learning (Sugiyama et al., 2012). Research in this area has largely followed two main trajectories. The first line of work is based on discriminative or contrastive objectives, such as in KLIEP (Sugiyama et al., 2012), NCE (Gutmann & Hyvärinen, 2012), and TR-DRE (Liu et al., 2017). While foundational, these methods often struggle with the “density-chasm” problem, where distributions with high discrepancies or complex settings lead to unstable training and poor estimates. Subsequent efforts to mitigate this issue within the same paradigm, such as FDRE (Choi et al., 2021), iterated regularization (Gruber et al., 2024), γ -DRE (Nagumo & Fujisawa, 2024), IMDRE (Kimura & Bondell, 2025) and PP-DRE (Wang et al., 2025), have often introduced significant computational overhead by requiring complex machinery like normalizing flows or additional importance sampling steps. A second, more recent line of research, known as score-based DRE, emerged as a powerful alternative for resolving the density-chasm problem. Pioneered by methods like TRE (Rhodes et al., 2020) and DRE- ∞ (Choi et al., 2022), this approach reframes the problem in a continuous setting, which inherently provides a smoother and more stable estimation path between the two distributions. Despite their robustness, subsequent innovations within this paradigm (Chen et al., 2025; Yu et al., 2025) have remained dependent on computationally expensive numerical solvers for integration. A related line of work, Guth et al. (2025), trains a time-varying energy via dual score matching, enabling single-step evaluation of normalized log-densities when p_0 or p_1 is Gaussian and global calibration is available. However, it does not address general DRE between two arbitrary non-Gaussian distributions, where aligning the global constants of separately trained energy models is infeasible. Our work, OS-DRE, operates within the robust score-based framework of the path integral but is the first to propose a *solver-free* approach that entirely eliminates the computational bottleneck by providing **an analytic solution to the integral itself, thereby preserving the core advantages of the integration paradigm**.

Problem Statement. Modern score-based DRE reframes the estimation of the ratio $r(\mathbf{x}) = p_1(\mathbf{x})/p_0(\mathbf{x})$ as the computation of an integral. By constructing a continuous path of densities $p_t(\mathbf{x})$ that interpolates between p_0 and p_1 , the log-density ratio is expressed as:

$$\log r(\mathbf{x}) = \log \frac{p_1(\mathbf{x})}{p_0(\mathbf{x})} = \log p_1(\mathbf{x}) - \log p_0(\mathbf{x}) = \int_0^1 \partial_t \log p_t(\mathbf{x}) dt. \quad (2)$$

108 The integrand, $\partial_t \log p_t(\mathbf{x})$, is known as the *time score*. In practice, the true time score is unknown and
 109 is approximated by a neural network, $s_t^\theta(\mathbf{x}, t)$, trained to match the true score, typically by minimizing
 110 a time score matching (TSM) objective (Choi et al., 2022). After training, the log-density ratio is
 111 estimated by computing the integral of the learned score model: $\log \hat{r}(\mathbf{x}) = \int_0^1 s_t^{\theta^*}(\mathbf{x}, t) dt$. **The**
 112 **central problem addressed in this work is the computational bottleneck of this final step.** Existing
 113 methods rely on expensive numerical techniques like ODE solvers or quadratures to approximate this
 114 integral, requiring numerous iterative evaluations of the model $s_t^{\theta^*}$. Our goal is to develop a method
 115 that computes this integral accurately and efficiently, without resorting to any numerical solvers.
 116

3 ONE-STEP DENSITY RATIO ESTIMATION

117 **Notations.** Let $\mathcal{S} \triangleq \{s_t \mid s_t(\mathbf{x}, t) \triangleq \partial_t \log p_t(\mathbf{x}), \mathbf{x} \in \mathcal{X}, p_t \in \mathcal{P}(\mathcal{X}), t \in [0, 1]\}$ denote the set
 118 of *time score* functions, where $\mathcal{P}(\mathcal{X})$ is a family of probability densities over the sample space \mathcal{X} .
 119

120 To ensure the analytical tractability of the time score function s_t , we impose some mild regularity
 121 conditions on the probability density $p_t(\mathbf{x})$, which are detailed in Sec. A.1. Under these conditions,
 122 the space \mathcal{S} is embedded in the Hilbert space $L^2(\mathcal{X} \times [0, 1])$.
 123

124 **Lemma 3.1.** *Under Assumptions A.1 and A.2, the space \mathcal{S} is a subset of $L^2(\mathcal{X} \times [0, 1])$.*

125 See Sec. A.3 for a detailed proof. This embedding allows us to leverage the tools of Hilbert space
 126 theory to analyze and approximate the time score function s_t .
 127

128 For notational convenience, we denote $L^2(\mathcal{X} \times [0, 1])$ by $\mathcal{H}_{\mathbf{x}, t}$ throughout this paper. The Hilbert
 129 space $\mathcal{H}_{\mathbf{x}, t}$ is isometrically isomorphic to the Hilbert tensor product $\mathcal{H}_{\mathbf{x}} \hat{\otimes} \mathcal{H}_t$ (Kadison & Ringrose,
 130 1986), where $\mathcal{H}_{\mathbf{x}} \triangleq L^2(\mathcal{X})$ and $\mathcal{H}_t \triangleq L^2([0, 1])$. This equivalence guarantees that any time score
 131 $s_t \in \mathcal{S}$ can be represented by separating its spatial and temporal components (see Lemma A.3).
 132

133 **Decomposition via Orthonormal Bases.** We first propose to represent the temporal component of
 134 the time score using a complete orthonormal basis $\{g_k\}_{k=1}^\infty$ for \mathcal{H}_t . This decomposition, analogous
 135 to the Karhunen-Loëve expansion (Karhunen, 1947; Loëve, 1977), allows us to express the time
 136 score $s_t(\mathbf{x}, t)$ for each fixed \mathbf{x} as a weighted sum of its spatial and temporal components:
 137

$$s_t(\mathbf{x}, t) = \sum_{k=1}^{\infty} h_k(\mathbf{x}) g_k(t), \quad \text{where } h_k(\mathbf{x}) = \langle s_t(\mathbf{x}, \cdot), g_k \rangle_{\mathcal{H}_t} \triangleq \int_0^1 s_t(\mathbf{x}, t) g_k(t) dt. \quad (3)$$

138 By integrating this series with respect to time, we derive our initial formulation for the $\log r(\mathbf{x})$.
 139

140 **Lemma 3.2.** *Let $\{g_k\}_{k=1}^\infty$ be a complete orthonormal basis for \mathcal{H}_t . The target log-density ratio
 141 $\log r(\mathbf{x})$ can be estimated by:*

$$\log r(\mathbf{x}) = \sum_{k=1}^{\infty} h_k(\mathbf{x}) \int_0^1 g_k(t) dt. \quad (4)$$

142 See Sec. A.4 for details. While theoretically sound, this approach faces a critical practical limitation.
 143 For many standard orthonormal bases (e.g., Fourier or Legendre bases), all basis elements except the
 144 constant function (say, g_1) have zero integrals, i.e., $\int_0^1 g_k(t) dt = \langle g_k, 1 \rangle_{\mathcal{H}_t} = 0, \forall k > 1$, causing the
 145 expansion of Eq. (4) to collapse to a single term and discard high-frequency information.
 146

147 **Generalization via Frame-Based Decomposition.** To resolve this degeneracy, we relax the strict
 148 orthogonality condition and adopt a more flexible *frame* for \mathcal{H}_t . Frames retain the completeness
 149 property of orthonormal bases but allow for redundancy and non-orthogonality, enabling the use of
 150 elements with non-zero integrals.
 151

152 **Definition 3.3** (Frame, Mallat (2009)). Let \mathcal{H} be a Hilbert space with inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}}$. A
 153 sequence $\{g_k\}_{k=1}^\infty$ in a Hilbert space \mathcal{H} is a frame if there exist constants $0 < A \leq B < \infty$, called
 154 the *frame bounds*, such that for any $g \in \mathcal{H}$:

$$A\|g\|_{\mathcal{H}}^2 \leq \sum_{k=1}^{\infty} |\langle g, g_k \rangle_{\mathcal{H}}|^2 \leq B\|g\|_{\mathcal{H}}^2. \quad (5)$$

155 The frame bounds ensure that $\{g_k\}_{k=1}^\infty$ provides a stable representation of any $g \in \mathcal{H}$, even if the
 156 frame elements g_k are not linearly independent (Mallat (2009)).
 157

162 By employing frames for both the spatial and temporal spaces, we arrive at our final, powerful
 163 representation for the time score and log-density ratio.

164 **Theorem 3.4.** *Let $\{f_l\}_{l=1}^{\infty}$ and $\{g_k\}_{k=1}^{\infty}$ be frames for \mathcal{H}_x and \mathcal{H}_t , respectively. Then, any time
 165 score function $s_t \in \mathcal{S}$ can be expressed as:*

$$167 \quad s_t(\mathbf{x}, t) = \sum_{k=1}^{\infty} \sum_{l=1}^{\infty} c_{l,k} f_l(\mathbf{x}) g_k(t), \quad (6)$$

170 where the coefficients $c_{l,k}$ depend on s_t . By defining spatial coefficients $h_k(\mathbf{x}) \triangleq \sum_{l=1}^{\infty} c_{l,k} f_l(\mathbf{x})$
 171 and integral $\bar{g}_k \triangleq \int_0^1 g_k(t) dt$, the time score and the corresponding log-density ratio can be expressed
 172 as:

$$173 \quad s_t(\mathbf{x}, t) = \sum_{k=1}^{\infty} h_k(\mathbf{x}) g_k(t), \quad \log r(\mathbf{x}) = \sum_{k=1}^{\infty} h_k(\mathbf{x}) \bar{g}_k. \quad (7)$$

176 This representation resolves the degeneracy issue, as the integrals \bar{g}_k are generally non-zero for all k
 177 if $\{g_k\}_{k=1}^{\infty}$ is a frame. Furthermore, Theorem 3.4 allows for the computation of derivatives.

178 **Corollary 3.5.** *If each function g_k in the frame expansion belongs to the Sobolev space $\mathcal{W}^{1,2}([0, 1])$
 179 and the coefficients $\{h_k(\mathbf{x})\}$ are such that the series $\sum_{k=1}^{\infty} h_k(\mathbf{x}) g'_k(t)$ converges in $\mathcal{H}_{x,t}$, then the
 180 weak derivative of the time score s_t with respect to t exists and is given by term-by-term differentiation:*

$$181 \quad \partial_t s_t(\mathbf{x}, t) = \sum_{k=1}^{\infty} h_k(\mathbf{x}) g'_k(t). \quad (8)$$

184 See Sec. A.5 and Sec. A.6 for the proofs of Theorem 3.4 and Corollary 3.5, respectively.

185 The infinite-dimensional representation in Theorem 3.4, while theoretically powerful, is not directly
 186 computable. This necessitates a transition to a practical, finite-dimensional approximation. The
 187 subsequent section is dedicated to this crucial step, detailing the construction of a suitable temporal
 188 basis $\{g_k\}_{k=1}^{\infty}$ using RBFs (Sec. 4.1) and providing a theoretical analysis of the error introduced by
 189 truncating the series to a finite number of terms (Sec. 4.2).

190 4 CONSTRUCTING THE TEMPORAL BASIS FOR OS-DRE

192 In the preceding section, we established the theoretical foundation for our method using an infinite-
 193 dimensional series expansion (Theorem 3.4). To operationalize this framework, we now transition
 194 from the infinite-dimensional ideal to a practical, finite-dimensional approximation scheme. This
 195 section details the construction of this scheme, analyzes its theoretical error bounds, and presents
 196 concrete examples of the basis functions used.

198 4.1 THE FINITE-DIMENSIONAL APPROXIMATION SCHEME

200 **General RBF Construction.** The core idea of our scheme is to project the target function onto
 201 a sequence of nested, finite-dimensional subspaces $\{V_K\}_{K=1}^{\infty}$, where each V_K is spanned by a set
 202 of RBFs. For this scheme to be a valid and stable implementation of the frame-based theory from
 203 Sec. 3, the chosen RBF family $\{g_k\}_{k=1}^{\infty}$ must inherit the two essential properties of a mathematical
 204 frame: *completeness*, which ensures the approximation can converge, and *stability*, which ensures the
 205 computation is robust. This leads to the following formal requirements.

206 **Proposition 4.1.** *Let $\{g_k\}_{k=1}^{\infty}$ be an infinite family of RBFs in \mathcal{H}_t , defined by $g_k(t) = \phi(|t - c_k|/\sigma_k)$.
 207 c_k and σ_k are the center and shape parameters of g_k . This family generates a convergent and
 208 well-posed approximation scheme if it meets two conditions: (i) *Dense*ness: The infinite family's
 209 linear span is dense in \mathcal{H}_t , i.e., $\overline{\text{span}\{g_k\}_{k=1}^{\infty}} = \mathcal{H}_t$. (ii) *Finite-dimensional stability*: For any finite
 210 $K \geq 1$, the subset $\{g_k\}_{k=1}^K$ is linearly independent.*

211 see Sec. A.8 for a detailed proof. Proposition 4.1 provides a clear blueprint for our construction.
 212 The abstract conditions (i) and (ii) can be satisfied by imposing concrete requirements on the RBF
 213 generating function ϕ . Specifically, the denseness condition (i) is fulfilled when ϕ and the RBF
 214 parameters are chosen to satisfy the premises of our Denseness Lemma (Lemma A.4). The stability
 215 condition (ii) is ensured by requiring ϕ to correspond to a *strictly positive definite kernel*, which
 guarantees that the basis functions generated from distinct centers are linearly independent.

With these requirements for ϕ in mind, we construct our basis functions in the general form $g_k(t) = \phi(|t - c_k|/\sigma_k)$. A key advantage of this approach is the potential for closed-form expressions for their integrals and derivatives, which are crucial for our application. The temporal integral \bar{g}_k and derivative $g'_k(t)$ are given by:

$$\bar{g}_k = \int_0^1 \phi\left(\frac{|t - c_k|}{\sigma_k}\right) dt, \quad g'_k(t) = \frac{\text{sgn}(t - c_k)}{\sigma_k} \phi'\left(\frac{|t - c_k|}{\sigma_k}\right). \quad (9)$$

Application to Time Score Approximation. We now connect this approximation scheme back to the central goal of our work. For a fixed \mathbf{x} , we approximate the true time score $s_t(\mathbf{x}, t)$ by its orthogonal projection onto the finite-dimensional subspace $V_K = \text{span}\{g_k\}_{k=1}^K$. Let this approximation be $s_t^{(K)}(\mathbf{x}, t)$. The stability guaranteed by Proposition 4.1 ensures that the coefficients $\{h_k^{(K)}(\mathbf{x})\}_{k=1}^K$ in the expansion are unique and can be robustly computed. By integrating this finite expansion, we obtain a practical, computable approximation for the log-density ratio, denoted $\log r^{(K)}(\mathbf{x})$:

$$s_t(\mathbf{x}, t) \approx s_t^{(K)}(\mathbf{x}, t) = \sum_{k=1}^K h_k^{(K)}(\mathbf{x}) g_k(t), \quad \log r(\mathbf{x}) \approx \log r^{(K)}(\mathbf{x}) = \sum_{k=1}^K h_k^{(K)}(\mathbf{x}) \bar{g}_k. \quad (10)$$

These equations form the basis of our numerical implementation. The subsequent sections will detail specific choices for the generating function ϕ and analyze the error introduced by this truncation.

4.2 TRUNCATION ERROR ANALYSIS

The truncation of the infinite series to a finite sum of K terms introduces an approximation error. We now provide a rigorous theoretical analysis of this error.

Convergence Rates for RBF Approximation. The convergence rate of the error $\|s_t - s_t^{(K)}\|_{\mathcal{H}_t}$ depends on the interplay between the smoothness of the target function s_t and the regularity of the RBF generating function ϕ . This regularity is characterized by the kernel's native space \mathcal{N}_ϕ , the Reproducing Kernel Hilbert Space (RKHS) for which the kernel of ϕ serves as the reproducing kernel. Informally, it consists of functions that are naturally smooth with respect to ϕ . To derive a rigorous error bound, we link this native space to standard Sobolev spaces, following the foundational work on Sobolev error estimates for RBFs (Narcowich et al., 2006).

Proposition 4.2. *Let the RBF generating function ϕ be such that its native space \mathcal{N}_ϕ is equivalent to $\mathcal{W}^{\tau,2}(\mathbb{R})$ for some $\tau > 1/2$. Let the target function $s_t(\mathbf{x}, \cdot)$ belong to a Sobolev space of lower smoothness, $s_t(\mathbf{x}, \cdot) \in \mathcal{W}^{\beta,2}([0, 1])$ with $1/2 < \beta \leq \tau$. Let $s_t^{(K)}(\mathbf{x}, \cdot)$ be the best approximation of s_t in the subspace $V_K = \text{span}\{g_k\}_{k=1}^K$, where the centers $\mathcal{C}_K = \{c_k\}_{k=1}^K$ are quasi-uniform. Then, there exists a constant C , independent of s_t and K , such that the approximation error is bounded by:*

$$\|s_t(\mathbf{x}, \cdot) - s_t^{(K)}(\mathbf{x}, \cdot)\|_{\mathcal{H}_t} \leq C \cdot K^{-\beta} \cdot \|s_t(\mathbf{x}, \cdot)\|_{\mathcal{W}^{\beta,2}([0,1])}. \quad (11)$$

See Sec. A.9 for details. This proposition complements Proposition 4.1 by establishing a quantitative convergence rate. It introduces a third requirement for the generating function ϕ , the native space condition, which ensures rapid convergence of the approximation error for smooth target functions.

4.3 A SUITE OF ANALYTIC RBF KERNELS

We conclude with specific choices for the RBF generating function ϕ . In our implementation, the centers $\{c_k\}_{k=1}^K$ are fixed to a quasi-uniform grid over $[0, 1]$ (e.g., equispaced points), while the shape parameters $\{\sigma_k\}_{k=1}^K$ are learnable. This design satisfies the denseness and quasi-uniformity conditions from our theory. The required linear independence is guaranteed when ϕ corresponds to a *strictly positive definite kernel*. The kernels below are chosen because they meet the denseness, stability and native space conditions and admit closed-form integrals and derivatives.

Example 1: Gaussian RBFs. The generating function is $\phi(r) = \exp(-r^2)$. It satisfies all theoretical requirements: (1) continuity and integrability for the Denseness Lemma, (2) strict positive

270 definiteness for stability, and (3) infinite smoothness, making its native space equivalent to $W^{\tau,2}$ for
 271 any $\tau > 1/2$. The basis function is $g_k(t) = \exp\left(-\frac{|t-c_k|^2}{\sigma_k^2}\right)$, with integral and derivative:
 272

$$273 \quad 274 \quad \bar{g}_k = \frac{\sigma_k \sqrt{\pi}}{2} \left[\operatorname{erf}\left(\frac{1-c_k}{\sigma_k}\right) + \operatorname{erf}\left(\frac{c_k}{\sigma_k}\right) \right], \quad g'_k(t) = -\frac{2(t-c_k)}{\sigma_k^2} g_k(t), \quad (12)$$

275 where $\operatorname{erf}(\cdot)$ is the error function, $\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z \exp(-x^2) dx$.

276 **Example 2: Inverse Multiquadric RBFs.** The generating function is $\phi(r) = (r^2 + 1)^{-1/2}$,
 277 which likewise meets the three conditions: (1) denseness, (2) stability via strict positive definiteness,
 278 and (3) infinite smoothness, ensuring a Sobolev-equivalent native space. The basis function is
 279 $g_k(t) = \frac{\sigma_k}{\sqrt{(t-c_k)^2 + \sigma_k^2}}$, with integral and derivative:
 280

$$281 \quad 282 \quad \bar{g}_k = \sigma_k \ln \left(\frac{(1-c_k) + \sqrt{(1-c_k)^2 + \sigma_k^2}}{-c_k + \sqrt{c_k^2 + \sigma_k^2}} \right), \quad g'_k(t) = -\frac{\sigma_k(t-c_k)}{((t-c_k)^2 + \sigma_k^2)^{3/2}}. \quad (13)$$

283 We also implement other RBFs, including rational quadratic and Matérn kernels (detailed in Sec. B).

284 4.4 TRAINING OBJECTIVE AND COMPUTATIONAL ADVANTAGES

285 To implement OS-DRE, we parameterize the spatial coefficients $\{h_k^{(K)}(\mathbf{x})\}$ using a single neu-
 286 ral network with parameters θ . Given an input sample \mathbf{x} , the network outputs K coefficients:
 287 $[h_1^\theta(\mathbf{x}), \dots, h_K^\theta(\mathbf{x})] = \text{NN}(\mathbf{x}; \theta)$. Our time score model and its derivative and integral are given by:
 288

$$289 \quad 290 \quad s_t^\theta(\mathbf{x}, t) = \sum_{k=1}^K h_k^\theta(\mathbf{x}) g_k(t), \quad \partial_t s_t^\theta(\mathbf{x}, t) = \sum_{k=1}^K h_k^\theta(\mathbf{x}) g'_k(t), \quad \int_0^1 s_t^\theta(\mathbf{x}, t) dt = \sum_{k=1}^K h_k^\theta(\mathbf{x}) \bar{g}_k. \quad (14)$$

291 We train this model by minimizing the sliced time score matching (STSM) objective from Choi et al.
 292 (2022), a tractable objective function independent of the unknown true score:

$$293 \quad 294 \quad \mathcal{L}_{\text{STSM}}(\theta) = 2\mathbb{E}_{p_0(\mathbf{x}_0)p_1(\mathbf{x}_1)} [\lambda(0)s_t^\theta(\mathbf{x}_0, 0) - \lambda(1)s_t^\theta(\mathbf{x}_1, 1)] \\ 295 \quad + \mathbb{E}_{p(t)p_t(\mathbf{x})} [2\lambda(t)\partial_t s_t^\theta(\mathbf{x}, t) + 2\lambda'(t)s_t^\theta(\mathbf{x}, t) + \lambda(t)s_t^\theta(\mathbf{x}, t)^2], \quad (15)$$

301 where $p(t) = \mathcal{U}[0, 1]$ and $\lambda(\cdot) : [0, 1] \rightarrow \mathbb{R}_+$ is a weighting function with λ' being its derivative.

302 Our framework offers key computational benefits in both training and inference. During training, the
 303 derivative term $\partial_t s_t^\theta$ is computed analytically using Eq. (14). This eliminates the need for automatic
 304 differentiation w.r.t. t , which in prior work (e.g., DRE- ∞) required expensive second-order gradients.
 305 By reducing optimization to a first-order problem, we enable faster and more stable training.

306 Once the optimal parameters θ^* are found, the log-density ratio is estimated in a single step:

$$307 \quad 308 \quad \log \hat{r}(\mathbf{x}) = \int_0^1 s_t^\theta(\mathbf{x}, t) dt = \sum_{k=1}^K h_k^{\theta^*}(\mathbf{x}) \bar{g}_k = \langle \text{NN}(\mathbf{x}; \theta^*), \bar{\mathbf{g}}^{(K)} \rangle, \quad (16)$$

309 where $\langle \cdot, \cdot \rangle$ denotes the inner product operator, $\text{NN}(\mathbf{x}; \theta^*) = [h_1^{\theta^*}(\mathbf{x}), h_2^{\theta^*}(\mathbf{x}), \dots, h_K^{\theta^*}(\mathbf{x})]$ and
 310 $\bar{\mathbf{g}}^{(K)} = [\bar{g}_1, \bar{g}_2, \dots, \bar{g}_K]$ are two vectors. Since the basis integrals \bar{g}_k are pre-computed analytic
 311 constants (e.g., Eq. (12)), estimation requires only a single forward pass to obtain the coefficients,
 312 leading to only 1 NFE and offering a substantial speedup over iterative ODE-based or quadrature
 313 methods. The training and inference procedures of OS-DRE are summarized in Algorithms 1 and 2.
 314 See Algorithm 3 for details of training procedure and Algorithm 4 for Pytorch implementation.

315 **Algorithm 1** One Training Step of OS-DRE

316 **Input:** A batch $\mathbf{x}_0 \sim p_0, \mathbf{x}_1 \sim p_1, t \sim \mathcal{U}(0, 1)$.

- 1: Derive \mathbf{x}_t with $(\mathbf{x}_0, \mathbf{x}_1)$ (see Sec. C.1.3).
- 2: Compute s_t^θ and $\partial_t s_t^\theta$ using Eq. (14).
- 3: Compute loss $\mathcal{L}_{\text{STSM}}(\theta)$ using Eq. (15).
- 4: Update trainable parameters θ and $\{\sigma_k\}_{k=1}^K$.

317 **Algorithm 2** One-Step Estimation

318 **Input:** Sample \mathbf{x} and pre-calculated $\{\bar{g}_k\}_{k=1}^K$.

319 **Output:** Estimated log-density ratio $\log \hat{r}(\mathbf{x})$.

- 1: $\{h_k^{\theta^*}(\mathbf{x})\}_{k=1}^K \leftarrow \text{NN}(\mathbf{x}; \theta^*)$.
- 2: Compute $\log \hat{r}(\mathbf{x})$ using Eq. (16).

324 5 EXPERIMENTAL SETTINGS AND RESULTS

325 We conduct extensive experiments to evaluate OS-DRE, using $\text{DRE-}\infty$ (Choi et al., 2022) and D^3RE 326 (Chen et al., 2025) as baselines. For fair comparison, all methods adopt the same quadrature scheme 327 (trapezoidal rule) and weighting function $\lambda(t) = t(1 - t)$. 328

329 **Density Estimation.** In density estimation, let $p_0(\mathbf{x}) = \mathcal{N}(\mathbf{0}, \mathbf{I}_d)$ be a simple noise distribution, 330 and $p_1(\mathbf{x})$ denote the complex and intractable data distribution. The log-likelihood of p_1 for a 331 given sample \mathbf{x} can be estimated as $\log p_1(\mathbf{x}) = \log r(\mathbf{x}) + \log p_0(\mathbf{x})$, where $r(\mathbf{x}) = p_1(\mathbf{x})/p_0(\mathbf{x})$ 332 is the density ratio between p_1 and p_0 . After training, the estimated log-density ratio $\log \hat{r}$ can 333 be derived based on Eq. (16). Thus, the log-likelihood of p_1 can be estimated as $\log p_1(\mathbf{x}) \approx \log \hat{r}(\mathbf{x}) + \log p_0(\mathbf{x})$. Detailed experimental settings can be found in Sec. C.3. 334

335 STRUCTURED AND MULTIMODAL DATASETS.

336 We evaluate OS-DRE on nine standard synthetic 337 benchmarks (Bansal et al., 2023; Chen et al., 2025). Results are shown part in Fig. 2 and 338 full in Fig. 7 (Sec. C.3). As shown in Fig. 2, 339 our solver-free method achieves accurate density 340 estimates with only one function evaluation 341 ($\text{NFE} = 1$), while $\text{DRE-}\infty$ and D^3RE with 342 $\text{NFE} = 2$ often yield blurred or distorted 343 results. OS-DRE reliably captures challenging 344 structures, including disconnected rings (circles), 345 curved manifolds (swissroll), sharp discontinuities 346 (checkerboard), and branching topologies (tree). 347 These results demonstrate that OS-DRE 348 learns complex multimodal densities 349 efficiently under tight inference constraints. 350

351 **REAL-WORLD TABULAR DATASETS.** We further 352 test OS-DRE on five real-world tabular 353 datasets (Grathwohl et al., 2019), spanning 354 domains from physics to image statistics. As 355 shown in Tab. 1, our one-step method ($\text{NFE} = 356 1$) not only demonstrates remarkable efficiency 357 but also achieves state-of-the-art (SOTA) 358 performance in terms of negative log-likelihood 359 (NLL). Notably, OS-DRE with the IMQ and RQ 360 kernels consistently outperforms the baseline 361 methods across all datasets, even when the 362 baselines are allocated a significantly larger 363 computational budget (NFE up to 50). This result is 364 particularly pronounced on the high-dimensional 365 MINIBOONE and BSDS300 datasets, where OS- 366 DRE achieves superior accuracy with a fraction 367 of the model parameters used by competing 368 methods. These findings confirm that our analytic 369 framework successfully resolves the efficiency-accuracy 370 trade-off, delivering both speed and SOTA 371 performance. 372

373 Table 1: Comparison of negative log-likelihood (NLL) and **wall-clock time** on five tabular datasets. 374 Lower is better. **All timing results were obtained on a single NVIDIA TITAN X GPU. The best NLL 375 in each dataset is shown in **bold**, and the best wall-clock time is underlined.**

| Method | NFE | RBF Kernel | POWER | | GAS | | HEPMASS | | MINIBOONE | | BSDS300 | |
|-----------------|-----|------------|-------------------------|--------------|--------------------------|--------------|-------------------------|--------------|------------------------|--------------|---------------------------|--------------|
| | | | NLL ↓ | Time (s) | NLL ↓ | Time (s) | NLL ↓ | Time (s) | NLL ↓ | Time (s) | NLL ↓ | Time (s) |
| DRE- ∞ | 2 | - | 0.05 \pm 1.84 | 0.317 | -4.37 \pm 1.44 | 0.207 | 19.30 \pm 1.31 | 0.311 | 41.55 \pm 2.07 | 0.099 | -130.68 \pm 4.17 | 0.448 |
| D ^3RE | 2 | - | 3.57 \pm 1.84 | 0.334 | 5.74 \pm 15.28 | 0.218 | 23.90 \pm 0.36 | 0.319 | 55.83 \pm 9.36 | 0.100 | -149.53 \pm 9.06 | 0.454 |
| DRE- ∞ | 5 | - | 0.35 \pm 0.50 | 0.561 | -3.63 \pm 0.78 | 0.310 | 20.24 \pm 0.47 | 0.612 | 20.90 \pm 0.84 | 0.113 | -83.70 \pm 1.35 | 1.061 |
| D ^3RE | 5 | - | 1.26 \pm 0.38 | 0.579 | -1.15 \pm 4.20 | 0.316 | 21.05 \pm 0.52 | 0.554 | 43.11 \pm 26.20 | 0.117 | -101.97 \pm 1.67 | 1.057 |
| DRE- ∞ | 10 | - | 0.03 \pm 0.17 | 0.982 | -4.34 \pm 0.60 | 0.517 | 20.43 \pm 0.52 | 0.987 | 20.57 \pm 0.93 | 0.146 | -87.65 \pm 2.24 | 2.043 |
| D ^3RE | 10 | - | 0.49 \pm 0.39 | 1.051 | -3.27 \pm 2.00 | 0.544 | 20.30 \pm 0.55 | 0.987 | 42.65 \pm 26.87 | 0.123 | -102.01 \pm 2.43 | 2.042 |
| DRE- ∞ | 50 | - | 0.25 \pm 0.28 | 4.128 | -4.33 \pm 0.71 | 2.018 | 20.67 \pm 0.57 | 4.078 | 20.97 \pm 0.51 | 0.223 | -90.24 \pm 2.14 | 10.035 |
| D ^3RE | 50 | - | 0.89 \pm 0.33 | 4.232 | -3.16 \pm 0.62 | 2.072 | 20.05 \pm 0.35 | 4.002 | 42.73 \pm 26.78 | 0.216 | -78.26 \pm 0.96 | 10.062 |
| OS-DRE (ours) | 1 | Matérn | 0.57 \pm 0.11 | 0.084 | -3.49 \pm 0.01 | <u>0.025</u> | 23.66 \pm 0.02 | 0.064 | 31.71 \pm 0.11 | <u>0.003</u> | -52.38 \pm 0.42 | 0.073 |
| OS-DRE (ours) | 1 | Gaussian | -0.35 \pm 0.10 | 0.104 | -16.39 \pm 0.17 | 0.038 | 17.44 \pm 0.00 | 0.118 | 10.95 \pm 0.33 | 0.005 | -191.22 \pm 3.19 | 0.076 |
| OS-DRE (ours) | 1 | IMQ | -0.69 \pm 0.18 | 0.084 | -18.33 \pm 0.04 | 0.039 | 17.45 \pm 0.05 | 0.071 | 9.97 \pm 0.37 | 0.005 | -217.99 \pm 3.39 | 0.070 |
| OS-DRE (ours) | 1 | RQ | -0.66 \pm 0.17 | <u>0.082</u> | -17.86 \pm 0.03 | 0.037 | 16.88 \pm 0.03 | <u>0.051</u> | 11.34 \pm 0.28 | <u>0.003</u> | -201.37 \pm 2.21 | 0.071 |

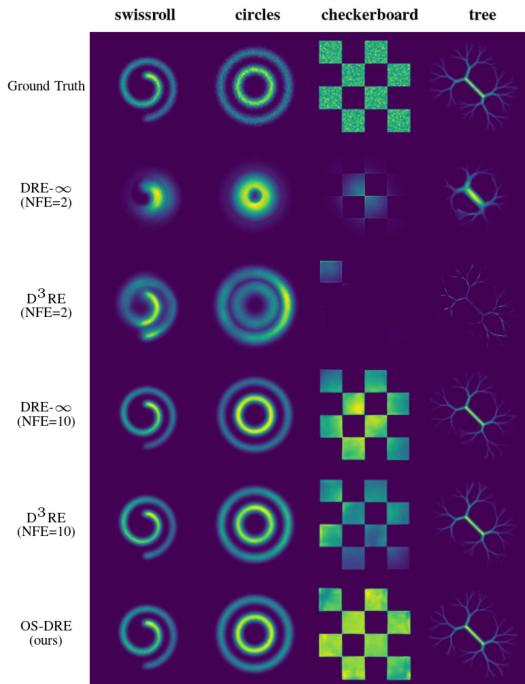


Figure 2: Comparison of density estimates from three score-based DRE methods on four structured and multimodal datasets. **DRE-∞** and **D ^3RE** use $\text{NFE} = 2$, whereas our **OS-DRE** uses only $\text{NFE} = 1$. Additional results are in Fig. 7 (Sec. C.3). OS-DRE is the best one with lowest NFE.

MINIBOONE and BSDS300 datasets, where OS-DRE achieves superior accuracy with a fraction of the model parameters used by competing methods.

These findings confirm that our analytic framework successfully resolves the efficiency-accuracy trade-off, delivering both speed and SOTA performance.

378 ENERGY-BASED MODELING ON MNIST. We
 379 conduct density estimation on the MNIST dataset,
 380 leveraging pre-trained energy-based models (EBMs)
 381 following (Choi et al., 2022; Chen et al., 2025). The
 382 log-likelihood of the data distribution $p_1(\mathbf{x})$ is esti-
 383 mated via the density ratio and reported in bits-per-
 384 dimension (BPD) (see Sec. C.3 for a detail). We use
 385 IMQ kernel. The results are summarized in Tab. 2.
 386 OS-DRE achieves a BPD of 1.278, setting a new
 387 SOTA for DRE-based methods on this benchmark, surpassing both D³RE (1.281) and DRE- ∞
 388 (1.302). Crucially, while achieving better accuracy, OS-DRE maintains its computational advantage.
 389 It estimates the BPD with NFE = 1, achieving a test-set inference time of 0.312 seconds, representing
 390 a $\sim 68\times$ speedup over D³RE and DRE- ∞ (NFE = 75, ~ 21 s).

391 **Mutual Information Estimation.** Mutual information (MI) quantifies the dependency between
 392 random variables $\mathbf{x} \sim p(\mathbf{x})$ and $\mathbf{y} \sim q(\mathbf{y})$, quantifying how much information one reveals about the
 393 other. We estimate MI between two d -dimensional variables using OS-DRE. Formally, $\text{MI}(\mathbf{x}, \mathbf{y}) =$
 394 $\mathbb{E}_{p(\mathbf{x}, \mathbf{y})} \left[\log \frac{p(\mathbf{x}, \mathbf{y})}{p(\mathbf{x})q(\mathbf{y})} \right]$, where the density ratio $\frac{p(\mathbf{x}, \mathbf{y})}{p(\mathbf{x})q(\mathbf{y})}$ is directly approximable via DRE.

395 BEYOND NORMAL: GEOMETRICALLY PATHOLOGICAL DISTRIBUTIONS. We further probe the
 396 robustness of OS-DRE on a suite of four MI estimation tasks involving geometrically pathological
 397 distributions. These benchmarks, inspired by the suite from Czyż et al. (2023), are specifically
 398 designed to challenge the underlying assumptions of many standard estimators by featuring properties
 399 like heavy tails, sharp density peaks, and non-differentiable boundaries. For each task, we compute
 400 the MI estimate over 10 random seeds and report the mean squared error (MSE) against the known
 401 ground-truth MI value. The results, presented in Tab. 3 (full in Tab. 6), demonstrate the stability and
 402 accuracy of our method. OS-DRE consistently achieves a lower MSE than the baseline methods
 403 across the wide range of challenging data geometries, particularly in scenarios with heavy tails
 404 (Half-Cube Map) and complex dependencies (Gamma-Exponential). This highlights the robustness
 405 of our analytic, one-step framework in scenarios where traditional score-based methods can struggle.

406 Table 3: MSE results on the Additive Noise (sharp discontinuities, top) and Gamma-Exponential
 407 (non-linear dependency, bottom) datasets. Across all correlation levels (top row of each sub-table),
 408 OS-DRE achieves consistently superior or competitive performance. Full results given in Tab. 6.

| Method | RBF Kernel | 0.1 | 0.2 | 0.3 | 0.4 | 0.5 | 0.6 | 0.7 | 0.8 | 0.9 |
|---------------|------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|
| DRE-infty | - | 0.0029 | 0.0018 | 0.0015 | 0.0012 | 0.0013 | 0.0013 | 0.0011 | 0.0011 | 0.000 |
| D3RE | - | 0.0108 | 0.0077 | 0.0065 | 0.0071 | 0.0085 | 0.0076 | 0.0064 | 0.0045 | 0.0055 |
| OS-DRE (ours) | Matérn | 0.0061 | 0.0029 | 0.0017 | 0.0015 | 0.0015 | 0.0013 | 0.0011 | 0.0009 | 0.0008 |
| OS-DRE (ours) | Gaussian | 0.0016 | 0.0015 | 0.0016 | 0.0011 | 0.0015 | 0.0014 | 0.0012 | 0.0010 | 0.0010 |
| OS-DRE (ours) | IMQ | 0.0010 | 0.0010 | 0.0010 | 0.0012 | 0.0009 | 0.0008 | 0.0007 | 0.0009 | 0.0007 |
| OS-DRE (ours) | RQ | 0.0019 | 0.0015 | 0.0015 | 0.0012 | 0.0010 | 0.0010 | 0.0010 | 0.0010 | 0.0009 |

| Method | RBF Kernel | 1.0 | 1.1 | 1.2 | 1.3 | 1.4 | 1.5 | 1.6 | 1.7 | 1.8 |
|---------------|------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|
| DRE-infty | - | 2.1328 | 0.8939 | 0.0725 | 0.0115 | 0.0213 | 0.0051 | 0.0114 | 0.0069 | 0.0051 |
| D3RE | - | 0.1919 | 0.1018 | 0.0154 | 0.0119 | 0.0063 | 0.0110 | 0.0050 | 0.0125 | 0.0114 |
| OS-DRE (ours) | Matérn | 0.1768 | 0.0315 | 0.0035 | 0.0026 | 0.0008 | 0.0017 | 0.0009 | 0.0006 | 0.0005 |
| OS-DRE (ours) | Gaussian | 0.2933 | 0.0503 | 0.0060 | 0.0028 | 0.0032 | 0.0014 | 0.0014 | 0.0007 | 0.0009 |
| OS-DRE (ours) | IMQ | 0.2821 | 0.1185 | 0.0901 | 0.0492 | 0.0200 | 0.0275 | 0.0072 | 0.0080 | 0.0087 |
| OS-DRE (ours) | RQ | 0.5182 | 0.0925 | 0.0330 | 0.0109 | 0.0052 | 0.0040 | 0.0015 | 0.0015 | 0.0012 |

421 HIGH-DISCREPANCY & HIGH-DIMENSIONAL DISTRIBUTIONS. To evaluate OS-DRE under
 422 extreme conditions, we test mutual information estimation between two high-dimensional Gaussians
 423 with large and increasing discrepancy, a setup that triggers the “density-chasm” problem (Rhodes
 424 et al., 2020). Results in Tab. 4 (full in Tab. 6) show that, unlike DRE- ∞ and D³RE, which fail at low
 425 NFE and remain unstable even with NFE = 50, OS-DRE with Gaussian or IMQ kernels achieves
 426 accurate and stable estimates across all dimensions. This demonstrates that our analytic framework
 427 effectively overcomes the density-chasm challenge where iterative methods falter.

428 **Continual Learning.** To evaluate OS-DRE in online scenarios such as real-time change point
 429 detection (Chen et al., 2021) and continuous covariate shift adaptation (Zhang et al., 2023), we test
 430 its ability to track evolving distributions across three challenging benchmarks, termed as Linearly
 431 Drifting Gaussian, Progressive Noise Corruption and Controlled Divergence Shift (see Sec. C.4 for
 a detail). In this continual learning setup, the target distribution p_t shifts over discrete timesteps,

Table 2: Energy-based modeling on MNIST. Results are reported in bits-per-dim (BPD). Timing measured over the full test set on a single TITAN X GPU. “BS” = batch size.

| Method | Params | BS | NFE | Time (s) | BPD \downarrow |
|-------------------|--------|-----|-----|--------------|------------------|
| DRE- ∞ | 11.2M | 512 | 75 | 21.443 | 1.302 |
| D ³ RE | 11.2M | 512 | 75 | 21.424 | 1.281 |
| OS-DRE | 11.5M | 512 | 1 | 0.312 | 1.278 |

Table 4: MI estimation under high-discrepancy settings ($MI \in \{10, 20, 30, 40\}$ nats). We report the estimated MI (mean \pm std over 3 seeds), MSE and wall-clock time. All timing results were obtained on a single NVIDIA TITAN X GPU. **Bolded** MSE values indicate the best performance for each setting. The best wall-clock time is underlined. Full results for $NFE \in \{2, 5, 10, 50\}$ given in Tab. 7.

| Method | NFE | RBF Kernel | MI = 10 | | | MI = 20 | | | MI = 30 | | | MI = 40 | | | | | | |
|---------------|-----|------------|------------------|-------------|--------------|------------------|-------------|--------------|------------------|-------------|--------------|------------------|-------------|----------|------|----|-----|----------|
| | | | Est. | MI | MSE | Time (s) | Est. | MI | MSE | Time (s) | Est. | MI | MSE | Time (s) | Est. | MI | MSE | Time (s) |
| DRE- ∞ | 2 | - | 1.40 \pm 0.01 | 73.91 | 0.045 | 3.16 \pm 0.01 | 283.52 | 0.045 | 5.21 \pm 0.01 | 614.62 | 0.045 | 5.13 \pm 0.02 | 1215.69 | 0.046 | | | | |
| D 3 RE | 2 | - | 11.61 \pm 0.08 | 2.58 | 0.048 | 21.91 \pm 0.08 | 3.65 | 0.047 | 27.51 \pm 0.07 | 6.21 | 0.046 | 17.64 \pm 0.17 | 500.04 | 0.044 | | | | |
| DRE- ∞ | 50 | - | 9.84 \pm 0.06 | 0.03 | 0.226 | 19.81 \pm 0.04 | 0.04 | 0.249 | 29.31 \pm 0.06 | 0.48 | 0.228 | 38.06 \pm 0.07 | 3.77 | 0.271 | | | | |
| D 3 RE | 50 | - | 10.07 \pm 0.04 | 0.01 | 0.234 | 20.30 \pm 0.03 | 0.09 | 0.256 | 27.01 \pm 0.03 | 8.94 | 0.256 | 32.37 \pm 0.04 | 58.19 | 0.260 | | | | |
| OS-DRE (ours) | 1 | Matérn | 10.31 \pm 0.02 | 0.09 | 0.024 | 15.73 \pm 0.05 | 18.30 | 0.028 | 15.55 \pm 0.02 | 208.98 | 0.032 | 18.65 \pm 0.15 | 456.11 | 0.028 | | | | |
| OS-DRE (ours) | 1 | Gaussian | 10.05 \pm 0.04 | 0.01 | 0.025 | 20.03 \pm 0.04 | 0.00 | 0.027 | 29.37 \pm 0.07 | 0.07 | 0.013 | 38.68 \pm 0.09 | 2.30 | 0.014 | | | | |
| OS-DRE (ours) | 1 | IMQ | 10.37 \pm 0.02 | 0.11 | 0.035 | 21.25 \pm 0.04 | 1.56 | 0.030 | 28.10 \pm 0.08 | 5.86 | 0.029 | 39.35 \pm 0.09 | 0.47 | 0.028 | | | | |
| OS-DRE (ours) | 1 | RQ | 9.89 \pm 0.03 | 0.03 | <u>0.022</u> | 19.49 \pm 0.04 | 0.83 | <u>0.012</u> | 28.94 \pm 0.10 | 1.52 | <u>0.012</u> | 38.92 \pm 0.07 | 1.41 | 0.019 | | | | |

creating a challenging environment that requires the model to continuously adapt to and quantify the change from a fixed source distribution p_0 . We measure this ability by estimating the KL-divergence between p_0 and the evolving target p_t at each step via DRE, i.e., $D_{\text{KL}}(p_t \| p_0) = \mathbb{E}_{p_t(\mathbf{x})} \left[\log \frac{p_t(\mathbf{x})}{p_0(\mathbf{x})} \right]$.

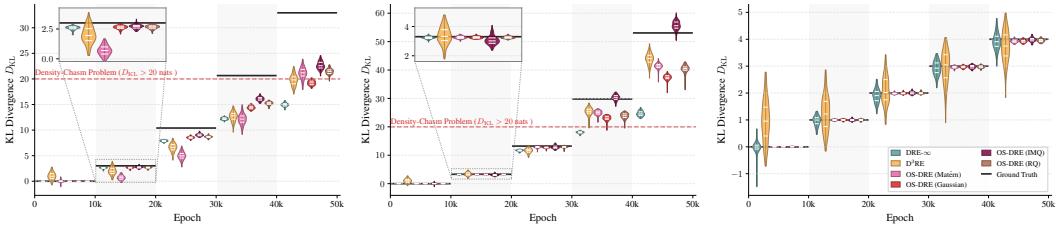


Figure 3: Kullback-Leibler (KL) divergence tracking on time-varying distributions. OS-DRE (NFE = 1) provides stable, low-variance estimates that track the ground truth (black line), while baselines (NFE = 50) exhibit significant lag and high variance.

As shown in Fig. 3, OS-DRE delivers real-time, low-variance KL estimates with only a single function evaluation (NFE = 1), closely matching the ground truth across dynamic shifts. In contrast, baseline methods, even with NFE = 50, suffer from lag, variance, and instability, especially under rapid or large shifts. **Together, these results demonstrate that our analytic, solver-free formulation avoids the error accumulation and instability inherent in iterative solvers, enabling real-time, reliable tracking of distributional dynamics in continual learning.**

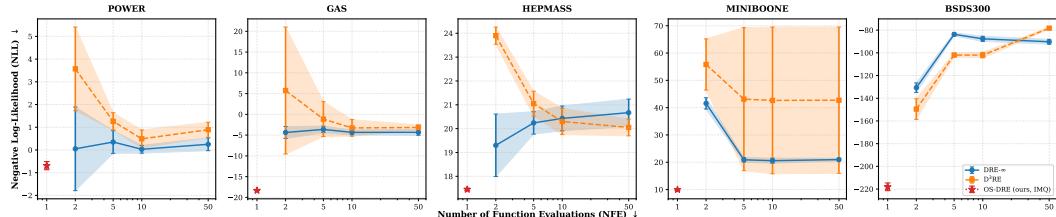
Ablation Studies. Proposition 4.2 highlights two key hyperparameters: the number of basis functions K and the choice of kernel ϕ , both governing the trade-off between accuracy and complexity.

NUMBER OF BASIS FUNCTIONS (K). We varied $K \in \{100, 200, 400, 800\}$ to study its effect. On GAS, performance improved with larger K up to 400 (NLLs: $-14.51, -15.82, -16.39$) but degraded at 800 (-11.12) due to overfitting, confirming that excessively large K harms generalization. For MI estimation, results were stable across K (e.g., MSEs at MI = 40 with IMQ: $0.55, 0.48, 0.47, 0.49$), indicating diminishing returns once K is sufficient. We thus use $K = 400$ for tabular data and $K = 200$ for pathological distributions as a balanced choice.

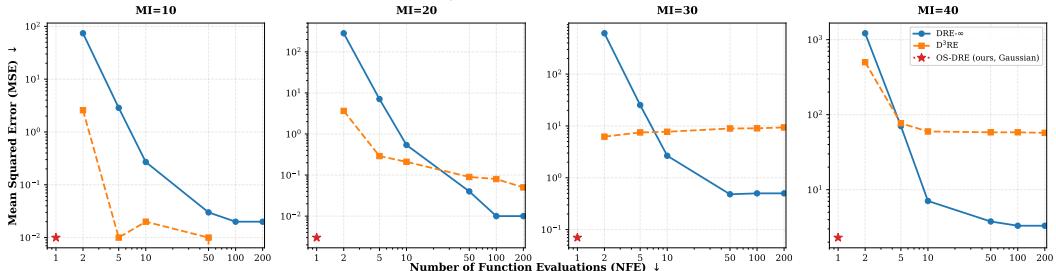
CHOICE OF RBF KERNEL (ϕ). The kernel ϕ determines inductive bias and approximation power. Among four tested kernels (Gaussian, Inverse Multiquadric (IMQ), Rational Quadratic (RQ), and Matérn), **IMQ** and **RQ** were strong general-purpose options, achieving state-of-the-art density estimation (Tab. 1 and Fig. 6) and robust MI estimation (Tab. 4), while also stabilizing continual learning tasks (Fig. 3). The **Gaussian** kernel, with localized influence, excelled at capturing sharp or disconnected structures in 2D synthetic benchmarks (Fig. 7) and moderate-discrepancy MI tasks. The **Matérn** kernel, with limited smoothness, was best on geometrically pathological tasks such as Gamma-Exponential, where less smooth inductive bias aligned with the target function.

Error of the Density Ratio (NLL / MSE) vs. Computational Cost (NFE). In score-based DRE, the overall error is often dominated by the bias introduced by numerical integration at low NFE, rather than by the score estimation itself. OS-DRE eliminates this bottleneck by replacing numerical integration with a closed-form, solver-free estimation. We measure computational cost using the NFE and evaluate the error of the density ratio using NLL for density estimation and MSE for MI

estimation. As shown in Fig. 4, OS-DRE consistently matches or surpasses the estimation quality of DRE_{∞} and D^3RE while using only $NFE = 1$. In the density estimation task (Tab. 1 and Fig. 4a), it achieves comparable or better NLL across all five tabular datasets, whereas the baseline methods require NFE values between 2 and 50 to reach similar performance. This corresponds to a $50\times$ reduction in computation. A similar pattern is observed in MI estimation (Tab. 4 and Fig. 4b), where OS-DRE attains near-zero MSE at $NFE = 1$ for $MI \in \{10, 20, 30\}$, while the other methods rely on substantially larger NFE . These results show that OS-DRE maintains high estimation quality without costly numerical integration and is therefore well suited for real-time applications.



(a) NLL (Error) vs. NFE (Cost) for density estimation on five tabular datasets. See Tab. 8 for a detail.



(b) MSE (Error) vs. NFE (Cost) for MI estimation under high-discrepancy settings. See Tab. 9 for a detail.

Figure 4: Trade-off between error of the density ratio and computational cost. The error is measured by negative log-likelihood (NLL) and mean squared error (MSE), and the computational cost by the number of function evaluations (NFE). OS-DRE maintains high estimation quality with minimal computational cost ($NFE = 1$), whereas the baseline methods require substantially larger NFE to reach comparable performance. **This shows that OS-DRE effectively resolves the longstanding trade-off between estimation quality and integration cost in score-based DRE methods.**

6 CONCLUSION

We proposed OS-DRE, a one-step, solver-free framework for score-based density ratio estimation that resolves the long-standing trade-off between accuracy and computational efficiency. By introducing a spatiotemporal decomposition of the time score, our method replaces expensive numerical integration with a single, analytic computation. This is achieved by representing the temporal component of the time score using what we term an analytic frame, a stable approximation basis constructed from radial basis functions, for which the necessary temporal integrals are known in closed form. Our theoretical analysis provides a complete framework for this approach, with proofs for the completeness and stability of the basis, alongside a rigorous truncation error bound that guarantees convergence. Our empirical results demonstrate that this analytic approach achieves competitive accuracy with only a single function evaluation, drastically outperforming iterative, solver-based methods in terms of speed. These findings establish OS-DRE as a powerful and practical tool, opening up new directions for efficient probabilistic inference and statistical estimation.

Limitations and Future Works. While OS-DRE achieves efficient and accurate DRE, its effectiveness partly depends on the choice of the target time score function $\{\partial_t \log p_t\}_{t \in [0,1]}$, analyzed in Proposition 4.2. When this target is misaligned with the ideal score (optimal yet unknown), approximation quality may deteriorate. While our work provides a comprehensive analysis of the approximation error, future research could explore training objectives beyond standard time score matching to improve robustness and calibration. For instance, integrating conditional score matching (Yu et al., 2025) or dual score matching (Guth et al., 2025) into our framework could merge analytic integration with energy consistency, potentially yielding more reliable density ratio estimates.

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REPRODUCIBILITY STATEMENT

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To ensure the reproducibility of our results, we provide a comprehensive account of our work. All experimental setups, including dataset descriptions and key hyperparameter settings, are detailed in the main paper and this appendix. We provide clear pseudocode for our core algorithms, detailing the training procedure (Algorithm 3) and the final one-step estimation process (Algorithm 2). A complete implementation of our OS-DRE framework, along with scripts to replicate all experiments, will be made publicly available upon publication. All experiments were conducted using the PyTorch framework on a single NVIDIA RTX 3070 GPU and four TITAN X GPUs.

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LLM DISCLAIMER

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The authors acknowledge the use of a large language model (LLM), specifically Google’s Gemini, to assist in the writing and editing process of this paper. The uses of the LLM were primarily for two purposes: (1) to assist in polishing the writing, including improving grammar, clarity, and phrasing of sentences; and (2) for retrieval and discovery, such as finding related work and summarizing existing literature to help situate our contributions within the broader academic context. The core ideas, theoretical derivations, experimental design, and interpretation of results were conducted by the authors.

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BROADER IMPACT

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This paper presents work whose goal is to advance the field of density ratio estimation, which does not involve any potential ethical risks. While direct societal impacts are limited, future extensions to applied domains (e.g., via our open-source codebase) should incorporate domain-specific ethical reviews per deployment contexts.

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|-----|---|-----------|
| 702 | APPENDIX | |
| 703 | | |
| 704 | APPENDIX CONTENTS | |
| 705 | | |
| 706 | 1 Introduction | 1 |
| 707 | | |
| 708 | 2 Related Works and Problem Statement | 2 |
| 709 | | |
| 710 | 3 One-Step Density Ratio Estimation | 3 |
| 711 | | |
| 712 | 4 Constructing the Temporal Basis for OS-DRE | 4 |
| 713 | | |
| 714 | 4.1 The Finite-Dimensional Approximation Scheme | 4 |
| 715 | | |
| 716 | 4.2 Truncation Error Analysis | 5 |
| 717 | | |
| 718 | 4.3 A Suite of Analytic RBF Kernels | 5 |
| 719 | | |
| 720 | 4.4 Training Objective and Computational Advantages | 6 |
| 721 | 5 Experimental Settings and Results | 7 |
| 722 | | |
| 723 | 6 Conclusion | 10 |
| 724 | | |
| 725 | Appendix | 14 |
| 726 | | |
| 727 | A Assumptions and Proofs | 16 |
| 728 | | |
| 729 | A.1 Assumptions | 16 |
| 730 | A.2 Theoretical Foundation for Spatiotemporal Decomposition | 16 |
| 731 | | |
| 732 | A.3 Proof of Lemma 3.1 | 17 |
| 733 | | |
| 734 | A.4 Proof of Lemma 3.2 | 17 |
| 735 | | |
| 736 | A.5 Proof of Theorem 3.4 | 18 |
| 737 | | |
| 738 | A.6 Proof of Corollary 3.5 | 19 |
| 739 | | |
| 740 | A.7 Denseness of Temporal Basis in \mathcal{H}_t | 19 |
| 741 | | |
| 742 | A.8 Proof of Proposition 4.1 | 21 |
| 743 | | |
| 744 | A.9 Proof of Proposition 4.2 | 21 |
| 745 | | |
| 746 | B Analytic Formulas for RBF Kernels | 22 |
| 747 | | |
| 748 | B.1 Gaussian RBFs | 22 |
| 749 | | |
| 750 | B.2 Inverse Multiquadric RBFs | 23 |
| 751 | | |
| 752 | B.3 Rational Quadratic RBFs | 24 |
| 753 | | |
| 754 | B.4 Matérn RBFs | 25 |
| 755 | | |
| 756 | C Experimental Details and More Results | 26 |
| 757 | | |
| 758 | C.1 Experimental Details | 26 |
| 759 | | |
| 760 | C.1.1 Interpolating Paths and the Temporal-Integral View | 26 |
| 761 | | |
| 762 | C.1.2 Joint Score Matching | 27 |
| 763 | | |
| 764 | C.1.3 Training Procedure | 27 |
| 765 | | |
| 766 | C.2 Model Parameterization and Implementation Details | 27 |

| | | |
|-----|--|----|
| 756 | C.2.1 Implementation Details | 27 |
| 757 | C.2.2 Neural Network Parameterization | 28 |
| 758 | | |
| 759 | C.3 Experimental Settings and Results for Density Estimation | 29 |
| 760 | C.4 Experimental Settings and Results for f -divergence Estimation | 31 |
| 761 | | |
| 762 | | |
| 763 | | |
| 764 | | |
| 765 | | |
| 766 | | |
| 767 | | |
| 768 | | |
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810 A ASSUMPTIONS AND PROOFS
811812 A.1 ASSUMPTIONS
813814 The theoretical results in Sec. 3 rely on the following mild assumptions regarding the analytical
815 properties of the probability density function $p_t(\mathbf{x})$.
816817 **Assumption A.1.** There exists a constant $C > 0$ such that $p_t(\mathbf{x}) \geq C$ for all $\mathbf{x} \in \mathcal{X}$ and $t \in [0, 1]$.
818819 **Assumption A.2** (Uniformly boundedness). The partial derivative $\partial_t p_t(\mathbf{x})$ is uniformly bounded;
820 that is, there exists a constant $D > 0$ such that $|\partial_t p_t(\mathbf{x})| \leq D$ for all $\mathbf{x} \in \mathcal{X}$ and $t \in [0, 1]$.
821822 Assumption A.1 ensures that $\log p_t(\mathbf{x})$ is well-defined, while Assumption A.2 ensures that the time
823 score s_t is well-behaved, specifically that it is an element of $L^2(\mathcal{X} \times [0, 1])$, as stated in Lemma 3.1.
824825 A.2 THEORETICAL FOUNDATION FOR SPATIOTEMPORAL DECOMPOSITION
826827 This section establishes the mathematical foundation for the frame-based decomposition of the
828 spatiotemporal Hilbert space $\mathcal{H}_{\mathbf{x},t}$, which underlies Theorem 3.4. The key observation is that $\mathcal{H}_{\mathbf{x},t}$
829 can be realized as the tensor product of the spatial and temporal Hilbert spaces (i.e., $\mathcal{H}_{\mathbf{x}}$ and \mathcal{H}_t), and
830 that frames of the product space can be constructed from those of the constituent spaces.
831832 We begin with the *algebraic tensor product* $\mathcal{H}_{\mathbf{x}} \otimes \mathcal{H}_t$, consisting of finite sums of elementary tensors
833 $f \otimes g$ with $f \in \mathcal{H}_{\mathbf{x}}$ and $g \in \mathcal{H}_t$. Although dense in $\mathcal{H}_{\mathbf{x},t}$, this space is not complete. Its completion
834 under the induced inner product is the *Hilbert tensor product*, $\mathcal{H}_{\mathbf{x}} \hat{\otimes} \mathcal{H}_t$, which is isometrically
835 isomorphic to the space of square-integrable functions on the product domain, $\mathcal{H}_{\mathbf{x},t} = L^2(\mathcal{X} \times [0, 1])$
836 (Kadison & Ringrose, 1986). This isomorphism allows us to construct a frame for the spatiotemporal
837 space from frames of the individual spaces, a result we formalize in the following lemma.
838839 **Lemma A.3.** Let $\{f_l\}_{l=1}^{\infty}$ be a frame for the spatial space $\mathcal{H}_{\mathbf{x}}$ with frame bounds A_f, B_f , and
840 let $\{g_k\}_{k=1}^{\infty}$ be a frame for the temporal space \mathcal{H}_t with frame bounds A_g, B_g . Then, the set of
841 elementary tensors $\{f_l \otimes g_k\}_{l,k=1}^{\infty}$ forms a frame for the Hilbert tensor product space $\mathcal{H}_{\mathbf{x}} \hat{\otimes} \mathcal{H}_t$, with
842 frame bounds $A_f A_g$ and $B_f B_g$.
843844 *Proof.* Let F be an arbitrary element in $\mathcal{H}_{\mathbf{x}} \hat{\otimes} \mathcal{H}_t \cong \mathcal{H}_{\mathbf{x},t}$. Let $h_k(\mathbf{x}) \triangleq \langle F(\mathbf{x}, \cdot), g_k \rangle_{\mathcal{H}_t}$. The sum of
845 the squared frame coefficients for F can be bounded as follows:
846

847
$$\begin{aligned} \sum_{l=1}^{\infty} \sum_{k=1}^{\infty} |\langle F, f_l \otimes g_k \rangle|^2 &= \sum_{k=1}^{\infty} \left(\sum_{l=1}^{\infty} |\langle h_k, f_l \rangle_{\mathcal{H}_{\mathbf{x}}}|^2 \right) \quad (\star) \\ &\leq \sum_{k=1}^{\infty} B_f \|h_k\|_{\mathcal{H}_{\mathbf{x}}}^2 = B_f \sum_{k=1}^{\infty} \|h_k\|_{\mathcal{H}_{\mathbf{x}}}^2 \quad (\star\star) \\ &= B_f \int_{\mathcal{X}} \left(\sum_{k=1}^{\infty} |\langle F(\mathbf{x}, \cdot), g_k \rangle_{\mathcal{H}_t}|^2 \right) d\mathbf{x} \quad (\star\star\star) \\ &\leq B_f \int_{\mathcal{X}} B_g \|F(\mathbf{x}, \cdot)\|_{\mathcal{H}_t}^2 d\mathbf{x} \quad (\star\star\star\star) \\ &= B_f B_g \|F\|_{\mathcal{H}_{\mathbf{x},t}}^2. \end{aligned} \tag{17}$$

848 An analogous derivation provides the lower bound, $A_f A_g \|F\|_{\mathcal{H}_{\mathbf{x},t}}^2 \leq \sum_{l,k} |\langle F, f_l \otimes g_k \rangle|^2$. The
849 key steps are: (\star) Rewriting the sum by substituting the definition of h_k . $(\star\star)$ Applying the upper
850 frame bound for the spatial frame $\{f_l\}$ for each fixed k . $(\star\star\star)$ Using Fubini's theorem to swap the
851 summation and integration. $(\star\star\star\star)$ Applying the upper frame bound for the temporal frame $\{g_k\}$
852 for each fixed \mathbf{x} . This completes the proof. \square
853854 This lemma provides the direct theoretical justification for the spatiotemporal expansion used in
855 Theorem 3.4, allowing us to represent any time score function $s_t \in \mathcal{S} \subseteq \mathcal{H}_{\mathbf{x},t}$ as a double summation
856 over the tensor product frame elements.
857

864 A.3 PROOF OF LEMMA 3.1
865866 **Lemma 3.1.** *Under Assumptions A.1 and A.2, the space \mathcal{S} is a subset of $L^2(\mathcal{X} \times [0, 1])$.*
867868
869 *Proof.* We want to show that for $\forall s_t \in \mathcal{S}$. It satisfies:
870

871
$$\|s_t\|_{L^2(\mathcal{X} \times [0, 1])}^2 = \int_{\mathcal{X}} \int_0^1 |s_t(\mathbf{x}, t)|^2 dt d\mathbf{x} < \infty. \quad (18)$$

872

873
874 Based on Assumption A.1 and Assumption A.2, we have: (1) $p_t(\mathbf{x}) \geq C > 0$, so $\frac{1}{p_t(\mathbf{x})} \leq \frac{1}{C}$; (2)
875 $|\partial_t p_t(\mathbf{x})| \leq D$. Then, using the chain rule, we write $s_t(\mathbf{x}, t)$ as:
876

877
$$|s_t(\mathbf{x}, t)|^2 = |\partial_t \log p_t(\mathbf{x})|^2 = \left| \frac{\partial_t p_t(\mathbf{x})}{p_t(\mathbf{x})} \right|^2 \leq \left(\frac{D}{C} \right)^2. \quad (19)$$

878

879
880 We now integrate over $\mathcal{X} \times [0, 1]$:
881

882
$$\begin{aligned} \|s_t\|_{L^2(\mathcal{X} \times [0, 1])}^2 &= \int_{\mathcal{X}} \int_0^1 |s_t(\mathbf{x}, t)|^2 dt d\mathbf{x} \\ &\leq \int_{\mathcal{X}} \int_0^1 \left(\frac{D}{C} \right)^2 dt d\mathbf{x} \\ &= \left(\frac{D}{C} \right)^2 \int_{\mathcal{X}} \int_0^1 dt d\mathbf{x} \\ &= \left(\frac{D}{C} \right)^2 \int_{\mathcal{X}} d\mathbf{x}. \end{aligned} \quad (20)$$

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893 Since $p_t(\mathbf{x})$ is a probability density function, we know that $\int_{\mathcal{X}} p_t(\mathbf{x}) d\mathbf{x} = 1, \forall t \in [0, 1]$, which
894 means that the integral over \mathcal{X} is finite, i.e., $\int_{\mathcal{X}} d\mathbf{x} < \infty$. Therefore, the space \mathcal{S} of functions s_t is a
895 subspace of $L^2(\mathcal{X} \times [0, 1])$. This complete the proof.
896□
897
898899 A.4 PROOF OF LEMMA 3.2
900901 **Lemma 3.2.** *Let $\{g_k\}_{k=1}^{\infty}$ be a complete orthonormal basis for \mathcal{H}_t . The target log-density ratio
902 $\log r(\mathbf{x})$ can be estimated by:*

903
$$\log r(\mathbf{x}) = \sum_{k=1}^{\infty} h_k(\mathbf{x}) \int_0^1 g_k(t) dt. \quad (4)$$

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908 *Proof.* The target log-density ratio is defined as the temporal integral of the time score function:
909

910
$$\log r(\mathbf{x}) = \int_0^1 s_t(\mathbf{x}, t) dt. \quad (21)$$

911

912 For a fixed \mathbf{x} , we can express this integral as an inner product in the Hilbert space $\mathcal{H}_t = L^2([0, 1])$
913 between the function $s_t(\mathbf{x}, \cdot)$ and the constant function $1(t) \equiv 1$.
914

915
$$\log r(\mathbf{x}) = \langle s_t(\mathbf{x}, \cdot), 1 \rangle_{\mathcal{H}_t}. \quad (22)$$

916

917 Since $\{g_k\}_{k=1}^{\infty}$ is a complete orthonormal basis for \mathcal{H}_t , the time score has the series expansion
918 $s_t(\mathbf{x}, t) = \sum_{k=1}^{\infty} h_k(\mathbf{x}) g_k(t)$, which converges in the L^2 -norm. Due to the continuity of the inner

product in a Hilbert space, we can interchange the inner product and the infinite summation:

$$\begin{aligned}
 \log r(\mathbf{x}) &= \left\langle \sum_{k=1}^{\infty} h_k(\mathbf{x}) g_k(t), 1(t) \right\rangle_{\mathcal{H}_t} \\
 &= \sum_{k=1}^{\infty} \langle h_k(\mathbf{x}) g_k(t), 1(t) \rangle_{\mathcal{H}_t} \\
 &= \sum_{k=1}^{\infty} h_k(\mathbf{x}) \langle g_k(t), 1(t) \rangle_{\mathcal{H}_t} \\
 &= \sum_{k=1}^{\infty} h_k(\mathbf{x}) \int_0^1 g_k(t) dt.
 \end{aligned} \tag{23}$$

This completes the proof. \square

A.5 PROOF OF THEOREM 3.4

Theorem 3.4. *Let $\{f_l\}_{l=1}^{\infty}$ and $\{g_k\}_{k=1}^{\infty}$ be frames for $\mathcal{H}_{\mathbf{x}}$ and \mathcal{H}_t , respectively. Then, any time score function $s_t \in \mathcal{S}$ can be expressed as:*

$$s_t(\mathbf{x}, t) = \sum_{k=1}^{\infty} \sum_{l=1}^{\infty} c_{l,k} f_l(\mathbf{x}) g_k(t), \tag{6}$$

where the coefficients $c_{l,k}$ depend on s_t . By defining spatial coefficients $h_k(\mathbf{x}) \triangleq \sum_{l=1}^{\infty} c_{l,k} f_l(\mathbf{x})$ and integral $\bar{g}_k \triangleq \int_0^1 g_k(t) dt$, the time score and the corresponding log-density ratio can be expressed as:

$$s_t(\mathbf{x}, t) = \sum_{k=1}^{\infty} h_k(\mathbf{x}) g_k(t), \quad \log r(\mathbf{x}) = \sum_{k=1}^{\infty} h_k(\mathbf{x}) \bar{g}_k. \tag{7}$$

Proof. The proof proceeds in three steps: establishing the existence of the expansion for s_t , deriving the corresponding expansion for $\log r(\mathbf{x})$, and simplifying the expressions.

By Lemma A.3, since $\{f_l\}$ and $\{g_k\}$ are frames for $\mathcal{H}_{\mathbf{x}}$ and \mathcal{H}_t respectively, the set of elementary tensors $\{f_l \otimes g_k\}_{l,k=1}^{\infty}$ forms a frame for the spatiotemporal space $\mathcal{H}_{\mathbf{x},t}$. A fundamental property of a frame is that any element in the Hilbert space can be represented as a series expansion of the frame elements. Therefore, for any $s_t \in \mathcal{S} \subseteq \mathcal{H}_{\mathbf{x},t}$, there exist coefficients $\{c_{l,k}\}$ such that:

$$s_t(\mathbf{x}, t) = \sum_{l=1}^{\infty} \sum_{k=1}^{\infty} c_{l,k} (f_l \otimes g_k)(\mathbf{x}, t) = \sum_{l=1}^{\infty} \sum_{k=1}^{\infty} c_{l,k} f_l(\mathbf{x}) g_k(t), \tag{24}$$

where the series converges in the norm of $\mathcal{H}_{\mathbf{x},t}$.

The log-density ratio is obtained by integrating the time score. For a fixed \mathbf{x} , the integration operator $I : h(t) \mapsto \int_0^1 h(t) dt$ is a continuous linear functional on \mathcal{H}_t . The continuity allows us to interchange the functional with the infinite summations:

$$\begin{aligned}
 \log r(\mathbf{x}) &= \int_0^1 s_t(\mathbf{x}, t) dt \\
 &= \int_0^1 \left(\sum_{l=1}^{\infty} \sum_{k=1}^{\infty} c_{l,k} f_l(\mathbf{x}) g_k(t) \right) dt \\
 &= \sum_{l=1}^{\infty} \sum_{k=1}^{\infty} c_{l,k} f_l(\mathbf{x}) \int_0^1 g_k(t) dt \\
 &= \sum_{l=1}^{\infty} \sum_{k=1}^{\infty} c_{l,k} f_l(\mathbf{x}) \bar{g}_k.
 \end{aligned} \tag{25}$$

972 By defining the spatial coefficient functions $h_k(\mathbf{x}) \triangleq \sum_{l=1}^{\infty} c_{l,k} f_l(\mathbf{x})$, we can group the terms in
 973 the double summations. This simplification yields the final expressions for the time score and the
 974 log-density ratio as presented in the theorem statement:

$$975 \quad s_t(\mathbf{x}, t) = \sum_{k=1}^{\infty} \left(\sum_{l=1}^{\infty} c_{l,k} f_l(\mathbf{x}) \right) g_k(t) = \sum_{k=1}^{\infty} h_k(\mathbf{x}) g_k(t), \quad (26)$$

$$976 \quad \log r(\mathbf{x}) = \sum_{k=1}^{\infty} \left(\sum_{l=1}^{\infty} c_{l,k} f_l(\mathbf{x}) \right) \bar{g}_k = \sum_{k=1}^{\infty} h_k(\mathbf{x}) \bar{g}_k. \quad (27)$$

981 This completes the proof. \square

983 A.6 PROOF OF COROLLARY 3.5

985 **Corollary 3.5.** *If each function g_k in the frame expansion belongs to the Sobolev space $\mathcal{W}^{1,2}([0, 1])$
 986 and the coefficients $\{h_k(\mathbf{x})\}$ are such that the series $\sum_{k=1}^{\infty} h_k(\mathbf{x}) g'_k(t)$ converges in $\mathcal{H}_{\mathbf{x}, t}$, then the
 987 weak derivative of the time score s_t with respect to t exists and is given by term-by-term differentiation:*

$$988 \quad \partial_t s_t(\mathbf{x}, t) = \sum_{k=1}^{\infty} h_k(\mathbf{x}) g'_k(t). \quad (8)$$

991 *Proof.* Let $v(\mathbf{x}, t) \triangleq \sum_{k=1}^{\infty} h_k(\mathbf{x}) g'_k(t)$. By assumption, this series converges to a function $v \in \mathcal{H}_{\mathbf{x}, t}$.
 992 We must show that v is the weak derivative of $s_t(\mathbf{x}, t)$ with respect to time.

994 By definition, this requires showing that for any smooth test function $\psi \in C_c^{\infty}((0, 1))$, the following
 995 equality holds for almost every $\mathbf{x} \in \mathcal{X}$:

$$996 \quad \int_0^1 s_t(\mathbf{x}, t) \psi'(t) dt = - \int_0^1 v(\mathbf{x}, t) \psi(t) dt. \quad (28)$$

999 Let's evaluate the left-hand side. For a fixed \mathbf{x} , we have:

$$1000 \quad \int_0^1 s_t(\mathbf{x}, t) \psi'(t) dt = \int_0^1 \left(\sum_{k=1}^{\infty} h_k(\mathbf{x}) g_k(t) \right) \psi'(t) dt$$

$$1001 \quad = \sum_{k=1}^{\infty} h_k(\mathbf{x}) \int_0^1 g_k(t) \psi'(t) dt \quad (\star)$$

$$1002 \quad = \sum_{k=1}^{\infty} h_k(\mathbf{x}) \left(- \int_0^1 g'_k(t) \psi(t) dt \right) \quad (\star\star)$$

$$1003 \quad = - \int_0^1 \left(\sum_{k=1}^{\infty} h_k(\mathbf{x}) g'_k(t) \right) \psi(t) dt \quad (\star\star\star)$$

$$1004 \quad = - \int_0^1 v(\mathbf{x}, t) \psi(t) dt.$$

1013 The key steps are justified as follows: (\star) The interchange of summation and integration is permitted
 1014 because the series for s_t converges in L^2 , and the operator $h \mapsto \int h \psi' dt$ is a continuous linear
 1015 functional on L^2 . $(\star\star)$ Since each $g_k \in \mathcal{W}^{1,2}([0, 1])$, it has a weak derivative g'_k . By the definition
 1016 of the weak derivative and the fact that ψ has compact support in $(0, 1)$ (meaning boundary terms
 1017 vanish), we can apply integration by parts. $(\star\star\star)$ The interchange of integration and summation is
 1018 again justified by the assumed L^2 convergence of the series defining $v(\mathbf{x}, t)$.

1019 This confirms that $v(\mathbf{x}, t)$ is the weak derivative of $s_t(\mathbf{x}, t)$, completing the proof. \square

1022 A.7 DENSENESS OF TEMPORAL BASIS IN \mathcal{H}_t

1023 **Lemma A.4.** *Let $\mathcal{H}_t \triangleq L^2([0, 1])$. Consider a family of radial basis functions $\{g_k\}_{k=1}^{\infty}$ defined by*

$$1024 \quad g_k(t) = \phi \left(\frac{|t - c_k|}{\sigma_k} \right), \quad t \in [0, 1], \quad (30)$$

1026 subject to the following conditions:

1027

- (i) The generating function $\phi : [0, \infty) \rightarrow \mathbb{R}_+$ is continuous, non-negative, not identically zero,
1028 and integrable, i.e., $\int_0^\infty \phi(r)dr < \infty$.
- (ii) The set of centers $\{c_k\}_{k=1}^\infty$ is dense in $[0, 1]$.
- (iii) For any point $t_0 \in (0, 1)$, there exists a subsequence of indices $\{k_n\}_{n=1}^\infty$ such that the
1033 centers $c_{k_n} \rightarrow t_0$ and the corresponding shape parameters $\sigma_{k_n} \rightarrow 0$ as $n \rightarrow \infty$.

1034
1035 Then, the linear span of this family, $\mathcal{A} \triangleq \text{span}\{g_k\}_{k=1}^\infty$, is dense in \mathcal{H}_t .

1036
1037 *Proof.* We use a proof by contradiction. Assume that the linear span \mathcal{A} is not dense in \mathcal{H}_t . A
1038 fundamental theorem of Hilbert spaces states that a subspace is dense if and only if its orthogonal
1039 complement contains only the zero vector. Therefore, our assumption implies the existence of a
1040 **non-zero** function $u \in \mathcal{H}_t$ (i.e., $\|u\|_{\mathcal{H}_t} > 0$) that is orthogonal to every function in the basis family
1041 $\{g_k\}_{k=1}^\infty$. This orthogonality condition is expressed as:

$$1042 \quad \langle u, g_k \rangle_{\mathcal{H}_t} = \int_0^1 u(t)g_k(t)dt = 0, \quad \forall k \geq 1. \quad (31)$$

1043 Our objective is to show that this assumption forces u to be the zero function in \mathcal{H}_t , which will
1044 establish the contradiction.

1045 By the Lebesgue Differentiation Theorem, for any function $u \in L^1([0, 1])$ (and thus for any $u \in$
1046 $L^2([0, 1])$), almost every point in $(0, 1)$ is a Lebesgue point. Let us choose an arbitrary such Lebesgue
1047 point, $t_0 \in (0, 1)$.

1048 Based on our assumptions, we can construct a specific sequence of functions. Since the centers
1049 $\{c_k\}$ are dense and condition (iii) holds, we can select a subsequence of indices $\{k_n\}_{n=1}^\infty$ such that
1050 $c_{k_n} \rightarrow t_0$ and $\sigma_{k_n} \rightarrow 0$ as $n \rightarrow \infty$. Let us denote the corresponding functions as $g_n(t) \triangleq g_{k_n}(t)$.

1051 We now define a sequence of normalized functions $\{F_n(t)\}_{n=1}^\infty$:

$$1052 \quad F_n(t) = \frac{g_n(t)}{D_n}, \quad \text{where } D_n = \int_{-\infty}^\infty g_n(s)ds. \quad (32)$$

1053 The normalization constant D_n is computed over \mathbb{R} to capture the total mass of the kernel, which
1054 is standard practice for constructing an approximate identity. It can be calculated via a change of
1055 variables:

$$1056 \quad D_n = \int_{-\infty}^\infty \phi\left(\frac{|s - c_{k_n}|}{\sigma_{k_n}}\right)ds = \sigma_{k_n} \int_{-\infty}^\infty \phi(|v|)dv = 2\sigma_{k_n} \int_0^\infty \phi(r)dr. \quad (33)$$

1057 Let $C_\phi = 2 \int_0^\infty \phi(r)dr$. By condition (i), C_ϕ is a finite positive constant, so $D_n = C_\phi \sigma_{k_n} > 0$. The
1058 sequence $\{F_n\}$ forms an “approximate identity” (or a summability kernel) centered around t_0 , which
1059 is characterized by three key properties:

1. Non-negativity: Since $\phi(r) \geq 0$ and $D_n > 0$, we have $F_n(t) \geq 0$ for all t .
2. Unit Integral: By construction, $\int_{-\infty}^\infty F_n(t)dt = 1$ for all n .
3. Concentration of Mass: For any fixed $\delta > 0$, the integral of F_n outside the neighborhood
1060 $(c_{k_n} - \delta, c_{k_n} + \delta)$ vanishes as $n \rightarrow \infty$.

$$1061 \quad \begin{aligned} \lim_{n \rightarrow \infty} \int_{|t - c_{k_n}| \geq \delta} F_n(t)dt &= \lim_{n \rightarrow \infty} \frac{1}{D_n} \int_{|t - c_{k_n}| \geq \delta} \phi\left(\frac{|t - c_{k_n}|}{\sigma_{k_n}}\right)dt \\ 1062 &= \lim_{n \rightarrow \infty} \frac{\sigma_{k_n}}{D_n} \int_{|v| \geq \delta/\sigma_{k_n}} \phi(|v|)dv \quad (\text{letting } v = (t - c_{k_n})/\sigma_{k_n}) \\ 1063 &= \frac{1}{C_\phi} \lim_{n \rightarrow \infty} 2 \int_{\delta/\sigma_{k_n}}^\infty \phi(r)dr. \end{aligned} \quad (34)$$

1064 Since $\sigma_{k_n} \rightarrow 0$, the lower limit of integration $\delta/\sigma_{k_n} \rightarrow \infty$. As $\int_0^\infty \phi(r)dr$ is finite, the tail
1065 of the integral must go to zero, i.e., $\lim_{x \rightarrow \infty} \int_x^\infty \phi(r)dr = 0$. Thus, this limit is zero.

Now, let us examine the convolution-like integral $\int_0^1 u(t)F_n(t)dt$. From our initial orthogonality assumption in Eq. (31), we have $\langle u, g_n \rangle_{\mathcal{H}_t} = 0$ for all n . This directly implies:

$$\int_0^1 u(t)F_n(t)dt = \frac{1}{D_n} \int_0^1 u(t)g_n(t)dt = \frac{1}{D_n} \langle u, g_n \rangle_{\mathcal{H}_t} = 0, \quad \forall n. \quad (35)$$

On the other hand, because t_0 is a Lebesgue point of u and $\{F_n\}$ is an approximate identity sequence concentrating at t_0 (since $c_{k_n} \rightarrow t_0$), a standard result of analysis (a key part of the Lebesgue Differentiation Theorem's proof) states that:

$$\lim_{n \rightarrow \infty} \int_0^1 u(t)F_n(t)dt = u(t_0). \quad (36)$$

Comparing Eq. (35) and Eq. (36), we must conclude that $u(t_0) = 0$.

Since t_0 was an arbitrary Lebesgue point and the set of Lebesgue points has full measure in $[0, 1]$, we have shown that $u(t) = 0$ almost everywhere on $[0, 1]$. In the space $L^2([0, 1])$, a function that is zero almost everywhere is equivalent to the zero vector.

This contradicts our initial assumption that u was a non-zero function. Therefore, the assumption that \mathcal{A} is not dense in \mathcal{H}_t must be false. This completes the proof. \square

A.8 PROOF OF PROPOSITION 4.1

Proposition 4.1. *Let $\{g_k\}_{k=1}^\infty$ be an infinite family of RBFs in \mathcal{H}_t , defined by $g_k(t) = \phi(|t - c_k|/\sigma_k)$. c_k and σ_k are the center and shape parameters of g_k . This family generates a convergent and well-posed approximation scheme if it meets two conditions: (i) Denseness: The infinite family's linear span is dense in \mathcal{H}_t , i.e., $\overline{\text{span}\{g_k\}_{k=1}^\infty} = \mathcal{H}_t$. (ii) Finite-dimensional stability: For any finite $K \geq 1$, the subset $\{g_k\}_{k=1}^K$ is linearly independent.*

Proof. The proof consists of verifying that these two conditions ensure the desired properties of the approximation scheme.

Convergence: Condition (i), established by our Denseness Lemma (Lemma A.4), guarantees the scheme's convergence. It ensures that for any function $h \in \mathcal{H}_t$ and any error tolerance $\epsilon > 0$, there exists a sufficiently large dimension K and a function $g \in V_K$ such that $\|h - g\|_{\mathcal{H}_t} < \epsilon$. This means the approximation error of the best-fit projection, $\inf_{g \in V_K} \|h - g\|$, can be made arbitrarily small.

Well-posed Approximation: Condition (ii) guarantees that for any fixed, finite K , the approximation problem within the subspace V_K is well-posed. Since $\{g_k\}_{k=1}^K$ is a linearly independent set, it forms a basis for the subspace $V_K = \text{span}\{g_k\}_{k=1}^K$. In a finite-dimensional Hilbert space, any basis is a Riesz basis (a specific type of frame). This implies the existence of frame bounds A_K and B_K that depend on K , satisfying $0 < A_K \leq B_K < \infty$. The existence of a strictly positive lower bound A_K ensures that the projection of any function onto V_K is a stable and well-defined operation. \square

A.9 PROOF OF PROPOSITION 4.2

Proposition 4.2. *Let the RBF generating function ϕ be such that its native space \mathcal{N}_ϕ is equivalent to $W^{\tau,2}(\mathbb{R})$ for some $\tau > 1/2$. Let the target function $s_t(\mathbf{x}, \cdot)$ belong to a Sobolev space of lower smoothness, $s_t(\mathbf{x}, \cdot) \in W^{\beta,2}([0, 1])$ with $1/2 < \beta \leq \tau$. Let $s_t^{(K)}(\mathbf{x}, \cdot)$ be the best approximation of s_t in the subspace $V_K = \text{span}\{g_k\}_{k=1}^K$, where the centers $\mathcal{C}_K = \{c_k\}_{k=1}^K$ are quasi-uniform. Then, there exists a constant C , independent of s_t and K , such that the approximation error is bounded by:*

$$\|s_t(\mathbf{x}, \cdot) - s_t^{(K)}(\mathbf{x}, \cdot)\|_{\mathcal{H}_t} \leq C \cdot K^{-\beta} \cdot \|s_t(\mathbf{x}, \cdot)\|_{W^{\beta,2}([0,1])}. \quad (11)$$

Proof. The proof is a direct application of the main results presented in Narcowich et al. (2006). Let $I_{\mathcal{C}_K} s_t$ denote the RBF interpolant to s_t at the centers \mathcal{C}_K . The best approximation error in the subspace V_K is, by definition, the infimum of the error over all functions in that subspace, which is bounded above by the error of any specific function in V_K , such as the RBF interpolant $I_{\mathcal{C}_K} s_t$. Thus,

$$\|s_t - s_t^{(K)}\|_{\mathcal{H}_t} = \inf_{h \in V_K} \|s_t - h\|_{\mathcal{H}_t} \leq \|s_t - I_{\mathcal{C}_K} s_t\|_{\mathcal{H}_t}. \quad (37)$$

We now bound the interpolation error using the results from [Narcowich et al. \(2006\)](#). The cited work provides error estimates for functions defined on a general compact domain $\Omega \subset \mathbb{R}^d$. Crucially, the validity of these results hinges on the assumption that the RBF generating function ϕ has a native space \mathcal{N}_ϕ equivalent to $W^{\tau,2}(\mathbb{R})$. Their key result, Theorem 4.2, provides an estimate for functions $f \in \mathcal{W}^{\beta,2}(\Omega)$ that are less smooth than the native space order τ . Applying this theorem to our specific one-dimensional case where $\Omega = [0, 1]$ and setting the error norm order $\mu = 0$ (for the L^2 norm) gives:

$$\|s_t - I_{\mathcal{C}_K} s_t\|_{L^2([0,1])} \leq A h_{\mathcal{C}_K, [0,1]}^\beta \rho_{\mathcal{C}_K, [0,1]}^\tau \|s_t\|_{\mathcal{W}^{\beta,2}([0,1])}, \quad (38)$$

where $h_{\mathcal{C}_K, [0,1]}$ is the fill distance and $\rho_{\mathcal{C}_K, [0,1]}$ is the mesh ratio.

The proposition assumes that the centers \mathcal{C}_K are quasi-uniform. For such a set of points, the mesh ratio is bounded by a constant independent of K , i.e., $\rho_{\mathcal{C}_K, [0,1]} \leq \rho_{\max}$. Furthermore, the fill distance is directly related to the number of points, $h_{\mathcal{C}_K, [0,1]} = \mathcal{O}(1/K)$.

Substituting these into the bound in Eq. (38):

$$\|s_t - I_{\mathcal{C}_K} s_t\|_{L^2([0,1])} \leq A(\mathcal{O}(1/K))^\beta (\rho_{\max})^\tau \|s_t\|_{\mathcal{W}^{\beta,2}([0,1])}. \quad (39)$$

By defining a new constant $C \triangleq A \cdot (\rho_{\max})^\tau$ that absorbs all terms independent of s_t and K , we arrive at the final error bound:

$$\begin{aligned} \|s_t(\mathbf{x}, \cdot) - s_t^{(K)}(\mathbf{x}, \cdot)\|_{\mathcal{H}_t} &\leq \|s_t(\mathbf{x}, \cdot) - I_{\mathcal{C}_K} s_t(\mathbf{x}, \cdot)\|_{\mathcal{H}_t} \\ &\leq A(\mathcal{O}(1/K))^\beta (\rho_{\max})^\tau \|s_t\|_{\mathcal{W}^{\beta,2}([0,1])} \quad (\mathcal{H}_t = L^2([0, 1])) \\ &= C \cdot K^{-\beta} \cdot \|s_t(\mathbf{x}, \cdot)\|_{\mathcal{W}^{\beta,2}([0,1])}. \end{aligned} \quad (40)$$

This completes the proof. \square

B ANALYTIC FORMULAS FOR RBF KERNELS

This section provides a summary of the Radial Basis Function (RBF) generating functions, $\phi(r)$, used and referenced in this work. All kernels listed below are *strictly positive definite*, satisfying the conditions of our approximation framework. Their respective closed-form integrals and derivatives are detailed in the subsequent sections.

Table 5: A summary of different RBF generating functions used in this paper.

| Kernel Name | $\phi(r)$ | Key Properties | Analytic Formulas |
|------------------------|------------------------------------|--|--------------------|
| Gaussian | $\exp(-r^2)$ | Infinitely smooth, localized influence (fast decay). | Eqs. (41) and (42) |
| Inverse Multiquadric | $(r^2 + 1)^{-1/2}$ | Infinitely smooth, global influence (slow decay). | Eqs. (43) and (44) |
| Rational Quadratic | $(r^2 + 1)^{-1}$ | Infinitely smooth, multi-scale, medium decay. | Eqs. (45) and (46) |
| Matérn ($\nu = 3/2$) | $(1 + \sqrt{3}r) \exp(-\sqrt{3}r)$ | Limited smoothness (C^2), local influence. | Eqs. (47) and (48) |

B.1 GAUSSIAN RBFs

The Gaussian RBF is defined by the generating function $\phi(r) = \exp(-r^2)$. The basis functions are therefore given by:

$$g_k(t) = \exp\left(-\frac{|t - c_k|^2}{\sigma_k^2}\right), \quad (41)$$

where c_k and $\sigma_k > 0$ are the center and shape parameters of g_k .

Closed-Form Expression for the Temporal Integral. The integral $\bar{g}_k = \int_0^1 g_k(t) dt$ is calculated as follows. We use the substitution $u = (t - c_k)/\sigma_k$, which implies $dt = \sigma_k du$.

$$\bar{g}_k = \int_0^1 \exp\left(-\frac{|t - c_k|^2}{\sigma_k^2}\right) dt = \sigma_k \int_{-c_k/\sigma_k}^{(1-c_k)/\sigma_k} \exp(-u^2) du.$$

1188 This integral can be expressed using the error function, $\text{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z \exp(-x^2) dx$. Since
 1189 $\int_a^b \exp(-u^2) du = \frac{\sqrt{\pi}}{2} (\text{erf}(b) - \text{erf}(a))$, we have:
 1190

$$\begin{aligned} \bar{g}_k &= \sigma_k \frac{\sqrt{\pi}}{2} \left[\text{erf} \left(\frac{1 - c_k}{\sigma_k} \right) - \text{erf} \left(-\frac{c_k}{\sigma_k} \right) \right] \\ &= \frac{\sigma_k \sqrt{\pi}}{2} \left[\text{erf} \left(\frac{1 - c_k}{\sigma_k} \right) + \text{erf} \left(\frac{c_k}{\sigma_k} \right) \right], \end{aligned}$$

1197 where the last step uses the property $\text{erf}(-z) = -\text{erf}(z)$.
 1198

1199 **Closed-Form Expression for the Temporal Derivative.** The derivative $g'_k(t)$ is found by applying
 1200 the chain rule:
 1201

$$\begin{aligned} g'_k(t) &= \frac{d}{dt} \exp \left(-\frac{(t - c_k)^2}{\sigma_k^2} \right) \\ &= \exp \left(-\frac{(t - c_k)^2}{\sigma_k^2} \right) \cdot \frac{d}{dt} \left(-\frac{(t - c_k)^2}{\sigma_k^2} \right) \\ &= \exp \left(-\frac{(t - c_k)^2}{\sigma_k^2} \right) \cdot \left(-\frac{2(t - c_k)}{\sigma_k^2} \right). \end{aligned}$$

1209 The final expressions for the integral and derivative are summarized below.
 1210

$$\begin{aligned} \bar{g}_k &= \frac{\sigma_k \sqrt{\pi}}{2} \left[\text{erf} \left(\frac{1 - c_k}{\sigma_k} \right) + \text{erf} \left(\frac{c_k}{\sigma_k} \right) \right], \\ g'_k(t) &= -\frac{2(t - c_k)}{\sigma_k^2} g_k(t). \end{aligned} \tag{42}$$

1217 B.2 INVERSE MULTIQUADRIC RBFs

1219 The Inverse Multiquadric (IMQ) RBF is defined by the generating function $\phi(r) = (r^2 + 1)^{-1/2}$.
 1220 The basis functions are therefore given by:
 1221

$$g_k(t) = \left(\frac{(t - c_k)^2}{\sigma_k^2} + 1 \right)^{-\frac{1}{2}} = \frac{\sigma_k}{\sqrt{(t - c_k)^2 + \sigma_k^2}}. \tag{43}$$

1226 **Closed-Form Expression for the Temporal Integral.** The temporal integral $\bar{g}_k = \int_0^1 g_k(t) dt$ is
 1227 calculated using the standard integral for the inverse hyperbolic sine function. We use the substitution
 1228 $u = t - c_k$, which implies $dt = du$.
 1229

$$\bar{g}_k = \int_0^1 \frac{\sigma_k}{\sqrt{(t - c_k)^2 + \sigma_k^2}} dt = \sigma_k \int_{-c_k}^{1 - c_k} \frac{1}{\sqrt{u^2 + \sigma_k^2}} du.$$

1233 The integral of $1/\sqrt{u^2 + a^2}$ is $\ln(u + \sqrt{u^2 + a^2})$. Applying this, we get:
 1234

$$\begin{aligned} \bar{g}_k &= \sigma_k \left[\ln \left(u + \sqrt{u^2 + \sigma_k^2} \right) \right]_{-c_k}^{1 - c_k} \\ &= \sigma_k \left(\ln \left((1 - c_k) + \sqrt{(1 - c_k)^2 + \sigma_k^2} \right) - \ln \left(-c_k + \sqrt{c_k^2 + \sigma_k^2} \right) \right) \\ &= \sigma_k \ln \left(\frac{(1 - c_k) + \sqrt{(1 - c_k)^2 + \sigma_k^2}}{-c_k + \sqrt{c_k^2 + \sigma_k^2}} \right). \end{aligned}$$

1242 **Closed-Form Expression for the Temporal Derivative.** The derivative $g'_k(t)$ is found by applying
 1243 the chain rule to $g_k(t) = \sigma_k ((t - c_k)^2 + \sigma_k^2)^{-1/2}$:

$$\begin{aligned} 1245 \quad g'_k(t) &= \sigma_k \cdot \frac{d}{dt} ((t - c_k)^2 + \sigma_k^2)^{-1/2} \\ 1246 \quad &= \sigma_k \cdot \left(-\frac{1}{2}\right) ((t - c_k)^2 + \sigma_k^2)^{-3/2} \cdot \frac{d}{dt} ((t - c_k)^2 + \sigma_k^2) \\ 1247 \quad &= \sigma_k \cdot \left(-\frac{1}{2}\right) ((t - c_k)^2 + \sigma_k^2)^{-3/2} \cdot 2(t - c_k) \\ 1248 \quad &= -\frac{\sigma_k(t - c_k)}{((t - c_k)^2 + \sigma_k^2)^{3/2}}. \\ 1249 \quad & \\ 1250 \quad & \\ 1251 \quad & \\ 1252 \quad & \\ 1253 \quad & \end{aligned}$$

1254 The final expressions for the integral and derivative are summarized below.

$$\begin{aligned} 1255 \quad \bar{g}_k &= \sigma_k \ln \left(\frac{(1 - c_k) + \sqrt{(1 - c_k)^2 + \sigma_k^2}}{-c_k + \sqrt{c_k^2 + \sigma_k^2}} \right), \\ 1256 \quad & \\ 1257 \quad & \\ 1258 \quad g'_k(t) &= -\frac{\sigma_k(t - c_k)}{((t - c_k)^2 + \sigma_k^2)^{3/2}}. \\ 1259 \quad & \\ 1260 \quad & \end{aligned} \tag{44}$$

1261 B.3 RATIONAL QUADRATIC RBFs

1262 The Rational Quadratic (RQ) kernel can be viewed as an infinite sum of Gaussian kernels of different
 1263 scales. This property makes it a robust choice, capable of modeling data at multiple scales. It is
 1264 strictly positive definite, and its generating function is $\phi(r) = (1 + r^2)^{-1}$. The basis functions are
 1265 therefore given by:

$$1266 \quad g_k(t) = \left(1 + \frac{(t - c_k)^2}{\sigma_k^2}\right)^{-1} = \frac{\sigma_k^2}{(t - c_k)^2 + \sigma_k^2}. \tag{45}$$

1267 **Closed-Form Expression for the Temporal Integral.** The temporal integral $\bar{g}_k = \int_0^1 g_k(t) dt$ is
 1268 calculated using the standard integral for the arctangent function. We use the substitution $u = t - c_k$,
 1269 which implies $dt = du$.

$$1270 \quad \bar{g}_k = \int_0^1 \frac{\sigma_k^2}{(t - c_k)^2 + \sigma_k^2} dt = \sigma_k^2 \int_{-c_k}^{1-c_k} \frac{1}{u^2 + \sigma_k^2} du.$$

1271 The integral of $1/(u^2 + a^2)$ is $\frac{1}{a} \arctan(\frac{u}{a})$. Applying this, we get:

$$\begin{aligned} 1272 \quad \bar{g}_k &= \sigma_k^2 \left[\frac{1}{\sigma_k} \arctan \left(\frac{u}{\sigma_k} \right) \right]_{-c_k}^{1-c_k} \\ 1273 \quad &= \sigma_k \left(\arctan \left(\frac{1 - c_k}{\sigma_k} \right) - \arctan \left(\frac{-c_k}{\sigma_k} \right) \right) \\ 1274 \quad &= \sigma_k \left(\arctan \left(\frac{1 - c_k}{\sigma_k} \right) + \arctan \left(\frac{c_k}{\sigma_k} \right) \right), \\ 1275 \quad & \\ 1276 \quad & \end{aligned}$$

1277 where the last step uses the property $\arctan(-z) = -\arctan(z)$.

1278 **Closed-Form Expression for the Temporal Derivative.** The derivative $g'_k(t)$ is found by applying
 1279 the chain rule to $g_k(t) = \sigma_k^2 ((t - c_k)^2 + \sigma_k^2)^{-1}$:

$$\begin{aligned} 1280 \quad g'_k(t) &= \sigma_k^2 \cdot \frac{d}{dt} ((t - c_k)^2 + \sigma_k^2)^{-1} \\ 1281 \quad &= \sigma_k^2 \cdot (-1) ((t - c_k)^2 + \sigma_k^2)^{-2} \cdot \frac{d}{dt} ((t - c_k)^2 + \sigma_k^2) \\ 1282 \quad &= -\sigma_k^2 ((t - c_k)^2 + \sigma_k^2)^{-2} \cdot 2(t - c_k) \\ 1283 \quad &= -\frac{2\sigma_k^2(t - c_k)}{((t - c_k)^2 + \sigma_k^2)^2}. \\ 1284 \quad & \\ 1285 \quad & \end{aligned}$$

1296 The final expressions for the integral and derivative are summarized below.
 1297

$$1298 \bar{g}_k = \sigma_k \left(\arctan \left(\frac{1 - c_k}{\sigma_k} \right) + \arctan \left(\frac{c_k}{\sigma_k} \right) \right), \quad g'_k(t) = -\frac{2\sigma_k^2(t - c_k)}{((t - c_k)^2 + \sigma_k^2)^2}. \quad (46)$$

1300
 1301 **B.4 MATÉRN RBFs**
 1302

1303 The Matérn family of RBFs is widely used in machine learning, particularly in Gaussian processes,
 1304 as their smoothness is controlled by a parameter ν . We consider the common case where $\nu = 3/2$,
 1305 which corresponds to a once-differentiable function. The generating function is strictly positive
 1306 definite and is given by $\phi(r) = (1 + \sqrt{3}r) \exp(-\sqrt{3}r)$. The basis functions, which are in the Sobolev
 1307 space $W_2^2(\mathbb{R})$, are:

$$1308 g_k(t) = \left(1 + \frac{\sqrt{3}|t - c_k|}{\sigma_k} \right) \exp \left(-\frac{\sqrt{3}|t - c_k|}{\sigma_k} \right). \quad (47)$$

1311 **Closed-Form Expression for the Temporal Integral.** The integral $\bar{g}_k = \int_0^1 g_k(t) dt$ is computed
 1312 by splitting the integral at the center c_k due to the absolute value. The indefinite integral of the
 1313 generating function is $\int \phi(r) dr = -re^{-\sqrt{3}r} - \frac{2}{\sqrt{3}}e^{-\sqrt{3}r}$. Evaluating this over the respective intervals
 1314 yields the final closed form.

1316 **Closed-Form Expression for the Temporal Derivative.** The derivative of the generating function
 1317 is $\phi'(r) = -3r \exp(-\sqrt{3}r)$. Applying the chain rule, we find the derivative of $g_k(t)$:

$$1319 g'_k(t) = \phi' \left(\frac{|t - c_k|}{\sigma_k} \right) \cdot \frac{\operatorname{sgn}(t - c_k)}{\sigma_k}$$

$$1320 = -3 \frac{|t - c_k|}{\sigma_k} \exp \left(-\frac{\sqrt{3}|t - c_k|}{\sigma_k} \right) \cdot \frac{t - c_k}{|t - c_k|} \cdot \frac{1}{\sigma_k}$$

$$1321 = -\frac{3(t - c_k)}{\sigma_k^2} \exp \left(-\frac{\sqrt{3}|t - c_k|}{\sigma_k} \right).$$

1327 The final expressions are summarized below.

$$1329 \bar{g}_k = \frac{2\sigma_k}{\sqrt{3}} - \sigma_k \left[\left(\frac{1 - c_k}{\sigma_k} + \frac{2}{\sqrt{3}} \right) e^{-\frac{\sqrt{3}(1 - c_k)}{\sigma_k}} + \left(\frac{c_k}{\sigma_k} + \frac{2}{\sqrt{3}} \right) e^{-\frac{\sqrt{3}c_k}{\sigma_k}} \right],$$

$$1330 g'_k(t) = -\frac{3(t - c_k)}{\sigma_k^2} \exp \left(-\frac{\sqrt{3}|t - c_k|}{\sigma_k} \right).$$

1350 **C EXPERIMENTAL DETAILS AND MORE RESULTS**
1351

1352 All experiments were conducted on four NVIDIA TITAN X (Pascal) 12GB GPUs using PyTorch
1353 (2.1.2) and PyTorch-Lightning (2.1.2). Our code is developed based on the official code for both DRE-
1354 ∞ at <https://github.com/ermongroup/dre-infinity> and Neural ODE at <https://github.com/rtqichen/torchdiffeq>. Our code will be made available once the paper
1355 is accepted.
1356

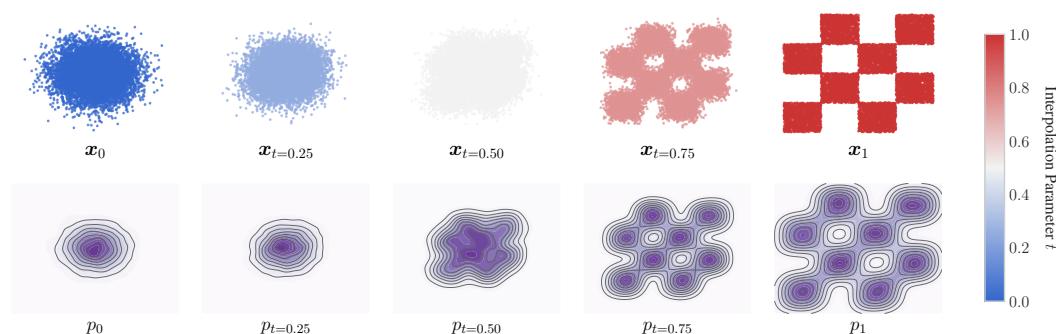
1358 **C.1 EXPERIMENTAL DETAILS**
1359

1360 **C.1.1 INTERPOLATING PATHS AND THE TEMPORAL-INTEGRAL VIEW**
1361

1362 This section clarifies how interpolating paths are constructed and why the resulting temporal integral
1363 offers a stable formulation of density ratio estimation (DRE), addressing a common source of
1364 confusion for readers outside the score-based modeling community.
1365

1366 **Temporal Integral Intuition.** The log-density ratio can be written as $\log r(\mathbf{x}) = \int_0^1 \partial_t \log p_t(\mathbf{x}) dt$.
1367 Here, $\partial_t \log p_t(\mathbf{x})$ is the instantaneous rate of change of the log-density along a smooth interpolation
1368 p_t . The integral simply accumulates these infinitesimal changes over $t \in [0, 1]$. Because the path
1369 is smooth and non-vanishing, this temporal accumulation remains numerically stable. This avoids
1370 the divergence that occurs when directly computing $\log \frac{p_1(\mathbf{x})}{p_0(\mathbf{x})}$ between distributions with little or no
1371 overlapping support (the density-chasm problem (Rhodes et al., 2020)).
1372

1373 **Path Schedules Used in This Paper.** Let \mathbf{x}_0 and \mathbf{x}_1 be samples drawn from p_0 and p_1 , respectively.
1374 We consider two standard path schedules. The first is the Linear path, a widely-used schedule in
1375 stochastic interpolants (Albergo et al., 2023), defined by $a_t = 1 - t$ and $b_t = t$. The second is the
1376 variance-preserving (VP) path (Song et al., 2021), satisfying $a_t = \exp(-0.25t^2(\beta_1 - \beta_0) - 0.5t\beta_0)$
1377 and $b_t = \sqrt{1 - a_t^2}$. We use the standard diffusion constants $\beta_0 = 0.1$ and $\beta_1 = 20$.
1378

1379 **Path Visualization.** Fig. 5 shows the VP path on the checkerboard dataset. The samples \mathbf{x}_t and
1380 densities p_t evolve smoothly from a simple Gaussian (p_0) to a complex multimodal target (p_1).
1381 The color-coded time steps illustrate that the support remains connected and well-behaved for all
1382 $t \in (0, 1)$, confirming the existence of a tractable and stable path integral.
1383

1404 Figure 5: Traditional DRE methods require directly estimating $\log \frac{p_1}{p_0}$ between potentially non-
1405 overlapping densities, leading to numerical instability. Continuous score-based DRE avoids this by
1406 constructing a smooth interpolating path $\{p_t\}_{t \in [0, 1]}$. The figure visualizes this path at five time steps
1407 ($t \in \{0, 0.25, 0.50, 0.75, 1.0\}$) under a variance-preserving (VP) schedule, showing the transition
1408 from a simple Gaussian (p_0) to a multimodal checkerboard distribution (p_1). Along the path, all
1409 intermediate densities remain connected and well-behaved, turning the hard ratio estimation into the
1410 tractable path integral $\int_0^1 \partial_t \log p_t(\mathbf{x}) dt$. The top row shows sample evolution (color-coded by t),
1411 and the bottom row shows the corresponding density contours.
1412

1404 C.1.2 JOINT SCORE MATCHING
1405

1406 Let $s_t = \partial_t \log p_t(\mathbf{x})$ and $\mathbf{s}_x = \nabla_{\mathbf{x}} \log p_t(\mathbf{x})$ be the **time score** and **data score**, respectively. In this
1407 section, we integrate the parameterized time score model $s_t^\theta \in \mathbb{R}$ and data score model $\mathbf{s}_x^\theta \in \mathbb{R}^d$
1408 to formulate the joint score model $\mathbf{s}_{t,x}^\theta : [s_t^\theta, \mathbf{s}_x^\theta] \in \mathbb{R}^{d+1}$. This joint score is incorporated into the
1409 training objective defined in Eq. (15), resulting in a joint score matching objective (Choi et al., 2022):

$$\begin{aligned} \mathcal{L}_{\text{joint}}(\theta) = & 2\mathbb{E}_{p_0(\mathbf{x}_0)p_1(\mathbf{x}_1)}[\lambda(0)s_{t,x}^\theta(\mathbf{x}_0, 0)[t] - \lambda(1)s_{t,x}^\theta(\mathbf{x}_1, 1)[t]] \\ & + \mathbb{E}_{p(t)p_t(\mathbf{x})}\mathbb{E}_{p(\mathbf{v})}[2\lambda(t)\partial_t s_{t,x}^\theta(\mathbf{x}, t)[t] + 2\lambda'(t)s_{t,x}^\theta(\mathbf{x}, t)[t] \\ & + \lambda(t)\|\mathbf{s}_{t,x}^\theta(\mathbf{x}, t)[\mathbf{x}]\|_2^2 + 2\lambda(t)\mathbf{v}^\top \nabla_{\mathbf{x}} s_{t,x}^\theta(\mathbf{x}, t)[\mathbf{x}]\mathbf{v}], \end{aligned} \quad (49)$$

1410 where $\mathbf{v} \sim p(\mathbf{v}) = \mathcal{N}(\mathbf{0}, \mathbf{I}_d)$ follows a standard Gaussian distribution, the terms $s_{t,x}^\theta(\mathbf{x}, t)[\mathbf{x}]$ and
1411 $s_{t,x}^\theta(\mathbf{x}, t)[t]$ represent the data and time score components of $\mathbf{s}_{t,x}^\theta(\mathbf{x}, t)$, respectively.

1412 C.1.3 TRAINING PROCEDURE
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1414 In each training step, we sample a batch of pairs $(\mathbf{x}_0, \mathbf{x}_1)$ from the source and target distributions, p_0
1415 and p_1 , respectively. We also sample a time t from a distribution $p(t)$ over $[0, 1]$. The interpolated
1416 sample \mathbf{x}_t is then constructed via a interpolation $\mathbf{x}_t = a_t \mathbf{x}_0 + b_t \mathbf{x}_1$. We use the coefficients (a_t, b_t)
1417 corresponding to the variance-preserving (VP) and linear path schedules following Choi et al. (2022);
1418 Chen et al. (2025), as detailed in Sec. C.1.1. The detailed training process is outlined in Algorithm 3.

1419 **Algorithm 3** Training of OS-DRE
1420

1421 **Input:** Data distributions p_0 and p_1 , number of basis functions K .
1422

1423 **Output:** Trained model parameters θ^* and $\{\sigma_k^*\}_{k=1}^K$.

- 1: Initialize trainable parameters θ of neural network NN and shape parameters $\{\sigma_k\}_{k=1}^K$.
- 2: Define fixed, quasi-uniform centers $\{c_k\}_{k=1}^K$ over $[0, 1]$.
- 3: **for** each training step **do**
- 4: Sample a batch: $\mathbf{x}_0 \sim p_0, \mathbf{x}_1 \sim p_1, t \sim p(t)$.
- 5: Construct interpolated samples $\mathbf{x}_t = a_t \mathbf{x}_0 + b_t \mathbf{x}_1$ (see Sec. C.1.1 for details).
- 6: Compute coefficients: $\{h_k^\theta(\mathbf{x})\}_{k=1}^K \leftarrow \text{NN}(\mathbf{x}; \theta)$ for each sample in the batch.
- 7: Construct score model s_t^θ and its derivative $\partial_t s_t^\theta$ using the model definition in Sec. 4.4.
- 8: Compute the STSM loss $\mathcal{L}_{\text{STSM}}(\theta)$ using Eq. (15).
- 9: Update trainable parameters θ and $\{\sigma_k\}_{k=1}^K$ via gradient descent on the loss.
- 10: **end for**

1424 C.2 MODEL PARAMETERIZATION AND IMPLEMENTATION DETAILS
1425

1426 Our implementation of the OS-DRE framework consists of two main components: the neural network
1427 that parameterizes the spatial coefficients and the RBF temporal basis itself.

1428 C.2.1 IMPLEMENTATION DETAILS
1429

1430 **Network Architecture.** Our model maps an input sample \mathbf{x} to its K spatial coefficients through
1431 a feed-forward network with a backbone and a single output head. The backbone is formed by a
1432 sequence of residual blocks that transform \mathbf{x} into a high-level feature embedding, which is then fed
1433 into the spatial-coefficient head, which applies another set of residual blocks and a final linear layer
1434 to produce a K -dimensional vector. The output directly corresponds to the spatial coefficients:

$$[h_1^\theta(\mathbf{x}), h_2^\theta(\mathbf{x}), \dots, h_K^\theta(\mathbf{x})] = \text{NN}(\mathbf{x}; \theta). \quad (50)$$

1435 For each input \mathbf{x} , the network computes all K scalar coefficients in a single forward pass.

1436 **Trainable Parameters.** The trainable parameters of our model consist of two groups: (1) The
1437 parameters (weights and biases) of NN, collectively denoted by θ ; (2) The shape parameters $\{\sigma_k\}_{k=1}^K$
1438 of the RBF temporal basis $\{g_k\}_{k=1}^K$. The RBF centers $\{c_k\}_{k=1}^K$ are fixed hyperparameters, chosen
1439 as a quasi-uniform grid over $[0, 1]$ to satisfy the theoretical conditions. All trainable parameters are
1440 optimized jointly by minimizing the STSM loss $\mathcal{L}_{\text{STSM}}$ defined in Eq. (15).

1458

C.2.2 NEURAL NETWORK PARAMETERIZATION

1459

To implement OS-DRE, we employ a neural network to approximate the joint score. Its core function is to map an input \mathbf{x} to the spatial coefficients $\{h_k(\mathbf{x})\}_{k=1}^K$ and data score. The network consists of a shared backbone and two lightweight task-specific heads for time and data score estimation.

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Architectural Overview. The model computes the time score $s_t(\mathbf{x}, t)$ and, optionally, the data score $s_{\mathbf{x}}(\mathbf{x}, t) \triangleq \nabla_{\mathbf{x}} \log p_t(\mathbf{x})$ for joint score matching (see Eq. (49)). The architecture consists of three main components:

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- **Shared Backbone:** Extracts a high-level feature embedding from \mathbf{x} . The backbone is a stack of residual blocks mapping \mathbf{x} to a latent representation $\Phi(\mathbf{x}) \in \mathbb{R}^{d_{\text{hidden}}}$. This shared embedding serves as input to both heads.
- **Spatial Coefficient Head:** Predicts the K spatial coefficients $\{h_k^{\theta}(\mathbf{x})\}_{k=1}^K$. This head processes $\Phi(\mathbf{x})$ through additional residual blocks and a final linear layer $\text{nn.Linear}(d_{\text{hidden}}, K)$, producing

$$[h_0^{\theta}(\mathbf{x}), h_1^{\theta}(\mathbf{x}), \dots, h_{K-1}^{\theta}(\mathbf{x})] = \text{SpatialCoefficientHead}(\Phi(\mathbf{x})). \quad (51)$$

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Hence, all K coefficients are predicted in one forward pass.

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Algorithm 4 PyTorch implementation of RBF-based Analytic Frame (for instance, Gaussian RBF).

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```

1  class GaussianRBFFrame(nn.Module):
2      """Gaussian Radial Basis Function (RBF)."""
3      def __init__(self, K):
4          super().__init__(K)
5          pi = torch.tensor(torch.pi)
6          self.register_buffer("sqrt_pi", torch.sqrt(pi))
7          self.sigma_fn = lambda : torch.exp(self.log_sigma)
8
9      @property
10      def sigma(self):
11          return self._compute_sigma()
12
13      def _compute_sigma(self):
14          return self.sigma_fn()
15
16      def forward(self, t):
17          sigma_squared = self.sigma ** 2
18          squared_dist = (t - self.c_k) ** 2      # [batch_size, K]
19          return torch.exp(-squared_dist / sigma_squared) #[batch_size, K]
20
21      def grad_function(self, t):
22          sigma_squared = self.sigma ** 2
23          squared_distances = (t - self.c_k) ** 2
24          exp_term = torch.exp(-squared_distances / sigma_squared)
25          return -2*(t-self.c_k)/sigma_squared*exp_term #[batch_size, K]
26
27      def _compute_integrals(self):
28          sigma = self.sigma
29          sigma_sqrt_pi = sigma * self.sqrt_pi
30          erf_term_1 = torch.erf((1 - self.c_k) / sigma)
31          erf_term_2 = torch.erf(self.c_k / sigma)
32          return (sigma_sqrt_pi / 2) * (erf_term_1 + erf_term_2)
33

```

1512 C.3 EXPERIMENTAL SETTINGS AND RESULTS FOR DENSITY ESTIMATION
1513

1514 In density estimation, let $p_0(\mathbf{x}) = \mathcal{N}(\mathbf{0}, \mathbf{I}_d)$ be a simple noise distribution, and $p_1(\mathbf{x})$ denote the
1515 complex and intractable data distribution. The log-likelihood of p_1 for a given sample \mathbf{x} can be
1516 estimated as $\log p_1(\mathbf{x}) = \log r(\mathbf{x}) + \log p_0(\mathbf{x})$, where $r(\mathbf{x}) = p_1(\mathbf{x})/p_0(\mathbf{x})$ is the density ratio
1517 between p_1 and p_0 . After training, the estimated log-density ratio $\log \hat{r}$ can be derived based on
1518 Eq. (16). Thus, the log-likelihood of p_1 can be estimated as $\log p_1(\mathbf{x}) \approx \log \hat{r}(\mathbf{x}) + \log p_0(\mathbf{x})$.

1519 **Structured and Multimodal Datasets.** This section provides a detailed analysis of the density
1520 estimation results presented in Fig. 7, covering all nine benchmark datasets. In all experiments, our
1521 OS-DRE model was configured with $K = 400$ basis functions using the RQ kernel and was restricted
1522 to $\text{NFE} = 1$ for inference. The baseline methods, DRE- ∞ and D 3 RE, were evaluated using a simple
1523 quadrature method (the trapezoidal rule) with a fixed $\text{NFE} = 2$. We optimize the model using the
1524 joint score matching loss with a learning rate of 0.01. The batch size is set to 10,000, with 100
1525 batches per epoch. The weighting function is defined as $\lambda(t) = t(1 - t)$.

- 1527 • **Disconnected Topologies.** The circles and rings datasets test the model’s ability to capture
1528 distributions with multiple, disconnected components and assign zero density to the regions
1529 between them. Fig. 7 shows that OS-DRE perfectly learns both topologies, generating
1530 crisp rings with sharp boundaries. The baselines, particularly DRE- ∞ , struggle with this,
1531 producing blurry estimates that incorrectly assign density to the space between the rings.
1532 The 8gaussians dataset, featuring eight distinct clusters, further showcases this strength.
1533 OS-DRE accurately identifies and models all eight modes, whereas the competing methods
1534 tend to merge some of the clusters.
- 1535 • **Intricate Structures.** The 2spirals, pinwheel, and swissroll datasets feature highly struc-
1536 tured, non-linear manifolds that require the model to learn complex, curving paths. OS-DRE
1537 demonstrates exceptional performance on all three, accurately tracing the thin spiral arms
1538 and the swiss roll manifold. D 3 RE captures the general shape but loses significant detail,
1539 while DRE- ∞ fails to resolve the structures, resulting in a single, diffuse cloud of density.
- 1540 • **Discontinuous and Branching Densities.** The checkerboard dataset presents a particularly
1541 difficult challenge with its discontinuous, grid-like density. OS-DRE successfully recovers
1542 the sharp, alternating high-density squares, a task where both baseline methods fail, produc-
1543 ing heavily smoothed and inaccurate approximations. Similarly, the tree dataset is designed
1544 to assess a model’s capacity to generate sharp, branching topological structures. OS-DRE
1545 excels, yielding crisp, well-defined branches. In contrast, the solver-based methods are
1546 unable to capture these fine details, illustrating a fundamental advantage of our analytic,
1547 one-step approach for modeling distributions with complex, high-frequency features. The
1548 moons dataset further confirms this, with OS-DRE producing significantly sharper and
1549 better-separated modes than the baselines.

1550 **Real-world Tabular Datasets.** We evaluate on five tabular datasets that are standard benchmarks in
1551 density estimation: POWER, GAS, HEPMASS, MINIBOONE, and BSDS300. These datasets pose
1552 challenging, non-Gaussian structures with unknown generative processes and complex correlations,
1553 making them suitable for testing model expressiveness. We follow the preprocessing and data
1554 splits of Papamakarios et al. (2017); Grathwohl et al. (2019) for a fair comparison. All baseline
1555 methods were evaluated using a quadrature scheme with varying numbers of function evaluations
1556 ($\text{NFE} = \{2, 5, 10, 50\}$). Our method, OS-DRE, was evaluated with a fixed $\text{NFE} = 1$. In this
1557 experiment, K is set to 400. We use joint score matching loss with learning rate 0.01. The weighting
1558 function is set to $\lambda(t) = t(1 - t)$.

1559 The full quantitative results are presented in Tab. 1. The results clearly demonstrate the superiority of
1560 OS-DRE. Across all five datasets, OS-DRE with an appropriate RBF kernel achieves a significantly
1561 lower (better) NLL than both DRE- ∞ and D 3 RE, regardless of the NFE allocated to the baselines.

1562 An interesting observation is the instability of the baseline methods. Their performance does not
1563 consistently improve with an increased NFE. For example, on MINIBOONE, the performance of
1564 DRE- ∞ is better at $\text{NFE} = 10$ than at $\text{NFE} = 50$. This highlights the inherent difficulty and potential
1565 instability of relying on numerical quadrature for complex, high-dimensional score functions. In
1566 contrast, OS-DRE’s analytic, one-step computation is deterministic and robust.

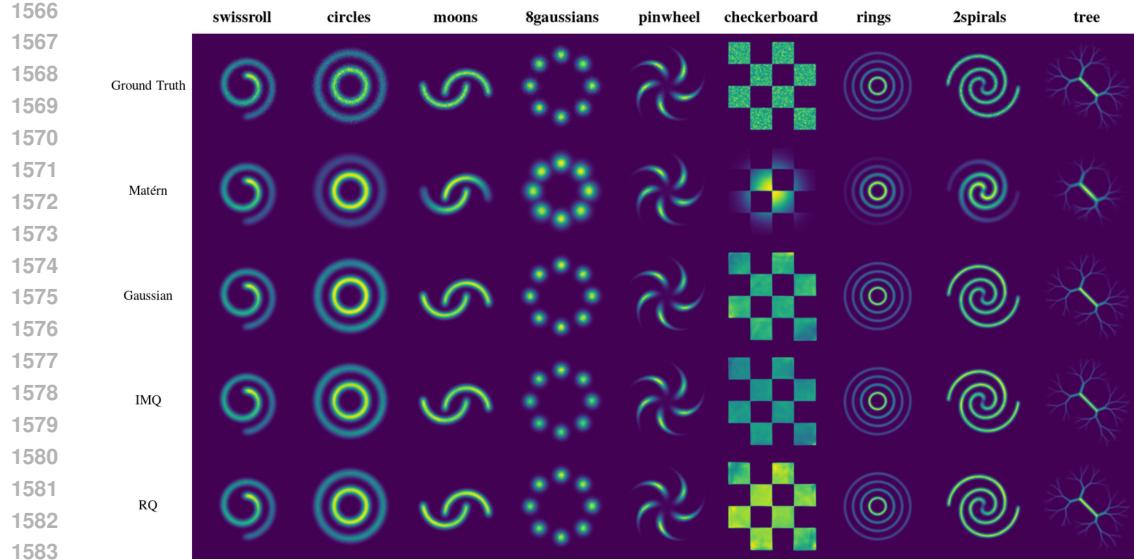


Figure 6: Ablation study on the choice of RBF kernel for structured and multimodal datasets.

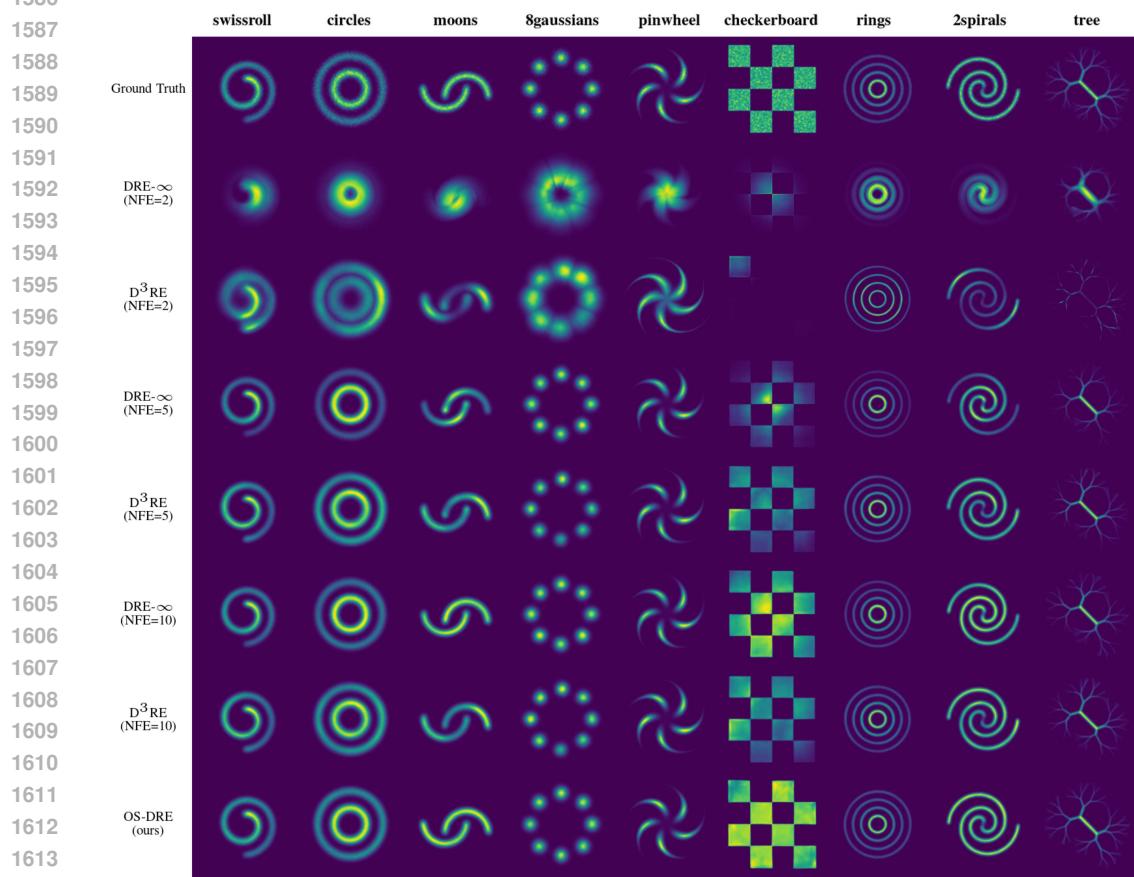


Figure 7: Comparison of density estimates using three score-based DRE methods on nine datasets.

1618
1619 Finally, we observe a clear performance difference among the RBF kernels within OS-DRE. While all kernels outperform the baselines, the IMQ and RQ kernels consistently deliver the best or near-best performance. The Gaussian kernel is also a strong performer, particularly on GAS and BSDS300.

1620 This confirms the importance of the kernel choice as a key hyperparameter, as discussed in our
 1621 theoretical analysis, with the heavier-tailed IMQ and RQ kernels often providing the best inductive
 1622 bias for these complex, real-world data distributions.
 1623

1624 **Energy-based modeling on MNIST.** We applied our OS-DRE framework for density estimation
 1625 on the MNIST dataset, leveraging pre-trained energy-based models (EBMs) as the target density
 1626 $p_1(\mathbf{x})$. We specifically use the setup described in Chen et al. (2025) and replicate the results for
 1627 DRE- ∞ and D 3 RE for a direct comparison. Let $p_1(\mathbf{x})$ denote the MNIST data distribution, and
 1628 $p_0(\mathbf{x}) = \mathcal{N}(\mathbf{0}, \mathbf{I}_d)$ be the simple Gaussian noise distribution. We applied an variance-preserving
 1629 interpolant (Song et al., 2021; Choi et al., 2022) of the form $\mathbf{x}_t = a_t \mathbf{x}_0 + b_t \text{EBM}(\mathbf{x}_1) + \sqrt{t(1-t)\gamma^2} \mathbf{z}$,
 1630 where $\mathbf{x}_0 \sim p_0(\mathbf{x})$, $\mathbf{x}_1 \sim p_1(\mathbf{x})$, $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_d)$, $a_t = \exp\{-0.25(b_{\max} - b_{\min})t^2 - 0.5b_{\min}t\}$ and
 1631 $b_t = \sqrt{1 - a_t^2}$. b_{\min} and b_{\max} are set to 0.1 and 20, respectively. We employ the joint score matching
 1632 objective and set $\gamma^2 = 2$, consistent with the framework used in Chen et al. (2025). We use IMQ
 1633 kernel.

1634 A specific advantage of OS-DRE is its one-step evaluation of the log-density ratio $\log \hat{r}(\mathbf{x}) =$
 1635 $\sum_{k=1}^K h_k^\theta(\mathbf{x}) \bar{g}_k$. We exploit this speed to introduce an additional regularization term during training.
 1636 This term minimizes the NLL of the MNIST datasets:

$$1637 \mathcal{L}_{\text{NLL-reg}}(\theta) = -\frac{1}{2 \ln 2} \mathbb{E}_{p_1(\mathbf{x})} [\log \hat{r}(\text{EBM}(\mathbf{x})) + \log p_0(\text{EBM}(\mathbf{x}))]. \quad (52)$$

1638 This regularization helps align the OS-DRE prediction directly with the desired log-density, which
 1639 we find beneficial for high-dimensional, complex data.
 1640

1642 C.4 EXPERIMENTAL SETTINGS AND RESULTS FOR f -DIVERGENCE ESTIMATION

1644 **Continual Learning.** To demonstrate the applicability of OS-DRE to online settings, such as
 1645 real-time change point detection, we evaluate its ability to track dynamically evolving distributions.
 1646 In this continual learning setup, the target distribution p_t shifts over discrete timesteps, creating a
 1647 challenging environment that requires the model to continuously adapt to and quantify the change
 1648 from a fixed source distribution p_0 . We measure this ability by estimating the KL-divergence between
 1649 p_0 and the evolving target p_t at each step. The following complex benchmarks are used.

- 1650 • **Linearly Drifting Gaussian.** This benchmark simulates a gradual, linear drift in both
 1651 the mean and covariance of a Gaussian distribution, testing the model’s ability to track a
 1652 smoothly evolving target. The source distribution is a standard d -dimensional Gaussian,
 1653 $p_0(\mathbf{x}) = \mathcal{N}(\mathbf{0}, \mathbf{I}_d)$. At each discrete step s , the target distribution p_t is defined as $p_t(\mathbf{x}) =$
 1654 $\mathcal{N}(\boldsymbol{\mu}_s, \boldsymbol{\Sigma}_s)$, where the parameters evolve linearly:

$$1655 \boldsymbol{\mu}_s = s \cdot \Delta \boldsymbol{\mu}, \quad \boldsymbol{\Sigma}_s = (1 - s \cdot \Delta \sigma) \mathbf{I}_d, \quad (53)$$

1656 with small, constant drift rates $\Delta \boldsymbol{\mu}$ and $\Delta \sigma$.

- 1658 • **Progressive Noise Corruption.** Inspired by the Gaussian noise corruption in the CIFAR-
 1659 10-C benchmark (Hendrycks & Dietterich, 2019), this task evaluates the model’s response
 1660 to a progressive increase in isotropic variance, simulating a common type of data corruption.
 1661 The source distribution is $p_0(\mathbf{x}) = \mathcal{N}(\mathbf{0}, \mathbf{I}_d)$. At each step s , the target distribution is a
 1662 zero-mean Gaussian with a linearly increasing covariance $p_t(\mathbf{x}) = \mathcal{N}(\mathbf{0}, \sigma_s^2 \mathbf{I}_d)$, where
 1663 $\sigma_s^2 = 1 + s \cdot \Delta \sigma^2$, with $\Delta \sigma^2$ being a constant factor determining the rate of variance
 1664 inflation.

- 1665 • **Controlled Divergence Shift.** We follow the setup in Zhang et al. (2023) to derive this
 1666 benchmark. This setup provides a stringent test of the model’s ability to track a distribution
 1667 whose mean shifts in a random direction at each step, while the KL divergence between
 1668 the current and initial distribution is precisely controlled. The source distribution is again
 1669 $p_0(\mathbf{x}) = \mathcal{N}(\mathbf{0}, \mathbf{I}_d)$. At each step s , the target distribution $p_t(\mathbf{x}) = \mathcal{N}(\boldsymbol{\mu}_s, \mathbf{I}_d)$ is defined
 1670 such that the KL divergence $\text{KL}(p_t \| p_0) = s$. Since the KL divergence for two Gaussians
 1671 with identity covariance is $0.5 \|\boldsymbol{\mu}_s\|^2$, the mean vector $\boldsymbol{\mu}_s$ is constructed to satisfy $\|\boldsymbol{\mu}_s\| =$
 1672 $\sqrt{2s}$, with its direction chosen uniformly at random on the unit hypersphere at each step.

1673 The full results are presented in Fig. 3. The plots clearly show the superior stability and responsiveness
 1674 of OS-DRE across all three dynamic scenarios.

- On the **Linearly Drifting Gaussian** benchmark (Fig. 3a), OS-DRE, particularly with the IMQ and RQ kernels, provides a smooth and low-variance estimate that closely follows the ground-truth KL divergence. In contrast, DRE- ∞ shows a significant underestimation bias, while D³RE’s estimates are plagued by extremely high variance, making them unreliable.
- The **Progressive Noise Corruption** task (Fig. 3b) presents a more challenging, accelerating shift. OS-DRE again provides stable estimates that follow the general trend of the ground truth. The baseline methods fail dramatically in this setting, with their estimates exhibiting massive variance and becoming completely decorrelated from the ground truth as the corruption intensifies.
- In the **Controlled Divergence Shift** experiment (Fig. 3c), the KL divergence increases in discrete steps. OS-DRE demonstrates excellent responsiveness. Its estimates are sharp and quickly adapt to the new ground truth level after each change point, with very low variance. The baselines, especially D³RE, are characterized by such high variance that they are unable to reliably detect these discrete changes.

These results collectively highlight the key advantage of our analytic, solver-free approach in continual learning settings. By avoiding the iterative computations that can accumulate error and lead to instability, OS-DRE provides a real-time, robust, and reliable tool for tracking distributional changes.

Mutual Information Estimation. Mutual information (MI) measures the dependency between two random variables $\mathbf{x} \sim p(\mathbf{x})$ and $\mathbf{y} \sim q(\mathbf{y})$, quantifying how much information one variable contains about the other. The MI between \mathbf{x} and \mathbf{y} is defined as $\text{MI}(\mathbf{x}, \mathbf{y}) = \mathbb{E}_{p(\mathbf{x}, \mathbf{y})} \left[\log \frac{p(\mathbf{x}, \mathbf{y})}{p(\mathbf{x})q(\mathbf{y})} \right]$, which we approximate using DRE.

BEYOND NORMAL: GEOMETRICALLY PATHOLOGICAL DISTRIBUTIONS. We evaluate the performance of OS-DRE and baseline methods on four mutual information (MI) estimation tasks involving geometrically challenging distributions, inspired by the benchmark suite from Czyż et al. (2023). The parameter ρ controls the strength of the dependency between the two random variables. The four benchmarks are detailed below:

- **Half-Cube Map.** This task tests robustness to heavy-tailed data. Correlated Gaussian variables (\mathbf{x}, \mathbf{y}) are transformed by the homeomorphism $\mathbf{x}' = \text{sign}(\mathbf{x})|\mathbf{x}|^{3/2}$ and $\mathbf{y}' = \text{sign}(\mathbf{y})|\mathbf{y}|^{3/2}$. While this preserves the true MI, $I(\mathbf{x}'; \mathbf{y}') = I(\mathbf{x}; \mathbf{y})$, it creates distributions with significantly heavier tails that challenge methods relying on local density assumptions.
- **Asinh Mapping.** Designed to test performance on distributions with highly concentrated densities, this task applies the inverse hyperbolic sine transformation, $\text{asinh}(z) = \log(z + \sqrt{z^2 + 1})$, to two independent Gaussian variables. This creates sharp peaks and regions of high curvature that can cause numerical instability in many estimators.
- **Additive Noise.** This scenario evaluates performance on distributions with sharp, non-differentiable boundaries. We define $\mathbf{y} = \mathbf{x} + \mathbf{n}$, where $\mathbf{x} \sim \mathcal{U}(0, 1)$ and $\mathbf{n} \sim \mathcal{U}(-\epsilon, \epsilon)$ are independent. The resulting joint distribution has a fragmented, piecewise-constant support that violates the smoothness assumptions of many score-based methods. The true MI is $I(\mathbf{x}; \mathbf{y}) = \log(2\epsilon) + 0.5$ for $\epsilon \leq 0.5$.
- **Gamma-Exponential.** This task features a complex, non-linear, and asymmetric dependency. One variable is drawn from a Gamma distribution, $\mathbf{x} \sim \text{Gamma}(\rho, 1)$, and its value is then used as the rate parameter for an Exponential distribution from which the second variable is drawn: $\mathbf{y} \mid \mathbf{x} = x \sim \text{Exponential}(x)$. The true mutual information is $I(\mathbf{x}; \mathbf{y}) = \psi(\rho + 1) - \log(\rho)$, where ψ is the digamma function.

The full results are presented in Tab. 6. OS-DRE demonstrates a clear advantage across all four challenging scenarios. On the **Half-Cube** and **Asinh mapping** tasks, OS-DRE, particularly with the Gaussian and Matérn kernels, achieves an MSE that is orders of magnitude lower than the baselines across nearly all correlation levels. This indicates that our analytic basis is better equipped to handle the heavy tails and high-curvature densities introduced by these transformations. In the **Additive Noise** scenario, which features sharp discontinuities, the IMQ kernel shows remarkable stability, consistently outperforming the baselines. This suggests that the global nature of the IMQ basis

functions provides a more robust representation for distributions with non-differentiable boundaries. Finally, the **Gamma-Exponential** task highlights the flexibility of our approach. The Matérn kernel, which has limited smoothness, provides the most accurate estimates, significantly outperforming the baselines, especially in the high-dependency regime ($\rho > 1.2$). This demonstrates the benefit of being able to select a kernel whose inductive bias (in this case, limited smoothness) matches the complex dependency structure of the data.

Table 6: MSE results for MI estimation on four geometrically pathological datasets. The top row of each sub-table indicates the varying correlation coefficient ρ . Our OS-DRE method demonstrates consistently superior or competitive performance across the wide range of challenging data geometries.

(a) MSE results for the Half-Cube Map dataset.

| Method | RBF Kernel | -0.9 | -0.8 | -0.7 | -0.6 | -0.5 | -0.4 | -0.3 | -0.2 | -0.1 | 0.0 | 0.1 | 0.2 | 0.3 | 0.4 | 0.5 | 0.6 | 0.7 | 0.8 | 0.9 |
|-------------------|------------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| DRE- ∞ | - | 0.0054 | 0.0029 | 0.0037 | 0.0023 | 0.0015 | 0.0021 | 0.0013 | 0.0010 | 0.0014 | 0.0015 | 0.0022 | 0.0015 | 0.0027 | 0.0032 | 0.0029 | 0.0030 | 0.0037 | 0.0056 | |
| D ³ RE | - | 0.0014 | 0.0006 | 0.0005 | 0.0003 | 0.0003 | 0.0004 | 0.0003 | 0.0003 | 0.0004 | 0.0009 | 0.0012 | 0.0006 | 0.0005 | 0.0004 | 0.0006 | 0.0008 | 0.0012 | | |
| OS-DRE (ours) | Matérn | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| OS-DRE (ours) | Gaussian | 0.0002 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | |
| OS-DRE (ours) | IMQ | 0.0001 | 0.0001 | 0.0001 | 0.0002 | 0.0001 | 0.0001 | 0.0001 | 0.0001 | 0.0001 | 0.0002 | 0.0001 | 0.0001 | 0.0001 | 0.0001 | 0.0002 | 0.0002 | 0.0001 | 0.0001 | 0.0002 |
| OS-DRE (ours) | RQ | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |

(b) MSE results for the Asinh Mapping dataset.

| Method | RBF Kernel | -0.9 | -0.8 | -0.7 | -0.6 | -0.5 | -0.4 | -0.3 | -0.2 | -0.1 | 0.0 | 0.1 | 0.2 | 0.3 | 0.4 | 0.5 | 0.6 | 0.7 | 0.8 | 0.9 |
|-------------------|------------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|-----|
| DRE- ∞ | - | 0.0005 | 0.0006 | 0.0005 | 0.0006 | 0.0005 | 0.0004 | 0.0004 | 0.0004 | 0.0002 | 0.0003 | 0.0005 | 0.0006 | 0.0007 | 0.0006 | 0.0006 | 0.0006 | 0.0007 | 0.0005 | |
| D ³ RE | - | 0.0014 | 0.0010 | 0.0006 | 0.0005 | 0.0003 | 0.0003 | 0.0003 | 0.0003 | 0.0003 | 0.0004 | 0.0004 | 0.0004 | 0.0005 | 0.0005 | 0.0005 | 0.0005 | 0.0011 | 0.0014 | |
| OS-DRE (ours) | Matérn | 0.0004 | 0.0001 | 0.0001 | 0.0001 | 0.0001 | 0.0001 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0001 | 0.0001 | 0.0001 | 0.0001 | 0.0001 | 0.0004 | |
| OS-DRE (ours) | Gaussian | 0.0002 | 0.0001 | 0.0001 | 0.0001 | 0.0001 | 0.0001 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0001 | 0.0001 | 0.0001 | 0.0001 | 0.0001 | 0.0001 | 0.0001 | 0.0002 | |
| OS-DRE (ours) | IMQ | 0.0002 | 0.0002 | 0.0002 | 0.0002 | 0.0002 | 0.0002 | 0.0002 | 0.0002 | 0.0002 | 0.0002 | 0.0002 | 0.0002 | 0.0003 | 0.0003 | 0.0003 | 0.0003 | 0.0003 | 0.0004 | |
| OS-DRE (ours) | RQ | 0.0002 | 0.0002 | 0.0001 | 0.0001 | 0.0001 | 0.0001 | 0.0001 | 0.0001 | 0.0001 | 0.0002 | 0.0002 | 0.0002 | 0.0002 | 0.0002 | 0.0002 | 0.0002 | 0.0002 | 0.0003 | |

(c) MSE results for the Additive Noise dataset.

| Method | RBF Kernel | 0.1 | 0.2 | 0.3 | 0.4 | 0.5 | 0.6 | 0.7 | 0.8 | 0.9 |
|-------------------|------------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| DRE- ∞ | - | 0.0029 | 0.0018 | 0.0015 | 0.0012 | 0.0013 | 0.0013 | 0.0011 | 0.0011 | 0.0000 |
| D ³ RE | - | 0.0108 | 0.0077 | 0.0065 | 0.0071 | 0.0085 | 0.0076 | 0.0064 | 0.0045 | 0.0055 |
| OS-DRE (ours) | Matérn | 0.0061 | 0.0029 | 0.0017 | 0.0015 | 0.0015 | 0.0013 | 0.0011 | 0.0009 | 0.0008 |
| OS-DRE (ours) | Gaussian | 0.0016 | 0.0015 | 0.0016 | 0.0011 | 0.0015 | 0.0014 | 0.0012 | 0.0010 | 0.0010 |
| OS-DRE (ours) | IMQ | 0.0010 | 0.0010 | 0.0010 | 0.0012 | 0.0009 | 0.0008 | 0.0007 | 0.0009 | 0.0007 |
| OS-DRE (ours) | RQ | 0.0019 | 0.0015 | 0.0015 | 0.0012 | 0.0010 | 0.0010 | 0.0010 | 0.0010 | 0.0009 |

(d) MSE results for the Gamma-Exponential dataset.

| Method | RBF Kernel | 1.0 | 1.1 | 1.2 | 1.3 | 1.4 | 1.5 | 1.6 | 1.7 | 1.8 |
|-------------------|------------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| DRE- ∞ | - | 2.1328 | 0.8939 | 0.0725 | 0.0115 | 0.0213 | 0.0051 | 0.0114 | 0.0069 | 0.0051 |
| D ³ RE | - | 0.1919 | 0.1018 | 0.0154 | 0.0119 | 0.0063 | 0.0110 | 0.0050 | 0.0125 | 0.0114 |
| OS-DRE (ours) | Matérn | 0.1768 | 0.0315 | 0.0035 | 0.0026 | 0.0008 | 0.0017 | 0.0009 | 0.0006 | 0.0005 |
| OS-DRE (ours) | Gaussian | 0.2933 | 0.0503 | 0.0060 | 0.0028 | 0.0032 | 0.0014 | 0.0014 | 0.0007 | 0.0009 |
| OS-DRE (ours) | IMQ | 0.2821 | 0.1185 | 0.0901 | 0.0492 | 0.0200 | 0.0275 | 0.0072 | 0.0080 | 0.0087 |
| OS-DRE (ours) | RQ | 0.5182 | 0.0925 | 0.0330 | 0.0109 | 0.0052 | 0.0040 | 0.0015 | 0.0012 | |

We also compare OS-DRE with KSG (Kraskov et al., 2004), MINE (Belghazi et al., 2018) and InfoNet (Hu et al., 2024), as illustrated in Fig. 8. Here, Gauss denotes 2-D complex Gaussian distributions, where $q(\mathbf{y}) = \mathcal{N}(\mathbf{0}, \Sigma)$ and $p(\mathbf{x}) = \mathcal{N}(\mathbf{0}, I_d)$, with $\Sigma = [[1, \rho], [\rho, 1]]$ and ρ varying in $[-0.9, 0.9]$. OS-DRE yields MI estimates that closely match the ground truth (with lower mean absolute error (MAE) values), demonstrating high accuracy in Gaussian scenarios.

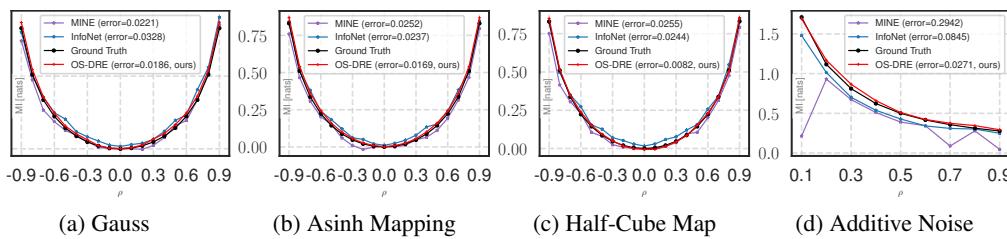


Figure 8: Comparison of MI estimates under four complex settings proposed in (Hu et al., 2024) (mean absolute error (MAE) included). OS-DRE consistently outperforms existing methods across all settings, providing estimates that are both accurate and robust. These results highlight the superiority of OS-DRE in estimating MI under challenging, nontrivial distributions.

HIGH-DISCREPANCY & HIGH-DIMENSIONAL DISTRIBUTIONS. To systematically evaluate model robustness as the density-chasm problem becomes progressively more severe, we designed an

1782 experiment for MI estimation between two high-dimensional Gaussian distributions. We define
 1783 the two distributions as $p_0(\mathbf{x}) = \mathcal{N}(\mathbf{0}, \mathbf{I}_d)$ and $p_1(\mathbf{x}) = \mathcal{N}(\mathbf{0}, \Sigma)$. The covariance matrix Σ is
 1784 constructed to be block-diagonal, where each 2×2 block along the diagonal is given by $\Lambda = \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix}$,
 1785 with $\rho = 0.5$. This structure creates strong pairwise correlations, leading to a highly ill-conditioned
 1786 covariance matrix, a known challenge for score-based DRE methods (Choi et al., 2022). The
 1787 experiments are conducted across several dimensions, $d \in \{40, 80, 120, 160\}$, which correspond
 1788 to true MI values of approximately $\{10, 20, 30, 40\}$ nats, respectively. We report the estimated MI
 1789 (mean \pm std over 3 seeds) and the Mean Squared Error (MSE).

1790 The full results are presented in Tab. 7. The data clearly illustrates the limitations of iterative, solver-
 1791 based methods in high-discrepancy scenarios. At low NFE (e.g., NFE= 2), both DRE- ∞ and D³RE
 1792 fail completely, severely underestimating the true MI. Even with a large computational budget of
 1793 NFE= 50, DRE- ∞ provides reasonable estimates, but D³RE remains unstable, collapsing entirely at
 1794 the highest discrepancy level (MI= 40).

1795 In stark contrast, our one-step OS-DRE demonstrates remarkable robustness. The choice of kernel
 1796 is critical. The Matérn kernel, which has limited smoothness, struggles as the dimensionality
 1797 and discrepancy increase, as predicted by theory. However, the infinitely smooth kernels deliver
 1798 exceptional performance. The Gaussian kernel provides the most accurate estimates for MI levels of
 1799 10, 20, and 30 nats, achieving an MSE that is competitive with or better than the best-performing
 1800 baseline (DRE- ∞ at NFE= 50), but with only a single function evaluation. At the most extreme
 1801 setting of MI= 40, the IMQ kernel proves to be the most robust, delivering the lowest MSE by a
 1802 significant margin. This highlights the key advantage of our analytic framework: by avoiding the
 1803 accumulation of numerical errors inherent in iterative solvers, OS-DRE can successfully navigate the
 1804 density chasm and provide stable, accurate estimates in a single step.

1805 Table 7: Mutual information estimation under high-discrepancy settings (MI $\in \{10, 20, 30, 40\}$ nats).
 1806 We report the estimated mutual information (mean \pm std) and MSE across different RBF kernels. All
 1807 timing results were obtained on a single NVIDIA TITAN X GPU. **Bolded** MSE values indicate the
 1808 best performance for each setting. The best wall-clock time is underlined.
 1809

| Method | NFE | RBF Kernel | MI = 10 | | | MI = 20 | | | MI = 30 | | | MI = 40 | | |
|-------------------|-----|------------|------------------|-------------|--------------|------------------|-------------|--------------|------------------|-------------|--------------|------------------|-------------|--------------|
| | | | Est. MI | MSE | Time (s) |
| DRE- ∞ | 2 | - | 1.40 \pm 0.01 | 73.91 | 0.045 | 3.16 \pm 0.01 | 283.52 | 0.045 | 5.21 \pm 0.01 | 614.62 | 0.045 | 5.13 \pm 0.02 | 1215.69 | 0.046 |
| D ³ RE | 2 | - | 11.61 \pm 0.08 | 2.58 | 0.048 | 21.91 \pm 0.08 | 3.65 | 0.047 | 27.51 \pm 0.07 | 6.21 | 0.046 | 17.64 \pm 0.17 | 500.04 | 0.044 |
| DRE- ∞ | 5 | - | 8.31 \pm 0.05 | 2.86 | 0.055 | 17.34 \pm 0.04 | 7.09 | 0.060 | 24.97 \pm 0.05 | 25.29 | 0.068 | 31.61 \pm 0.06 | 70.36 | 0.057 |
| D ³ RE | 5 | - | 9.91 \pm 0.04 | 0.01 | 0.056 | 19.46 \pm 0.04 | 0.29 | 0.061 | 27.26 \pm 0.03 | 7.50 | 0.058 | 31.24 \pm 0.05 | 76.80 | 0.058 |
| DRE- ∞ | 10 | - | 9.48 \pm 0.06 | 0.27 | 0.075 | 19.27 \pm 0.04 | 0.54 | 0.100 | 28.37 \pm 0.05 | 2.66 | 0.085 | 37.34 \pm 0.06 | 7.08 | 0.083 |
| D ³ RE | 10 | - | 10.13 \pm 0.04 | 0.02 | 0.075 | 20.45 \pm 0.03 | 0.21 | 0.094 | 27.22 \pm 0.03 | 7.72 | 0.076 | 32.27 \pm 0.04 | 59.70 | 0.080 |
| DRE- ∞ | 50 | - | 9.84 \pm 0.06 | 0.03 | 0.226 | 19.81 \pm 0.04 | 0.04 | 0.249 | 29.31 \pm 0.06 | 0.48 | 0.228 | 38.06 \pm 0.07 | 3.77 | 0.271 |
| D ³ RE | 50 | - | 10.07 \pm 0.04 | 0.01 | 0.234 | 20.30 \pm 0.03 | 0.09 | 0.256 | 27.01 \pm 0.03 | 8.94 | 0.256 | 32.37 \pm 0.04 | 58.19 | 0.260 |
| DRE- ∞ | 100 | - | 9.87 \pm 0.06 | 0.02 | 0.475 | 19.89 \pm 0.04 | 0.01 | 0.493 | 29.30 \pm 0.06 | 0.50 | 0.478 | 38.18 \pm 0.07 | 3.31 | 0.554 |
| D ³ RE | 100 | - | 10.01 \pm 0.04 | 0.00 | 0.498 | 20.29 \pm 0.03 | 0.08 | 0.546 | 27.00 \pm 0.03 | 9.00 | 0.487 | 32.37 \pm 0.04 | 58.20 | 0.514 |
| DRE- ∞ | 200 | - | 9.86 \pm 0.06 | 0.02 | 0.819 | 19.89 \pm 0.04 | 0.01 | 0.954 | 29.29 \pm 0.06 | 0.50 | 0.879 | 38.18 \pm 0.07 | 3.31 | 0.956 |
| D ³ RE | 200 | - | 10.04 \pm 0.04 | 0.00 | 0.816 | 20.23 \pm 0.03 | 0.05 | 0.922 | 26.94 \pm 0.03 | 9.36 | 0.907 | 32.43 \pm 0.04 | 57.28 | 0.955 |
| OS-DRE (ours) | 1 | Matérn | 10.31 \pm 0.02 | 0.09 | 0.024 | 15.73 \pm 0.05 | 18.30 | 0.028 | 15.55 \pm 0.02 | 208.98 | 0.032 | 18.65 \pm 0.15 | 456.11 | 0.028 |
| OS-DRE (ours) | 1 | Gaussian | 10.05 \pm 0.04 | 0.01 | 0.025 | 20.03 \pm 0.04 | 0.00 | 0.027 | 29.37 \pm 0.07 | 0.07 | 0.013 | 38.68 \pm 0.09 | 2.30 | 0.014 |
| OS-DRE (ours) | 1 | IMQ | 10.37 \pm 0.02 | 0.11 | 0.035 | 21.25 \pm 0.04 | 1.56 | 0.030 | 28.10 \pm 0.08 | 5.86 | 0.029 | 39.35 \pm 0.09 | 0.47 | 0.028 |
| OS-DRE (ours) | 1 | RQ | 9.89 \pm 0.03 | 0.03 | <u>0.022</u> | 19.49 \pm 0.04 | 0.83 | <u>0.012</u> | 28.94 \pm 0.10 | 1.52 | <u>0.012</u> | 38.92 \pm 0.07 | 1.41 | 0.019 |

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Table 8: Accuracy-efficiency trade-off on tabular datasets. Accuracy is measured by NLL, and
 1841 efficiency is measured by NFE. Lower is better. Each method is evaluated at different NFE settings.
 1842 The best results are highlighted in **bold**. In this table, OS-DRE uses the IMQ kernel. See Fig. 4a for a
 1843 visual comparison of this trade-off.
 1844

| Dataset | Method | NFE = 1 | NFE = 2 | NFE = 5 | NFE = 10 | NFE = 50 |
|-----------|----------------------|--------------------------------------|--------------------|--------------------|--------------------|-------------------|
| POWER | DRE- ∞ | – | 0.05 ± 1.84 | 0.35 ± 0.50 | 0.03 ± 0.17 | 0.25 ± 0.28 |
| | D ³ RE | – | 3.57 ± 1.84 | 1.26 ± 0.38 | 0.49 ± 0.39 | 0.89 ± 0.33 |
| | OS-DRE (ours) | -0.69 ± 0.18 | – | – | – | – |
| GAS | DRE- ∞ | – | -4.37 ± 1.44 | -3.63 ± 0.78 | -4.34 ± 0.60 | -4.33 ± 0.71 |
| | D ³ RE | – | 5.74 ± 15.28 | -1.15 ± 4.20 | -3.27 ± 2.00 | -3.16 ± 0.62 |
| | OS-DRE (ours) | -18.33 ± 0.04 | – | – | – | – |
| HEPMASS | DRE- ∞ | – | 19.30 ± 1.31 | 20.24 ± 0.47 | 20.43 ± 0.52 | 20.67 ± 0.57 |
| | D ³ RE | – | 23.90 ± 0.36 | 21.05 ± 0.52 | 20.30 ± 0.55 | 20.05 ± 0.35 |
| | OS-DRE (ours) | 17.45 ± 0.05 | – | – | – | – |
| MINIBOONE | DRE- ∞ | – | 41.55 ± 2.07 | 20.90 ± 0.84 | 20.57 ± 0.93 | 20.97 ± 0.51 |
| | D ³ RE | – | 55.83 ± 9.36 | 43.11 ± 26.20 | 42.65 ± 26.87 | 42.73 ± 26.78 |
| | OS-DRE (ours) | 9.97 ± 0.37 | – | – | – | – |
| BSDS300 | DRE- ∞ | – | -130.68 ± 4.17 | -83.70 ± 1.35 | -87.65 ± 2.24 | -90.24 ± 2.14 |
| | D ³ RE | – | -149.53 ± 9.06 | -101.97 ± 1.67 | -102.01 ± 2.43 | -78.26 ± 0.96 |
| | OS-DRE (ours) | -217.99 ± 3.39 | – | – | – | – |

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Table 9: Accuracy-efficiency trade-off in MI estimation. Accuracy is measured by MSE, and
 1869 efficiency is measured by NFE (NFE = $\in \{1, 2, 5, 10, 50, 100, 200\}$). Lower is better. Results are
 1870 shown across different MI settings (MI $\in \{10, 20, 30, 40\}$). The best results are highlighted in **bold**.
 1871 OS-DRE uses the Gaussian RBF kernel. See Fig. 4b for a visual comparison of this trade-off.
 1872

| MI Setting | Method | 1 | 2 | 5 | 10 | 50 | 100 | 200 |
|------------|----------------------|-------------|---------|-------|-------|-------|-------------|-------------|
| MI = 10 | DRE- ∞ | – | 73.91 | 2.86 | 0.27 | 0.03 | 0.02 | 0.02 |
| | D ³ RE | – | 2.58 | 0.01 | 0.02 | 0.01 | 0.00 | 0.00 |
| | OS-DRE (ours) | 0.01 | – | – | – | – | – | – |
| MI = 20 | DRE- ∞ | – | 283.52 | 7.09 | 0.54 | 0.04 | 0.01 | 0.01 |
| | D ³ RE | – | 3.65 | 0.29 | 0.21 | 0.09 | 0.08 | 0.05 |
| | OS-DRE (ours) | 0.00 | – | – | – | – | – | – |
| MI = 30 | DRE- ∞ | – | 614.62 | 25.29 | 2.66 | 0.48 | 0.50 | 0.50 |
| | D ³ RE | – | 6.21 | 7.50 | 7.72 | 8.94 | 9.00 | 9.00 |
| | OS-DRE (ours) | 0.07 | – | – | – | – | – | – |
| MI = 40 | DRE- ∞ | – | 1215.69 | 70.36 | 7.08 | 3.77 | 3.31 | 3.31 |
| | D ³ RE | – | 500.04 | 76.80 | 59.70 | 58.19 | 58.20 | 57.28 |
| | OS-DRE (ours) | 2.30 | – | – | – | – | – | – |