Nonparametric Score Estimators

Yuhao Zhou  Jiaxin Shi  Jun Zhu

Abstract
Estimating the score, i.e., the gradient of log density function, from a set of samples generated by an unknown distribution is a fundamental task in inference and learning of probabilistic models that involve flexible yet intractable densities. Kernel estimators based on Stein’s methods or score matching have shown promise, however their theoretical properties and relationships have not been fully-understood. We provide a unifying view of these estimators under the framework of regularized nonparametric regression. It allows us to analyse existing estimators and construct new ones with desirable properties by choosing different hypothesis spaces and regularizers. A unified convergence analysis is provided for such estimators. Finally, we propose score estimators based on iterative regularization that enjoy computational benefits from curl-free kernels and fast convergence.

1. Introduction
Intractability of density functions has long been a central challenge in probabilistic learning. This may arise from various situations such as training implicit models like GANs (Goodfellow et al., 2014), or marginalizing over a non-conjugate hierarchical model, e.g., evaluating the output density of stochastic neural networks (Sun et al., 2019). In these situations, inference and learning often require evaluating such intractable densities or optimizing an objective that involves them.

Among various solutions, one important family of methods are based on score estimation, which rely on a key step of estimating the score, i.e., the derivative of the log density \( \nabla_x \log p(x) \) from a set of samples drawn from some unknown probability density \( p \). These methods include parametric score matching (Hyvärinen, 2005; Sasaki et al., 2014; Song et al., 2019), its denoising variants as autoencoders (Vincent, 2011), nonparametric score matching (Sriperumbudur et al., 2017; Sutherland et al., 2018), and kernel score estimators based on Stein’s methods (Li & Turner, 2018; Shi et al., 2018). They have been successfully applied to applications such as estimating gradients of mutual information for representation learning (Wen et al., 2020), score-based generative modeling (Song & Ermon, 2019; Saremi & Hyvärinen, 2019), gradient-free adaptive MCMC (Strathmann et al., 2015), learning implicit models (Warde-Farley & Bengio, 2016), and solving intractability in approximate inference algorithms (Sun et al., 2019).

Recently, nonparametric score estimators are growing in popularity, mainly because they are flexible, have well-studied statistical properties, and perform well when samples are very limited. Despite a common goal, they have different motivations and expositions. For example, the work Sriperumbudur et al. (2017) is motivated from the density estimation perspective and the richness of kernel exponential families (Canu & Smola, 2006; Fukumizu, 2009), where the estimator is obtained by score matching. Li & Turner (2018) and Shi et al. (2018) are mainly motivated by Stein’s methods. The solution of Li & Turner (2018) gives the score prediction at sample points by minimizing the kernelized Stein discrepancy (Chwialkowski et al., 2016; Liu et al., 2016) and at an out-of-sample point by adding it to the training data, while the estimator of Shi et al. (2018) is obtained by a spectral analysis in function space.

As these estimators are studied in different contexts, their relationships and theoretical properties are not fully-understood. In this paper, we provide a unifying view of them under the regularized nonparametric regression framework. This framework allows us to construct new estimators with desirable properties, and to justify the consistency and improve the convergence rate of existing estimators. It also allows us to clarify the relationships between these estimators. We show that they differ only in hypothesis spaces and regularization schemes.

Our contributions are both theoretical and algorithmic:

- We provide a unifying perspective of nonparametric score estimators. We show that the major distinction of the KEF estimator (Sriperumbudur et al., 2017) from the other two estimators lies in the use of curl-free kernels, while Li & Turner (2018) and Shi et al. (2018)
We denote by $A$ the RKHS associated to $\sum_2$. Background: a block matrix $K$ under the norm induced by the inner product $\langle \cdot, \cdot \rangle$. The closure of $\{K\}$ is the Hilbert space $\mathcal{H}_K$. We show that the structure of curl-free estimators can further accelerate such algorithms.

Our results suggest favoring curl-free estimators in high dimensions. To address the scalability challenge, we propose iterative score estimators under our framework by adopting the $\nu$-method (Engl et al., 1996) as the regularizer. We show that the structure of curl-free kernels can further accelerate such algorithms. Inspired by the similar idea, we propose a conjugate gradient solver of KEF that is significantly faster than previous approximations.

**Notation**

We always assume $\rho$ is a probability measure with probability density function $p(x)$ supported on $\mathcal{X} \subseteq \mathbb{R}^d$, and $\mathcal{L}^2(\mathcal{X}, \rho; \mathbb{R}^d)$ is the Hilbert space of all square integrable functions $f : \mathcal{X} \rightarrow \mathbb{R}^d$ with inner product $\langle f, g \rangle_{\mathcal{L}^2(\mathcal{X}, \rho; \mathbb{R}^d)} = \mathbb{E}_\rho[f(x)g(x)]$. We denote by $\langle \cdot, \cdot \rangle_{\mathcal{L}^2}$ and $\|\cdot\|_{\mathcal{L}^2}$ the inner product and the norm in $\mathcal{L}^2(\mathcal{X}, \rho; \mathbb{R}^d)$, respectively. We denote $k$ as a scalar-valued kernel, and $\mathcal{K}$ as a matrix-valued kernel $\mathcal{K} : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}^{d \times d}$ satisfying the following conditions: (1) $\mathcal{K}(x, x') = \mathcal{K}(x', x)$ for all $x, x' \in \mathcal{X}$; (2) $\sum_{i,j=1}^d c_i^\top \mathcal{K}(x_i, x_j) c_j \geq 0$ for any $\{x_i\} \subset \mathcal{X}$ and $\{c_i\} \subset \mathbb{R}^d$. We denote a vector-valued reproducing kernel Hilbert space (RKHS) associated to $\mathcal{K}$ by $\mathcal{H}_\mathcal{K}$, which is the closure of $\{\sum_{i=1}^d K(x_i, \cdot)c_i : x_i \in \mathcal{X}, c_i \in \mathbb{R}^d, m \in \mathbb{N}\}$ under the norm induced by the inner product $\langle K(x_i, \cdot)c_i, K(x_j, \cdot)c_j \rangle := c_i^\top \mathcal{K}(x_i, x_j) c_j$. We define $K_\mathcal{K} := \mathcal{K}(\cdot, \cdot)$ and $[\mathcal{M}] := \{1, \ldots, M\}$ for $M \in \mathbb{Z}_+$. For $A_1, \ldots, A_n \in \mathbb{R}^{n \times 1}$, we use $(A_1, \ldots, A_n)$ to represent a block matrix $A \in \mathbb{R}^{n \times n}$ with $A_{(i-1)n+j,k}$ being the $(j, k)$-th component of $A_i$, and we similarly define $[A_1, \ldots, A_n] := (A_1^\top, \ldots, A_n^\top)^\top$.

## 2. Background

In this section, we briefly introduce the nonparametric regression method of learning vector-valued functions (Baladassarre et al., 2012). We also review existing kernel-based approaches to score estimation.

### 2.1. Vector-Valued Learning

Supervised vector-valued learning amounts to learning a vector-valued function $f_\lambda : \mathcal{X} \rightarrow \mathcal{Y}$ from a training set $z = \{(x^m, y^m)\}_{m \in [M]}$, where $\mathcal{X} \subseteq \mathbb{R}^d$, $\mathcal{Y} \subseteq \mathbb{R}^q$. Here we assume the training data is sampled from an unknown distribution $p(x, y)$, which can be decomposed into $p(y|x)p(x)$. A criterion for evaluating such an estimator is the mean squared error (MSE) $\mathcal{E}(f) := \mathbb{E}_{p(x,y)}[\|f(x) - y\|_2^2]$. It is well-known that the conditional expectation $f_\lambda(x) := \mathbb{E}_{\rho(y|x)}[y]$ minimizes $\mathcal{E}$. In practice, we minimize the empirical error $\mathcal{E}_\lambda(f) := \frac{1}{M} \sum_{m=1}^M \|f(x^m) - y^m\|_2^2$ in a certain hypothesis space $\mathcal{F}$. However, the minimization problem is typically ill-posed for large $\mathcal{F}$. Hence, it is convenient to consider the regularized problem:

$$f_{\lambda, \lambda} := \arg \min_{f \in \mathcal{F}} \mathcal{E}_\lambda(f) + \lambda \|f\|^2_{\mathcal{F}},$$

where $\|\cdot\|_{\mathcal{F}}$ is the norm in $\mathcal{F}$. In the vector-valued case, it is typical to consider a vector-valued RKHS $\mathcal{H}_\mathcal{K}$ associated with a matrix-valued kernel $\mathcal{K}$ as the hypothesis space. Then the estimator is $f_{\lambda, \lambda} = \sum_{m=1}^M K_m x^m$ for $K_m \in \mathcal{K}$. The estimator now can be written as $f_{\lambda, \lambda} = \frac{1}{\lambda} M S \lambda x + \lambda I$, the estimator now can be written as $f_{\lambda, \lambda} = \frac{1}{\lambda} M S \lambda x + \lambda I$. In fact, if we consider the data-free limit of (1): $\arg \min_{f \in \mathcal{H}_\mathcal{K}} \mathcal{E}(f) + \lambda \|f\|^2_{\mathcal{H}_\mathcal{K}}$, the minimizer is unique when $\lambda > 0$ and is given by $f := (L_{\mathcal{K}} + \lambda I)^{-1} L_{\mathcal{K}} f_{\lambda, \lambda}$, where $L_{\mathcal{K}} : \mathcal{H}_\mathcal{K} \rightarrow \mathcal{H}_\mathcal{K}$ is the integral operator defined as $L_{\mathcal{K}} f := L_{\mathcal{K}} f(x) dQ(x)$ (Smale & Zhou, 2007). It turns out that $\frac{1}{\lambda} M S \lambda x$ is an empirical estimate of $L_{\mathcal{K}} f$. It can also be shown that $L_{\mathcal{K}} f_{\lambda, \lambda} = \frac{1}{\lambda} M S \lambda x$. Hence, we can write $f_{\lambda, \lambda} = (L_{\mathcal{K}} + \lambda I)^{-1} L_{\mathcal{K}} f_{\lambda, \lambda}$.

As we have mentioned, the role of regularization is to deal with the ill-posedness. Specifically, $L_{\mathcal{K}} f_{\lambda, \lambda}$ is not always invertible as it has finite rank and $\mathcal{H}_\mathcal{K}$ is usually of infinite dimension. Many regularization methods are studied in the context of solving inverse problems (Engl et al., 1996) and statistical learning theory (Bauer et al., 2007). The regularization method we presented in (1) is the famous Tikhonov regularization, which belongs to a class of regularization techniques called spectral regularization (Bauer et al., 2007). Specifically, spectral regularization corresponds to a family of estimators defined as $f_{\lambda, \lambda} := g_\lambda L_{\mathcal{K}} f_{\lambda, \lambda}$.
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where \( g_\lambda : \mathbb{R}^+ \rightarrow \mathbb{R} \) is a regularizer such that \( g_\lambda(\hat{L}_K) \) approximates the inverse of \( L_K \). Note that \( L_K \) can be decomposed into \( \sum \sigma_i (e_i, e_i) \), where \((\sigma_i, e_i)\) is a pair of eigenvalue and eigenfunction, we can define \( g_\lambda(\hat{L}_K) := \sum g_\lambda(\sigma_i) (e_i, e_i) \). The Tikhonov regularization corresponds to \( g_\lambda(\sigma) = (\lambda + \sigma)^{-1} \). There are several different regularizers. For example, the spectral cut-off regularizer is defined by \( g_\lambda(\sigma) = \sigma^{-1} \) for \( \sigma \geq \lambda \) and \( g_\lambda(\sigma) = 0 \) otherwise. We refer the readers to Smale & Zhou (2007); Bauer et al. (2007); Baldassarre et al. (2012) for more details.

2.2. Related Work

We assume \( \log p(x) \) is differentiable, and define the score as \( s_p := \nabla \log p \). By score estimation we aim to estimate \( s_p \) from a set of i.i.d. samples \( \{x_m\}_{m \in [M]} \) drawn from \( p \). There have been many kernel-based score estimators studied in different contexts (Sriperumbudur et al., 2017; Sutherland et al., 2018; Li & Turner, 2018; Shi et al., 2018). Below we give a brief review of them.

Kernel Exponential Family Estimator The kernel exponential family (KEF) (Canu & Smola, 2006; Fukumizu, 2009) was originally proposed as an infinite-dimensional generalization of exponential families. It was shown to be useful in density estimation as it can approximate a broad class of densities arbitrarily well (Sriperumbudur et al., 2017). The KEF is defined as:

\[
P_k := \{p_f(x) = e^{f(x) - A(f)} : f \in \mathcal{H}_k, e^{A(f)} < \infty\},
\]

where \( \mathcal{H}_k \) is a scalar-valued RKHS, and \( A(f) := \log \int_X e^{f(x)} dx \) is the normalizing constant. Since \( A(f) \) is typically intractable, Sriperumbudur et al. (2017) proposed to estimate \( f \) by matching the model score \( \nabla \log p_f \) and the data score \( s_p \), thus the KEF can naturally be used for score estimation (Strathmann et al., 2015). This approach works by minimizing the regularized score matching loss:

\[
\min_{f \in \mathcal{H}_k} J(p||p_f) + \lambda \|f\|^2_{\mathcal{H}_k},
\]

where \( J(p||q) := \mathbb{E}_p \|\nabla \log p - \nabla \log q\|^2_2 \) is the Fisher divergence between \( p \) and \( q \). Integration by parts was used to eliminate \( \nabla \log p \) from \( J(p||q) \) (Hyvärinen, 2005) and the exact form of (2) was given as follows (Sriperumbudur et al., 2017, Theorem 5):

\[
\hat{f}_{p,\lambda} = \sum_{m=1}^M \sum_{j=1}^d \xi_{m+1,-1} dj k(x^m, x^j) - \hat{c} \mathbf{1},
\]

where \( \hat{\xi}(x) \) obtained by solving \( (G + M\mathbf{1}) \mathbf{c} = \mathbf{b} / \lambda \) with \( G_{m+1,-1} dj = \partial_i \partial_j d k(x^m, x^j) \) and \( \mathbf{b} = G_{m+1,-1} \mathbf{1} \). The derivative w.r.t. the \( j \)-th component of the second parameter \( x^j \). This solution suffers from computational drawbacks due to the large linear system of size \( M d \times M d \). Sutherland et al. (2018) proposed to use the Nyström method to accelerate KEF. Instead of minimizing the loss in the whole RKHS, they minimized it in a low dimensional subspace.

Stein Gradient Estimator The Stein gradient estimator proposed by Li & Turner (2018) is based on inverting the following generalized Stein’s identity (Stein, 1981; Gorham & Mackey, 2015)

\[
\mathbb{E}_p[h(x) \nabla \log p(x)^T + \nabla h(x)] = 0,
\]

where \( h : \mathcal{X} \rightarrow \mathbb{R}^d \) is a test function satisfying some regularity conditions. An empirical approximation of the identity is \( \frac{1}{M} \mathbf{H} = \nabla h_i \), where \( \mathbf{H} = (h(x^1), \ldots, h(x^M)) \in \mathbb{R}^{d \times M} \), \( \mathbf{S} = (\nabla \log p(x^1), \ldots, \nabla \log p(x^M)) \in \mathbb{R}^{M \times d} \) and \( \nabla h_i = \frac{1}{M} \sum_{m=1}^M \nabla \log p(x^m)^T h(x^m) \). Li & Turner (2018) proposed to minimize \( \|\nabla h_i + \frac{1}{M} \mathbf{H} \|^2_F + \frac{\nu}{M} \|\mathbf{S}\|^2 \) to estimate \( \mathbf{S} \), where \( \|\cdot\|_F \) denotes the Frobenius norm. The kernel trick \( k(x^i, x^j) := h(x^i)^T h(x^j) \) was then exploited to obtain the estimator. From the above we only have score estimates at the sample points. Li & Turner (2018) proposed a heuristic out-of-sample extension at \( x \) by adding it to \( \{x^m\} \) and recompute the minimizer. Such an approach is expensive and unjustified. It is still unclear whether the estimator is consistent.

Spectral Stein Gradient Estimator The Spectral Stein Gradient Estimator (SSGE) (Shi et al., 2018) was derived by a spectral analysis of the score function. Unlike Li & Turner (2018) it was shown to have convergence guarantees and principled out-of-sample extension. The idea is to expand each component of the score in a scalar-valued function space \( L^2(\mathcal{X}, \rho) \); \( g_i(x) = \sum_{j=1}^J \beta_{ij} \psi_j(x) \), where \( g_i \) is the \( i \)-th component of the score and \( \{\psi_j\} \) are the eigenfunctions of the integral operator \( L_k f := \int_X k(x, \cdot) f(x) d\rho(x) \) associated with a scalar-valued kernel \( k \). By using the Stein’s identity in (4) Shi et al. (2018) showed that \( \beta_{ij} = -\mathbb{E}_p[\partial_i \psi_j(x)] \). The Nyström method (Baker, 1977; Williams & Seeger, 2001) was then used to estimate \( \psi_j \):

\[
\hat{\psi}_j(x) = \frac{\sqrt{M}}{\lambda_j} \sum_{m=1}^M k(x, x^m) w_{jm},
\]

where \( \{x^m\}_{m \in [M]} \) are i.i.d. samples drawn from \( \rho \), \( w_{jm} \) is the \( m \)-th component of the eigenvector that corresponds to its \( j \)-th largest eigenvalue of the kernel matrix constructed from \( \{x^m\}_{m \in [M]} \). The final estimator was obtained by truncating \( g_i \) to \( \sum_{j=1}^J \beta_{ij} \hat{\psi}_j(x) \) and plugging in \( \hat{\psi}_j \). Shi et al. (2018, Theorem 2) provided an error bound of SSGE depending on \( J \) and \( M \). However, the convergence rate is still unknown.
3. Nonparametric Score Estimators

The kernel score estimators discussed in Sec. 2.2 were proposed in different contexts. The KEF estimator is motivated from the density estimation perspective, while Stein and SSGE have no explicit density models. SSGE relies on spectral analysis in the function space, while the other two are derived by minimizing a loss function. Despite sharing a common goal, it is still unclear how these estimators relate to each other. In this section, we present a unifying framework of score estimation using regularized vector-valued regression. We show that existing kernel score estimators are special cases under the framework, which allows us to thoroughly investigate their strengths and weaknesses.

3.1. A Unifying Framework

As introduced in Sec. 2.2, the goal is to estimate the score \( s_p \) from a set of i.i.d. samples \( \{x^m\}_{m \in [M]} \) drawn from \( \rho \). We first consider the ideal case where we have the ground truth values of \( s_p \) at the sample locations. Then we can estimate \( s_p \) with vector-valued regression as described in Sec. 2.1:

\[
\hat{s}_{p,\lambda} = \arg \min_{s \in \mathcal{H}_K} \frac{1}{M} \sum_{m=1}^{M} \| s(x^m) - s_p(x^m) \|^2 + \frac{\lambda}{2} \| s \|^2_{\mathcal{H}_K}.
\]

The solution is given by \( \hat{s}_{p,\lambda} = (\hat{L}_K + \lambda I)^{-1} \hat{L}_K s_p \).

We could replace the Tikhonov regularizer with other spectral regularization, for which the general solution is

\[
\hat{s}^g_{p,\lambda} := g_{\lambda}(\hat{L}_K) \hat{L}_K s_p.
\]

In reality, the values of \( s_p \) at \( x^{1:M} \) are unknown and we cannot compute \( \hat{L}_K s_p \) as \( \frac{1}{M} \sum_{m=1}^{M} \mathcal{K}_x s_p(x^m) \). Fortunately, we could exploit integration by parts to avoid this problem. Under some mild regularity conditions (Assumptions B.1-B.3), we have

\[
\mathcal{L}_K s_p = \mathbb{E}_\rho[\mathcal{K}_x \nabla \log p(x)] = -\mathbb{E}_\rho[\text{div} \mathcal{K}_x^T],
\]

where the divergence of \( \mathcal{K}_x^T \) is defined as a vector-valued function, whose \( i \)-th component is the divergence of the \( i \)-th column of \( \mathcal{K}_x^T \). The empirical estimate \( \hat{L}_K s_p \) is then available as \( -\frac{1}{M} \sum_{m=1}^{M} \text{div} \mathcal{K}_x^T \mathcal{K}_x x^m \), which results in the following general formula of nonparametric score estimators:

\[
\hat{s}^g_{p,\lambda} = -g_{\lambda}(\hat{L}_K) \hat{\zeta},
\]

where \( \hat{\zeta} := \frac{1}{M} \sum_{m=1}^{M} \text{div} \mathcal{K}_x^T \mathcal{K}_x x^m \).

3.2. Regularization Schemes

We now derive the final form of the estimator under three regularization schemes (Bauer et al., 2007). The choice of regularization will impact the convergence rate of the estimator, which will be studied in Sec. 4.

**Theorem 3.1 (Tikhonov Regularization).** Let \( \hat{s}^g_{p,\lambda} \) be defined as in (8), and \( g_\lambda(\sigma) = (\sigma + \lambda)^{-1} \). Then

\[
\hat{s}^g_{p,\lambda}(x) = \mathcal{K}_x c - \hat{\zeta}(x)/\lambda,
\]

where \( c \) is obtained by solving

\[
(K + M\lambda I)c = h/\lambda.
\]

**Lemma 3.2.** Let \( \sigma \) be a non-zero eigenvalue of \( \frac{1}{M} \mathcal{K}_x = \mathbb{E}_\rho[\mathcal{K}_x^T \mathcal{K}_x] \) such that \( \frac{1}{M} \mathcal{K}_x u = \sigma u \), where \( u \in \mathbb{R}^d \) is the unit eigenvector. Then \( \sigma \) is an eigenvalue of \( \hat{L}_K \) and the corresponding unit eigenfunction is

\[
v = \frac{1}{\sqrt{M}\sigma} \sum_{m=1}^{M} \mathcal{K}_x u^{(m)},
\]

where \( u \) is splitted into \( (u^{(1)}, \ldots, u^{(M)}) \) and \( u^{(i)} \in \mathbb{R}^d \).

The lemma is a direct generalization of Rosasco et al. (2010, Proposition 9) to vector-valued operators.

**Theorem 3.3 (Spectral Cut-Off Regularization).** Let \( \hat{s}^g_{p,\lambda} \) be defined as in (8), and

\[
g_\lambda(\sigma) = \begin{cases} 
\sigma^{-1} & \sigma > \lambda, \\
0 & \sigma \leq \lambda.
\end{cases}
\]

Let \( (\sigma_j, u_j) \geq 1 \) be the eigenvalue and eigenvector pairs that satisfy \( \frac{1}{M} \mathcal{K}_x u_j = \sigma_j u_j \). Then we have

\[
\hat{s}^g_{p,\lambda}(x) = -\mathcal{K}_x \left( \sum_{\sigma_j \geq \lambda} \frac{u_j u_j^T}{M\sigma_j^2} \right) h,
\]

where \( \mathcal{K}_x \) and \( h \) are defined as in Theorem 3.1.

Apart from the above methods with closed-form solutions, early stopping of iterative solvers like gradient descent can also play the role of regularization (Engl et al., 1996). Iterative methods replace the expensive inversion or eigendecomposition of the \( Md \times Md \) size kernel matrix with
We consider two iterative methods: the Landweber iteration and the $\nu$-method (Engl et al., 1996). The former minimizes $\| \hat{c} - L K \hat{c} \|_H^2$ by $\hat{c}^{(t+1)} = \hat{c}^{(t)} - \nu (L K \hat{c}^{(t)} - \hat{c}^{(t)})$. It is equivalent to $g_\nu(\hat{c}) = \eta \sum_{i=0}^{d-1} (1 - \eta \sigma)^i$, where we let $t = \lfloor \nu^{-1} \rfloor$ and $\eta$ is a stepsize parameter. It turns out that $\hat{c}^{(t)} = -t \nu \hat{c} + K \hat{c} c$, where $c_0 = 0$ and $c_{i+1} = (I_d - \eta K/M) c_i - t \nu^2 h/M$. The Landweber iteration often requires a large number of iterations, and an accelerated version of it is the $\nu$-method, where $\nu$ is a parameter controlling the maximal convergence rate (see Sec. 4). As it is more complicated, we defer its algorithm to Example C.3 in appendix C.2.3.

3.3. Hypothesis Spaces

In this framework, the hypothesis space is characterized by the matrix-valued kernel that induces the RKHS (Alvarez et al., 2012). Below we discuss two choices of the kernel: the diagonal ones are computationally more efficient, while curl-free kernels capture the conservative property of score vector fields.

**Diagonal Kernels** The simplest way to define a diagonal matrix-valued kernel is $K(x,y) = k(x,y) I_d$, where $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a scalar-valued kernel. This induces a product RKHS $\mathcal{H}_k^d := \otimes_{i=1}^d H_k$ where all output dimensions of a function are independent. In this case the kernel matrix for $X = (x^1, \ldots, x^M)$ is $K = k(X,X) \otimes I_d$, where $k(X,X)$ denotes the Gram matrix of the scalar-valued kernel $k$. Therefore, the computational cost of matrix inversion and eigendecomposition is the same as in the scalar-valued case. On the other hand, the independence assumption may not hold for score functions, whose output dimensions are correlated as they form the gradient of the log density. As we shall see in Sec. 5, such misspecification of the hypothesis space degrades the performance in high dimensions.

**Curl-Free Kernels** Noticing that score vector fields are gradient fields, we can use curl-free kernels (Fuselier Jr, 2007; Macêdo & Castro, 2010) to capture this property. A curl-free kernel can be constructed from the negative Hessian of a translation-invariant kernel $k(x,y) = \phi(x - y)$: $K_{\text{cf}}(x,y) := -\nabla^2 \phi(x - y)$, where $\phi : \mathcal{X} \to \mathbb{R} \in \mathbb{C}^2$. It is easy to see that $K_{\text{cf}}$ is positive definite. A nice property of $K_{\text{cf}}$ is that any element in it is a gradient of some function. To see this, notice that the $j$-th column of $K_{\text{cf}}$ is $-\nabla(\partial_j \phi)$ and each element in $K_{\text{cf}}$ is a linear combination of columns of $K_{\text{cf}}$. The cost of inversion and eigendecomposition of the kernel matrix is $O(M^3 d^3)$, compared to $O(M^3)$ for diagonal kernels.

### 3.4. Examples

In the following we provide examples of nonparametric score estimators derived from the framework. We show that existing estimators can be recovered with certain types of kernels and regularization schemes (Table 1).

**Example 3.4 (KEF).** Consider using curl-free kernels for the Tikhonov regularized estimator in (9). By substituting $K_{\text{cf}}(x,y) = -\nabla^2 \phi(x - y)$ for $K$, we get

$$s^g_{p,\lambda}(x) = -\sum_{m=1}^d \sum_{j=1}^d c(m-1)d+j \nabla \partial_j \phi(x - x^m) - \frac{\zeta_{\text{cf}}(x)}{\lambda},$$

where $\zeta_{\text{cf}}(x)_i := -\frac{1}{M} \sum_{m=1}^M \sum_{j=1}^d \partial_i \partial_j \phi(x - x^m)$. Noticing that $K_{\text{cf}}(x,y)_{ij} = -\partial_i \partial_j \phi(x - y) = \partial_i \partial_j k(x,y)$, we could check that the definition of $c$ here, which follows from (9), is the same as in (3). Thus by comparing with (3), we have

$$s^g_{p,\lambda}(x) = \nabla \hat{f}_{p,\lambda}(x) = \nabla \log p_f(x,\lambda).$$

Therefore, the KEF estimator is equivalent to choosing curl-free kernels and the Tikhonov regularization in (8).

We note that, although the solutions are equivalent, the space $\{ \nabla \log p_f, f \in H_k \}$ is different from the curl-free RKHS constructed from the negative Hessian of $k$. Such equivalence of regularized minimization problems may be of independent interest.

**Example 3.5 (SSGE).** For the estimator (12) obtained from the spectral cut-off regularization. Consider letting $K(x,y) = k(x,y) I_d$. Then $K = k(X,X) \otimes I_d$, and it can be decomposed as $\sum_{m=1}^M \sum_{j=1}^d \lambda_m (w_m \psi_m^j \otimes e_i e_i^T)$, where $\{ (\lambda_m, w_m) \}$ is the eigenpairs of $k(X,X)$ with $\lambda_1 \geq \lambda_2 \cdots \geq \lambda_M$ and $\{ e_i \}$ is the standard basis of $\mathbb{R}^d$. The estimator reduces to

$$s^g_{p,\lambda}(x)_i = -k(x,x) \left( \sum_{j=1}^d \frac{w_i w_j^T}{\lambda_j} \right) r_i,$$

where $r_i := (h_i, h_{d+1}, \ldots, h_{(M-1)d+i})$. When we choose $\lambda = \lambda_f$, simple calculations (see appendix C.1) show that (14) equals the SSGE estimator $s^g_{p,\lambda}(x)_i = -\frac{1}{M} \sum_{j=1}^d \sum_{m=1}^M \partial_i \psi_j(x^m) \hat{\psi}_j(x)$, where $\hat{\psi}_j$ is defined as in (5). Therefore, SSGE is equivalent to choosing the diagonal kernel $K(x,y) = k(x,y) I_d$ and the spectral cut-off regularization in (8).

**Example 3.6 (Stein).** We consider modifying the Tikhonov regularizer to $g_\nu(\sigma) = (\lambda + \sigma)^{-1} I_{1(\sigma > 0)}$. In this case, we obtain an estimator $s^g_{p,\lambda}(x) = -K_{\text{cf}} K^{-1} \left( \frac{1}{M} K + \lambda I \right)^{-1} h$ by Lemma C.1. At sample points, the estimated score is $-\left( \frac{1}{M} K + \lambda I \right)^{-1} h$, which coincides with the Stein gradient estimator. This suggests a principled out-of-sample extension of the Stein gradient estimator.
To gain more insights, we consider to minimize (6) in the subspace generated by \( \{ K_m^c : m \in [M], c_m \in \mathbb{R}^d \} \). Compared with (11), the one-dimensional subspace \( \mathbb{R}^c \) is ignored. We could check that (in appendix C.1) this is equivalent to exploiting the previous mentioned regularizer. Therefore, the Stein estimator is equivalent to using the diagonal kernel \( K(x, y) = k(x, y) I_d \) and the Tikhonov regularization with a one-dimensional subspace ignored. We also find that when using the curl-free kernel, this estimator is equivalent to the Nyström version of KEF with full samples (Sutherland et al., 2018).

### 3.5. Scalability

When using curl-free kernels, we need to deal with an \( M^d \times M^d \) matrix. In such cases, the Tikhonov and the spectral cut-off regularization cost \( O(M^3 d^3) \) and have difficulties scaling with the sample size and the input dimensions. Fortunately, as the unifying perspective suggests, we could modify the regularization schemes with iterative methods that only require matrix-vector multiplications, e.g., the Landweber iteration and the \( \nu \)-method (see Sec. 3.2). Interestingly, we get further acceleration by utilizing the structure of curl-free kernels.

**Example 3.7 (Iterative curl-free estimators).** We observe that when using a curl-free kernel \( K_{cf} \) constructed from a radial scalar-valued kernel \( k(x, y) = \phi(\|x - y\|) \).

\[
K_{cf}(x, y) = \left( \frac{\phi'(r)}{r^2} - \frac{\phi''(r)}{r^2} \right) r^T r - \frac{\phi'(r)}{r} I,
\]

where \( r = x - y \), \( r = \|r\|_2 \). Consider in matrix-vector multiplications, for a vector \( a \in \mathbb{R}^d \), \( K_{cf}(x, y)a \) can be computed as \( \left( \frac{\phi'(r)}{r^2} - \frac{\phi''(r)}{r^2} \right) (r^T a) r - \frac{\phi'(r)}{r} a \), where only a vector-vector multiplication is required with time complexity \( O(d) \), compared to general \( O(d^2) \). Thus, we only need \( O(M^2 d) \) time to compute \( Kb \) for any \( b \in \mathbb{R}^{Md} \). In practice, we only need to store samples for computing \( Kb \) instead of constructing the whole kernel matrix. This reduces the memory usage from \( O(M^2 d^2) \) to \( O(M^2 d) \).

We note that the same idea in Example 3.7 can be used to accelerate the KEF estimator if we adopt the conjugate gradient methods (Van Loan & Golub, 1983) to solve (10), because we have shown that the KEF estimator is equivalent to our Tikhonov regularized estimators with curl-free kernels. As we shall see in experiments, this method is extremely fast in high dimensions.

### 4. Theoretical Properties

In this section, we give a general theorem on the convergence rate of score estimators in our framework, which provides a tighter error bound of SSGE (Shi et al., 2018).

| Algorithm   | Kernel | Regularizer                |
|-------------|--------|----------------------------|
| SSGE        | \( k(x, y)I_d \) | \( 1_{\{\sigma \geq \lambda\}} \sigma^{-1} \) |
| Stein       | \( k(x, y)I_d \) | \( 1_{\{\sigma \geq \lambda\}} (\lambda + \sigma)^{-1} \) |
| KEF         | \(-\nabla^2 \phi(x - y)\) | \( (\lambda + \sigma)^{-1} \) |
| NKEF        | \(-\nabla^2 \phi(x - y)\) | \( 1_{\{\sigma \geq \lambda\}} (\lambda + \sigma)^{-1} \) |

We also investigate the case where samples are corrupted by a small set of points, and provide the convergence rate of the heuristic out-of-sample extension proposed in Li & Turner (2018). Proofs and assumptions are deferred to appendix B.

First, we follow Bauer et al. (2007); Baldassarre et al. (2012) to characterize the regularizer.

**Definition 4.1 (Bauer et al. (2007)).** We say a family of functions \( g_\lambda : [0, \kappa^2] \to \mathbb{R}, 0 < \lambda \leq \kappa^2 \) is a regularizer if there are constants \( B, D, \gamma \) such that \( \sup_{0 < \sigma \leq \kappa^2} |g_\lambda(\sigma)| \leq D, \sup_{0 < \sigma \leq \kappa^2} |\sigma g_\lambda(\sigma)| \leq B/\lambda \) and \( \sup_{0 < \sigma \leq \kappa^2} |1 - \sigma g_\lambda(\sigma)| \leq \gamma \). The qualification of \( g_\lambda \) is the maximal \( r \) such that \( \sup_{0 < \sigma \leq \kappa^2} |1 - \sigma g_\lambda(\sigma)| \sigma^r \leq \gamma r, \) where \( \gamma \) does not depend on \( \lambda \).

Now, we can use the idea of Bauer et al. (2007, Theorem 10) to obtain an error bound of our estimator as follows.

**Theorem 4.2.** Assume Assumptions B.1-B.5 hold. Let \( \bar{r} \) be the qualification of the regularizer \( g_\lambda \), and \( s^g_{p, \lambda} \) be defined as in (8). Suppose there exists \( f_0 \in H_\kappa \) such that \( s^p = L^p_k f_0 \) for some \( r \in [0, \bar{r}] \). Then we have for \( \lambda = M^{-\frac{1}{\bar{r} + 1/2}} \),

\[
\|s^p_{p, \lambda} - s^p\|_{H_\kappa} = O_p \left( M^{-\frac{1}{\bar{r} + 1/2}} \right),
\]

and for \( r \in [0, \bar{r} - 1/2] \), we have

\[
\|s^g_{p, \lambda} - s^g\|_\rho = O_p \left( M^{-\frac{1}{\bar{r} + 1/2}} \right),
\]

where \( O_p \) is the Big-O notation in probability.

Note the qualification impacts the maximal convergence rate. As the qualification of Tikhonov regularization is 1, from the error bound, we observe the well-known saturation phenomenon of Tikhonov regularization (Engl et al., 1996), i.e., the convergence rate does not improve even if \( s^p = L^p_k f_0 \) for \( r > 1 \). To alleviate this, we can choose the regularizer with larger qualification. For example, the spectral cut-off regularization and the Landweber iteration have qualification \( \infty \), and the \( \nu \)-method has qualification \( \nu \). This suggests \( \nu \)-method is appealing as it has smaller iteration number than the Landweber iteration and better maximal convergence rate than Tikhonov regularization.

**Remark 4.3.** The consistency and convergence rate of the original Stein estimator and its out-of-sample extension suggested in Example 3.6 follow from Theorem 4.2.
Remark 4.4. From Theorem 4.2, the convergence rate in \( \| \cdot \|_p \) of SSGE is \( O_p(M^{-\beta}) \), where \( \beta \in [1/4, 1/2) \), which improves Shi et al. (2018, Theorem 2). To see this, we assume the eigenvalues of \( \mathbf{L}_K \) are \( \mu_1 \geq \mu_2 \geq \cdots \) and they decay as \( \mu_j = O(J^{-\beta}) \). The error bound provided by Shi et al. (2018) is

\[
\| \hat{s}_{p,\lambda} - s_p \|_p^2 = O_p \left( \frac{J^2}{\mu_j (\mu_j - \mu_{j+1})^2 M + \mu_j} \right).
\]

We can choose \( J = M^{-1/4+\epsilon} \) to obtain \( \| \hat{s}_{p,\lambda} - s_p \|_p = O_p(M^{-1/4}) \). The convergence rate is slower than \( O_p(M^{-1/4}) \), i.e., the worst case of Theorem 4.2.

Next, we consider the case where estimators are not obtained from i.i.d. samples. Specifically, we consider how the convergence rate is affected when our data is the mixture of a set of i.i.d. samples and a set of fixed points.

**Theorem 4.5.** Under the same assumption of Theorem 4.2, we define \( g_\lambda(x) := (\lambda + \sigma)^{-1} \), and choose \( Z := \{z^n\}_{n \in [N]} \subseteq X \). Let \( Y := \{y^n\}_{m \in [M]} \) be a set of i.i.d. samples drawn from \( p \), and \( \hat{s}_{p,\lambda,z} \) be defined as in (8) with \( X = Z \cup Y \). Suppose \( N = O(M^\alpha) \), then we have for \( \lambda = M^{-\frac{1}{\alpha+\epsilon}} \),

\[
\sup_{Z} \| \hat{s}_{p,\lambda,z} - s_p \|_{H_K} = O_p \left( M^{-\frac{1}{\alpha+\epsilon}} \right) + O \left( M^{\alpha - \frac{1}{\alpha+\epsilon}} \right),
\]

where the \( \sup_Z \) is taken over all \( \{z^n\}_{n \in [N]} \subseteq X \).

**Proof Outline.** Define \( T_Z := \frac{1}{N} S_Z^* S_Z \), where \( S_Z \) is the sampling operator. Let \( \hat{s}_{p,\lambda} \) be defined as in (8) with \( X = Y \). We can write the estimator as \( \hat{s}_{p,\lambda,z} = \frac{g_\lambda(L_K + R_Z)^{-1}(L_K + R_Z)s_p}{Z} \), where \( R_Z := \frac{N}{M+N}(T_Z - L_K) \), and bound \( \| \hat{s}_{p,\lambda,z} - \hat{s}_{p,\lambda} \| \) by \( \| g_\lambda(L_K + R_Z) - g_\lambda(L_K) \|_K s_p \| + \| g_\lambda(L_K + R_Z) R_Z s_p \| \). It can be shown that the first term is \( O \left( (NM^{-1})^{-\frac{1}{\alpha+\epsilon}} \right) \), and the second term is \( O \left( (NM^{-1})^{-\frac{1}{\alpha+\epsilon}} \right) \). Combining with Theorem 4.2, we can obtain the result. □

From Theorem 4.5, we see that the convergence rate is not affected when data is corrupted by at most \( O(M^{-\frac{1}{\alpha+\epsilon}}) \) points. Under the same notation of this theorem, the out-of-sample extension of Stein estimator provided by Li & Turner (2018) can be written as \( \hat{s}_{p,\lambda,x}(x) \), which can be regarded as corrupting data by one point. Then we can obtain the following bound on this estimator

**Corollary 4.6.** Under the same assumption and notation of Theorem 4.5, we have

\[
\sup_{x \in X} \| \hat{s}_{p,\lambda,x}(x) - s_p(x) \|_2 = O_p(M^{-\frac{1}{\alpha+\epsilon}}).
\]

5. Experiments

We evaluate our estimators on both synthetic and real data. In Sec. 5.1, we consider a challenging grid distribution as described in the experiment of Sutherland et al. (2018) to test the accuracy of nonparametric score estimators in high dimensions and out-of-sample points. In Sec. 5.2 we train Wasserstein autoencoders (WAE) with score estimation and compare the accuracy and the efficiency of different estimators. We mainly compare the following score estimators:

**Existing nonparametric estimators:** Stein (Li & Turner, 2018), SSGE (Shi et al., 2018), KEF (Sriperumbudur et al., 2017), and its low rank approximation NKEF_\alpha (Sutherland et al., 2018), where \( \alpha \) represents to use \( \alpha M/10 \) samples.

**Parametric estimators:** In the WAE experiment, we also consider the sliced score matching (SSM) estimator (Song et al., 2019), which is a parametric method and requires amortized training.

**Proposed:** The iterative curl-free estimator with the \( \nu \)-method, and the conjugate gradient version of the KEF estimator (KEF-CG), both described in Sec. 3.5.

5.1. Synthetic Distributions

We follow Sutherland et al. (2018, Sec. 5.1) to construct a \( d \)-dimensional grid distribution. It is the mixture of \( d \) standard Gaussian distributions centered at \( d \) fixed vertices in the unit hypercube. We change \( d \) and \( M \) respectively to test the accuracy and the convergence of different estimators, and use 1024 samples from the grid distribution to evaluate the \( \ell^2 \) norm. We report the result of 32 runs in Fig. 1.

We can see that the effect of hypothesis space is significant. The diagonal kernels used in SSGE and Stein degrade the accuracy in high dimensions, while curl-free kernels provide better performance. In low dimensions, all estimators are comparable, and the computational cost of diagonal kernels is lower than that of curl-free kernels. This suggests favoring the diagonal kernels in low dimensions. Possibly because this dataset does not make the convergence rate saturate, we find different regularization schemes produce similar results. The iterative score estimator based on the \( \nu \)-method is among the best and KEF-CG closely tracked them even with large \( d \) and \( M \).

5.2. Wasserstein Autoencoders

Wasserstein autoencoder (WAE) (Tolstikhin et al., 2017) is a latent variable model \( p(z, x) \) with observed and latent variables \( x \in X \) and \( z \in Z \), respectively. \( p(z, x) \) is defined by a prior \( p(z) \) and a distribution of \( z \) conditioned on \( x \),

\[\text{Code is available at https://github.com/miskcoo/kscore}.
\]
Figure 1. Normalized distance $E[\|s_p - \hat{s}_{p,\lambda}\|_2^2]/d$ on grid data. In the first row, $M$ is fixed and $d$ varies. In the second row, $d$ is fixed and $M$ varies. Shaded areas are three times the standard deviation.

(a) $M = 128$
(b) $M = 512$
(c) $d = 16$
(d) $d = 128$

Figure 2. (a) Computational costs of KEF-CG for $\lambda = 10^{-5}$ on MNIST; (b) The ratio of the maximum and the minimum eigenvalues of kernel matrices.

and can be written as $p(z, x) = p(z)p_0(x|z)$. WAEs aim at minimizing Wasserstein distance $W_1(p_X, p_{CG})$ between the data distribution $p_X(x)$ and $p_{CG}(x) := \int p(z, x)dz$, where $c$ is a metric on $\mathcal{X}$. Tolstikhin et al. (2017) showed that when $p_0(x|z)$ maps $z$ to $x$ deterministically by a function $G : \mathcal{Z} \rightarrow \mathcal{X}$, it suffices to minimize $E_{p_X(x)}[\E_{q_\phi(z|x)}[\|x - G(z)\|_2^2] + \lambda D(q_\phi(z), p(z))]$, where $D$ is a divergence of two distributions and $q_\phi(z|x)$ is a parametric approximation of the posterior. When we choose $D$ to be the KL divergence, the entropy term of $q_\phi(z) := \int q_\phi(z|x)p_X(x)dx$ in the loss function is intractable (Song et al., 2019). If $z$ can be parameterized by $p_\phi(x)$ with $x \sim p_X$, the gradient of the entropy can be estimated using score estimators as $E_{p_X(x)}[\nabla_z \log q_\phi(z)\nabla_\phi f_\phi(x)]$ (Shi et al., 2018; Song et al., 2019).

We train WAEs on MNIST and CelebA and repeat each configuration 3 times. The average negative log-likelihoods for MNIST estimated by AIS (Neal, 2001) are reported in Table 2. The results for CelebA are reported in appendix A. We can see that the performance of these estimators is close in low latent dimensions, and the parametric method is slightly better than nonparametric ones as we have continuously generated samples. However, in high dimensions, estimators based on curl-free kernels significantly outperform those based on diagonal kernels and parametric methods. This is probably due to guarantee that the estimates at all locations form a gradient field.

As discussed in Sec. 3.5, curl-free kernels are computationally expensive. This is shown in Table 2 by the running time of the original KEF algorithm. By comparing the time and performance of NKEF, with $\alpha = 2, 4, 8$, we see that in order to get meaningful speed-up in high dimensions, low-rank approximation methods have to sacrifice the performance, which are outperformed by the iterative curl-free estimators based on the $\nu$-method. KEF-CG is the fastest curl-free method in high dimensions while the performance is comparable with the original KEF. Fig. 2a shows the training time of KEF-CG in different latent dimensions. Surprisingly, the speed rapidly increases with increasing latent dimension and then flattens out. The convergence rate of conjugate gradient is determined by the condition number, which means the kernel matrix $K$ becomes well-conditioned in high dimensions (see Fig. 2b).

We found with large $d$, SSGE required at least 97% eigenvalues to attain the reported likelihood. We also ran SSGE with curl-free kernels and found only 13% eigenvalues are required to attain a comparable result when $d = 8$. From these observations, a possible reason why diagonal kernels degrade the performance in high dimensions is that the distribution is complicated while the hypothesis set is simple, so the small number of eigenfunctions are insufficient to approximate the target. This can also be observed from Fig. 1, where the performance of diagonal kernels and curl-free kernels are closer as $M$ increases since more eigenfunctions are provided.

6. Conclusion

Our contributions are two folds. Theoretically, we present a unifying view of nonparametric score estimators, and clarify the relationships of existing estimators. Under this
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perspective, we provide a unified convergence analysis of existing estimators, which improves existing error bounds. Practically, we propose an iterative curl-free estimator with nice theoretical properties and computational benefits, and use the similar idea to develop a fast conjugate gradient solver for the KEF estimator.

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In appendix A we provide additional details and further results of experiments. In appendix B, we list the assumptions we used, and prove the non-asymptotic version of Theorem 4.2 and 4.5. In appendix C, we give the details of Sec. 3, including deriving algorithms presented in Sec. 3.2, examples in Sec. 3.4 and a general formula for curl-free kernels. Appendix D includes some technical results used in proofs. Finally, We present samples drawn from trained WAEs in appendix E.

A. Experiment Details and Additional Results

In experiments, we use the IMQ kernel \(k(x, y) := (1 + ||x - y||^2/\sigma^2)^{-1/2}\) and its curl-free version in corresponding kernel estimators. We use the median of the pairwise Euclidean distances between samples as the kernel bandwidth. The parameter \(\nu\) of the \(\nu\)-method is set to 1. The maximum iteration number of KEF-CG is 40 and the convergence tolerance of it is \(10^{-4}\).

A.1. Grid Distributions

We use \(\alpha M\) eigenvalues in SSGE with \(\alpha\) searched in \([0.99, 0.97, 0.95, 0.9, 0.8, 0.7, 0.6, 0.5, 0.4]\). We search the number of iteration steps of the \(\nu\)-method in \([20, 30, 40, 50, 60, 70, 80, 90, 100]\). We search the regularization coefficient \(\lambda\) of Stein, NKEF, KEF-CG in \(10^{-k} : k = 0, 1, \cdots, 8\). The experiments are repeated 32 times.

A.2. Wasserstein Autoencoders

We use the standard Gaussian distribution \(\mathcal{N}(0, I)\) as the prior \(p(z)\), and \(\mathcal{N}(\mu^v(x), \sigma_v^2(x))\) as the approximated posterior \(q_v(z|x)\), and Bernoulli\((G_0(z))\) as the generator \(p_0(x|z)\). We use minibatch size 64. Models are optimized by the Adam optimizer with learning rate \(10^{-4}\). Each configuration is repeated 3 times, and the mean and the standard deviation are reported in Table 3 and Table 4. All models are timed on GeForce GTX TITAN X GPU.

### Table 3. Negative log-likelihoods on the MNIST dataset and per epoch time on 128 latent dimension.

| Latent Dim | 8       | 32      | 64      | 128     | Time  |
|------------|---------|---------|---------|---------|-------|
| STEIN      | 97.15 ± 0.14 | 92.10 ± 0.07 | 101.60 ± 0.44 | 114.41 ± 0.25 | 4.2s  |
| SSGE       | 97.24 ± 0.07 | 92.24 ± 0.17 | 101.92 ± 0.08 | 114.57 ± 0.23 | 9.2s  |
| KEF        | 97.07 ± 0.03 | 90.93 ± 0.23 | 91.58 ± 0.03 | 92.40 ± 0.34 | 201.1s |
| NKEF_2     | 97.71 ± 0.24 | 92.29 ± 0.41 | 92.82 ± 0.18 | 94.14 ± 0.69 | 36.4s |
| NKEF_3     | 97.59 ± 0.15 | 91.19 ± 0.08 | 91.80 ± 0.12 | 92.94 ± 0.58 | 97.5s |
| NKEF_8     | 97.23 ± 0.06 | 90.86 ± 0.09 | 92.39 ± 1.32 | 92.49 ± 0.41 | 301.2s |
| KEF-CG     | 97.39 ± 0.22 | 90.77 ± 0.12 | 92.66 ± 0.67 | 92.05 ± 0.06 | 13.7s |
| \(\nu\)-method | 97.28 ± 0.17 | 90.94 ± 0.02 | **91.48** ± 0.09 | 92.10 ± 0.06 | 78.1s |
| SSM        | **96.98** ± 0.27 | 89.06 ± 0.01 | 93.06 ± 0.68 | 96.92 ± 0.08 | 6.0s  |

### Table 4. Fréchet Inception Distances on the CelebA dataset and per epoch time on 128 latent dimension.

| Latent Dim | 8       | 32      | 64      | 128     | Time  |
|------------|---------|---------|---------|---------|-------|
| STEIN      | 73.85 ± 1.39 | 58.29 ± 0.46 | 57.54 ± 0.57 | 76.31 ± 1.33 | 164.4s |
| SSGE       | 72.49 ± 1.09 | 58.01 ± 0.60 | 58.39 ± 1.00 | 76.85 ± 1.12 | 172.2s |
| NKEF_2     | 75.12 ± 1.55 | 53.92 ± 0.29 | 51.16 ± 0.30 | 55.17 ± 0.43 | 244.7s |
| NKEF_3     | 73.15 ± 0.77 | 54.54 ± 1.02 | 50.76 ± 0.19 | 53.70 ± 0.10 | 412.5s |
| KEF-CG     | 72.92 ± 0.60 | 54.32 ± 0.31 | 50.44 ± 0.20 | **50.66** ± 0.89 | 166.2s |
| \(\nu\)-method | 72.02 ± 1.22 | 52.86 ± 0.20 | **50.16** ± 0.23 | 52.80 ± 0.43 | 220.9s |
| SSM        | **69.72** ± 0.25 | **49.93** ± 0.74 | 72.68 ± 1.75 | 94.07 ± 3.57 | 163.3s |

**MNIST** We parameterize \(\mu^v, \sigma_v^2\) and \(G_0(x)\) by fully-connected neural networks with two hidden layers, both of which consist of 256 units activated by ReLU. For SSM, the score is parameterized by a fully-connected neural network with two hidden layers consisting of 256 units activated by tanh. The regularization coefficients of Stein, KEF, NKEF, KEF-CG are searched in \(10^{-k} : k = 2, 3, \cdots, 7\) for the best log-likelihood, and the number of iteration steps of the \(\nu\)-method are searched in \(\{50, 70, \cdots, 150\}\), and we use \(\alpha M\) eigenvalues in SSGE with \(\alpha\) searched in \([0.99, 0.97, 0.95, 0.93, 0.91, 0.89, 0.87]\). We run 1000 epoches and evaluate the model by AIS (Neal, 2001), where the parameters are the same as in SSGE. Specifically,
we set the step size of HMC to $10^{-6}$, and the leapfrog step to 10. We use 5 chains and set the temperature to $10^3$.

**CelebA** We parameterize $\mu_\theta$, $G_\theta$ by convolutional neural networks similar to Song et al. (2019). $\sigma_\phi^2$ is set to 1. For SSM, we use the same network as in MNIST to parameterize the score. The regularization coefficients of Stein, KEF, NKEF, KEF-CG are searched in $\{10^{-k} : k = 2, 3, \ldots, 7\}$ for the best log-likelihood, and the number of iteration steps of the $\nu$-method are searched in $\{20, 30, 40, 50, 60, 70\}$, and we use $\alpha M$ eigenvalues in SSGE with $\alpha$ searched in $\{0.99, 0.97, 0.95, 0.93, 0.91, 0.89, 0.87\}$. We run 100 epochs and evaluate the model using the Fréchet Inception Distance (FID). As KEF and NKEF are slow, we do not compare them in this dataset. Results are reported in Table 4.

**B. Error Bounds**

In the following, we suppress the dependence of $\mathcal{H}_K$ on $K$ for simplicity. We use $\| \cdot \|_{\text{HS}}$ to denote the Hilbert-Schmidt norm of operators. The assumptions required in obtaining an error bound are listed below.

**Assumption B.1.** $\mathcal{X}$ is a non-empty open subset of $\mathbb{R}^d$, with piecewise $C^1$ boundary.

**Assumption B.2.** $p$, $\log p$ and each element of $K$ are continuously differentiable. $p$ and its total derivative $Dp : \mathcal{X} \to \mathbb{R}^d$ can both be continuously extended to $\mathcal{X}$, where $\mathcal{X}$ is the closure of $\mathcal{X}$. Each element of $K$ and its total derivative can be continuously extended to $\mathcal{X} \times \mathcal{X}$.

**Assumption B.3.** For all $i, j \in [d]$, $K(x, x)_{ij}p(x) = 0$ on $\partial \mathcal{X}$, and $\sqrt{|K(x, x)_{ij}|}p(x) = o(\|x\|_2^{-d})$ as $x \to \infty$, where $\partial \mathcal{X} := \mathcal{X} \setminus \mathcal{X}$.

**Assumption B.4.** Define an $\mathcal{H}_K$-valued random variable $\xi_s := \text{div}_x K_T^s$, let $\xi := \int_{\mathcal{X}} \xi_s dp$. There are two constants $\Sigma$, $K$, such that

$$
\int_{\mathcal{X}} \left\{ \exp \left( \frac{\|\xi_s - \xi\|_H}{K} \right) - \frac{\|\xi_s - \xi\|_H}{K} - 1 \right\} dp \leq \frac{\Sigma^2}{2K^2}.
$$

**Assumption B.5.** There is a constant $\kappa > 0$ such that $\sup_{x \in \mathcal{X}} \text{tr} K(x, x) \leq \kappa^2$.

Assumptions B.1-B.3 are similar to those in Sriperumbudur et al. (2017). They guarantee the integration by parts is valid, so we can obtain $\mathbb{E}_p[\text{div}_x K_T^s] = -\mathbb{E}_p[\text{div}_x K_T^s]$. Assumptions B.4 and B.5 come from Bauer et al. (2007), and are used in the concentration inequalities. Note that Assumption B.4 can be replaced by a stronger one that $\|\xi_s - \xi\|_H$ is uniformly bounded on $\mathcal{X}$.

We follows the idea of Bauer et al. (2007, Theorem 10) to prove Theorem 4.2. The non-asymptotic version is given as follows.

**Theorem B.1.** Assume Assumptions B.1-B.5 hold. Let $\hat{r}$ be the qualification of the regularizer $g_\lambda$, and $\hat{s}_p^\lambda$ be defined as in (8). Suppose there exists $f_0 \in \mathcal{H}_K$ such that $s_p = L_K^s f_0$, for some $r \in [0, \hat{r}]$. Then for any $0 < \delta < 1, M \geq (2\sqrt{2}\kappa^2 \log(4/\delta))^{\frac{p+2}{p+2}}$, choosing $\lambda = M^{-\frac{4}{p+2}}$, the following inequalities hold with probability at least $1 - \delta$

$$
\|\hat{s}_p, - s_p\|_H \leq C_1 M^{-\frac{4}{p+2}} \log \frac{4}{\delta},
$$

and for $r \in [0, \hat{r} - 1/2]$, we have

$$
\|\hat{s}_p, - s_p\|_\rho \leq C_2 M^{-\frac{4}{p+4}} \log \frac{4}{\delta},
$$

where $C_1 = 2B(K + \Sigma) + 2\sqrt{2}B\kappa^2\|s_p\|_H + (\gamma_r + \kappa^2 \gamma_r c_r)\|f_0\|_H$, and $C_2 = 2B(K + \Sigma)\kappa + 2\sqrt{2}B\kappa^3\|s_p\|_H + ((\gamma_r + \kappa^2 \gamma_r c_r) + c_r (\gamma_r + \kappa^2 \gamma_r c_r))\|f_0\|_H$, and $c_r$ is a constant depending on $r$. $O_p$ is the Big-O notation in probability.

**Proof.** We consider the following decomposition

$$
\|\hat{s}_p, - s_p\|_H \leq \|g_\lambda(L_K)(\tilde{\xi} - \xi)\|_H + \|g_\lambda(L_K) L_K s_p - s_p\|_H
\leq \|g_\lambda(L_K)(\tilde{\xi} - \xi)\|_H + \|g_\lambda(L_K)(L_K - \tilde{L}_K)s_p\|_H + \|r_\lambda(L_K)s_p\|_H,
$$

where $r_\lambda(\sigma) := g_\lambda(\sigma)\sigma - 1$. By Definition 4.1, we have $\|g_\lambda(L_K)\| \leq B/\lambda$. From Lemma D.3 and D.4, with probability at least $1 - \delta$, we have

$$
\|g_\lambda(L_K)(\tilde{\xi} - \xi)\|_H + \|g_\lambda(L_K) L_K - \tilde{L}_K)s_p\|_H \leq \frac{2B(K + \Sigma) + 2\sqrt{2}B\kappa^3\|s_p\|_H \log \frac{4}{\delta}}{\lambda M}.
$$

Nonparametric Score Estimators
By Definition 4.1, \(|r_\lambda(L_K)L_K^c| \leq \gamma r \lambda^r\) and \(|r_\lambda(\hat{L}_K)| \leq \gamma\), then
\[
\|r_\lambda(\hat{L}_K) s_p\|_H \leq \|r_\lambda(\hat{L}_K) L_K^c f_0\|_H + \|r_\lambda(\hat{L}_K)(L_K \hat{L}_K) f_0\|_H \\
\leq \gamma r \lambda^r \|f_0\|_H + \gamma \|L_K - \hat{L}_K\| \|f_0\|_H.
\]
When \(r \in [0, 1]\), from Bauer et al. (2007, Theorem 1), there exists a constant \(c_r\) such that \(|L_K - \hat{L}_K| \leq c_r \|L_K - \hat{L}_K\|^r\). Then by Lemma D.4, and choose \(\lambda \geq 2\sqrt{2}\kappa^2 M^{-1/2} \log(4/\delta)\), we have
\[
\|L_K^c - \hat{L}_K^c\| \leq c_r \left(\frac{2\sqrt{2}\kappa^2}{\sqrt{M}} \log \frac{4}{\delta}\right)^r \leq c_r \lambda^r.
\]
Collecting the above results,
\[
\|\hat{s}_{p, \lambda} - s_p\|_H \leq \frac{A_1}{\lambda \sqrt{M}} + A_2 \lambda^r \log \frac{4}{\delta},
\]
where \(A_1, A_2\) are constants which do not depend on \(\lambda\) and \(M\). Then, we can choose \(\lambda = M^{-\frac{1}{2\tau+2}}\) to obtain the bound. Combining with \(\lambda \geq 2\sqrt{2}\kappa^2 M^{-1/2} \log(4/\delta)\), we require \(M^{-\frac{1}{2\tau+2}} \geq 2\sqrt{2}\kappa^2 M^{-1/2} \log(4/\delta)\).

When \(r > 1\), from Lemma D.5, there exists a constant \(c'_r\) such that \(|L_K^c - \hat{L}_K^c| \leq c'_r \|L_K - \hat{L}_K\|_{HS}\). Then \(|L_K^c - \hat{L}_K^c| \leq 2\sqrt{2}c'_r \kappa^2 M^{-1/2} \log(4/\delta)\), and a similar discussion can be applied to obtain the bound.

Note that \(|\hat{s}_{p, \lambda} - s_p|_\rho = \|\sqrt{L_K^c}(\hat{s}_{p, \lambda} - s_p)\|_H\). Then we can apply the above discussion to obtain the bound for \(|\|\rho\|_\rho\|^r\).

Next, we give the non-asymptotic version of Theorem 4.5 as follows

**Theorem B.2.** Under the same assumption of Theorem B.1, we define \(g_\lambda(\sigma) := (\lambda + \sigma)^{-1}\), and choose \(Z := \{z^n\}_{n \in [N]} \subseteq X\). Let \(Y := \{y^n\}_{n \in [N]}\) be a set of i.i.d. samples drawn from \(\rho\). Let \(\hat{s}_{p, \lambda}X\) be defined as in (8) with \(X = Z \cup Y\). Suppose \(N = M^\alpha\), then for any \(0 < \delta < 1\), \(M \geq (2\sqrt{2}\kappa^2 \log(4/\delta))^{2\tau+2}\), choosing \(\lambda = M^{-\frac{1}{2\tau+2}}\), the following inequalities hold with probability at least \(1 - \delta\)
\[
\sup_Z \|\hat{s}_{p, \lambda}X - s_p\|_H \leq C_1 M^{-\frac{1}{2\tau+2}} \log \frac{4}{\delta} + C_3 M^{\alpha - \frac{1}{2\tau+2}}
\]
where \(C_3 := 2(\kappa^2 + 1)^2 \|s_p\|_H\), and the \(\sup_Z\) is taken over all \(\{z^n\}_{n \in [N]} \subseteq X\).

In particular, when \(\alpha = \frac{1}{2\tau+2}\), we have
\[
\sup_Z \|\hat{s}_{p, \lambda}X - s_p\|_H \leq (C_1 + C_3) M^{-\frac{1}{2\tau+2}} \log \frac{4}{\delta}.
\]

**Proof.** We define \(T_Z := \frac{1}{N} S^T Z S_Z\), where \(S_X f := (f(z^1), \ldots, f(z^N))\) is the sampling operator. Let \(\hat{L}_K := T_Y\) and \(\hat{s}_{p, \lambda}\) be the estimator obtained from \(Y\). Then we can write \(\hat{s}_{p, \lambda} := g_\lambda(\hat{L}_K + R_Z)(\hat{L}_K + R_Z)s_p\), where \(R_Z := \frac{N}{M+N}(T_Z - \hat{L}_K)\).

We can bound the error as follows
\[
\|\hat{s}_{p, \lambda}X - s_p\|_H \leq \|\hat{s}_{p, \lambda}X - \hat{s}_{p, \lambda}\|_H + \|\hat{s}_{p, \lambda} - s_p\|_H \\
\leq \|(g_\lambda(\hat{L}_K + R_Z) - g_\lambda(\hat{L}_K))\hat{L}_K s_p\|_H + \|g_\lambda(\hat{L}_K + R_Z)R_Z s_p\|_H + \|\hat{s}_{p, \lambda} - s_p\|_H.
\]
The last term has been bounded by Theorem B.1, and we consider the first two terms. Since \(g_\lambda(\sigma) = (\lambda + \sigma)^{-1}\) is Lipschitz in \([0, \infty)\), from Lemma D.5, we have \(|g_\lambda(\hat{L}_K + R_Z) - g_\lambda(\hat{L}_K)| \leq \|R_Z\|_{HS}/\lambda^2\). Note \(|g_\lambda(\hat{L}_K + R_Z)R_Z\|_{HS} \leq \|R_Z\|_{HS}/\lambda\), we obtain
\[
\|\hat{s}_{p, \lambda}X - \hat{s}_{p, \lambda}\|_H \leq \left(\frac{\kappa^2}{\lambda^2} + \frac{1}{\lambda}\right) \|R_Z\|_{HS} \|s_p\|_H \leq \left(\frac{\kappa^2}{\lambda^2} + \frac{1}{\lambda}\right) \frac{2\kappa^2 N}{M+N} \|s_p\|_H \\
\leq \frac{2(\kappa^2 + 1)^2 N}{\lambda^2 M} \|s_p\|_H = 2(\kappa^2 + 1)^2 M^{\alpha - \frac{1}{2\tau+2}} \|s_p\|_H.
\]
Combining with Theorem B.1, and noticing that the right hand does not depend on \(Z\), we obtain the final bound. □
Finally, we prove the error bound of the Stein estimator with its original out-of-sample extension.

**Proof of Corollary 4.6.** The Stein estimator at point \( x \in \mathcal{X} \) can be written as

\[
\hat{s}_{p,\lambda}(x) = \sum_{i=1}^{d} \langle K(x, \hat{s}_{p,\lambda} x) \rangle e_i,
\]

where \( \{e_i\} \) is the standard basis of \( \mathbb{R}^d \). Note that

\[
\sup_{x \in \mathcal{X}} \|\hat{s}_{p,\lambda}(x) - s_p(x)\|_2 \leq \sum_{i=1}^{d} \sup_{x \in \mathcal{X}} |\langle K(x, \hat{s}_{p,\lambda} x - s_p) \rangle| \leq \kappa^2 \sup_{x \in \mathcal{X}} \|\hat{s}_{p,\lambda} - s_p\|_H.
\]

Then, the bound of Stein estimator immediately follows from Theorem 4.5. \( \square \)

### C. Details in Section 3

#### C.1. Computational Details

**Details of Example 3.5** Using the notation in Example 3.5 and Sec. 2.2, we can reformulate SSGE into a matrix form as follows:

\[
\hat{g}_j(x) = -\sum_{j=1}^{J} \left( \frac{1}{M} \sum_{m=1}^{M} \partial_i \hat{\psi}_j(x^m) \right) \psi_j(x)
\]

\[
= -\sum_{j=1}^{J} \left( \frac{1}{M} \sum_{m=1}^{M} \partial_i \psi_j(x^n) \sum_{m=1}^{M} w_j^{(m)} \right) \left( \sum_{i=1}^{M} k(x^n, x^n) \right)
\]

\[
= -\sum_{j=1}^{J} \left( \sum_{m=1}^{M} \frac{w_j^{(m)}}{w_j^{(m)}} \right) \partial_i \psi_j(x^n)
\]

\[
= -k(x, X) \left( \sum_{j=1}^{J} \frac{w_j w_j^T}{\lambda_j^2} \right) r_i,
\]

where \( r_{i,j} = \sum_{m=1}^{M} \partial_i k(x^n, x^m) \), and \( w_1, \ldots, w_M \) is the unit eigenvectors of \( k(X, X) \) corresponding to eigenvalues \( \lambda_1 \geq \cdots \geq \lambda_M \). \( w_j^{(m)} \) is the \( m \)-th component of \( w_j \). Note that when using diagonal kernels, we have \( K(x, y) = k(x, y) \otimes I_d \), then the eigenvectors of \( K(X, X) \) are \( \{w_i \otimes e_j : i \in [M], j \in [d]\} \) and the eigenvalue corresponds to \( w_i \otimes e_j \) is \( \lambda_i \), where \( \{e_j\} \) is the standard basis of \( \mathbb{R}^d \). We also note that in this case

\[
h_{(m-1)d+i} = \hat{\zeta}(x^n)_i = \frac{1}{M} \sum_{j=1}^{M} (\text{div} \xi_j k(x^n, x^n))_i = \frac{1}{M} \sum_{j=1}^{M} \partial_i k(x^n, x^n) = Mr_{i,m}.
\]

Comparing with (12), we find that SSGE is equivalent to use diagonal kernels and spectral cut-off regularization.

**Details of Example 3.6** For the regularizer \( g_\lambda(\sigma) := (\lambda + \sigma)^{-1} 1_{\sigma > 0} \), from Lemma C.1 we know when \( K \) is non-singular, \( \hat{s}^2_{p,\lambda}(x) = -K_{xX} K^{-1} (\frac{1}{M} K + \lambda I)^{-1} h \). Next, we consider the minimization problem in (6), and ignore the one-dimensional subspace \( \mathbb{R}^2 \) of the solution space, and assume the solution is \( K_{xX} c \) as before. We can rewrite the objective in (6) to

\[
\frac{1}{M} c^T K^2 c + \lambda c K c + 2e^T h.
\]

By taking gradient, we find \( c \) satisfies \( (\frac{1}{M} K^2 + \lambda K) c = -h \), so it is equivalent to use the previously mentioned regularization.
Curl-Free Kernels Suppose $K_{cf}$ is a curl-free kernel defined by $\nabla^2 \phi(r)$, where $r = (x - x')^T$ and $r = \|r\|$. Then

$$
\frac{\partial}{\partial r_i} \phi = \phi' r_i, \\
\nabla \frac{\partial}{\partial r_i} \phi = \phi'' r_i r + \phi' e_i r - r_i \hat{r},
$$

where $e_i$ is the $i$-th column of the identity matrix. Then the curl-free kernel is of the form

$$
K_{cf}(x, y) = \left( \frac{\phi'}{r^3} - \frac{\phi''}{r^2} \right) r r^T - \frac{\phi'}{r} I.
$$

(15)

We also obtain a divergence formula for such kernel. Note that

$$
\partial_{jj} \partial_i \phi = \phi''' r_j^2 r_i + \phi'' (r_i + r_j \delta_{ij}) r^2 - 2 r_j^2 r_i
$$

$$
+ \phi' \left( \frac{r_j^2}{r^2} + \frac{3 r_j^2}{r^2} \right) (r_j \delta_{ij} - r_i),
$$

where $\delta_{ij} = [i = j]$. Next, we sum out $j$ and then obtain

$$
div_x K_{cf}(x, x') = -\Delta (\partial_i \phi)(r) = -\frac{r}{r} \left[ \phi'''(r) + \frac{d - 1}{r} \left( \phi''(r) - \frac{\phi'(r)}{r} \right) \right].
$$

(16)

C.2. Details of Different Regularization Schemes

C.2.1. Tikhonov Regularization

**Proof of Theorem 3.1.** When $g_\lambda(\sigma) = (\sigma + \lambda)^{-1}$, the estimator is $\hat{s}_{p, \lambda} = -(\hat{L}_K + \lambda I)^{-1} \hat{\zeta}$. We need to compute the explicit formula of the inverse of $\hat{L}_K + \lambda I$. Note that $(\hat{L}_K + \lambda I)^{-1} \hat{\zeta}$ is the solution of the following minimization problem

$$
\hat{s}_{p, \lambda} = \arg \min_{s \in \mathcal{H}_K} \frac{1}{M} \sum_{i=1}^M s(x_i)^T s(x_i) + 2 \langle s, \hat{\zeta} \rangle_{\mathcal{H}} + \lambda \|s\|_{\mathcal{H}}^2.
$$

From the general representer theorem (Sriperumbudur et al., 2017, Theorem A.2), the minimizer lies in the space generated by

$$
\{K_x c : i \in [M], c \in \mathbb{R}^d \} \cup \{\hat{\zeta}\}.
$$

We can assume

$$
\hat{s}_{p, \lambda} = \sum_{i=1}^M K_x c_i + a \hat{\zeta}.
$$

Define $c := (c_1, \ldots, c_M)$ and $h := (\hat{\zeta}(x^1), \ldots, \hat{\zeta}(x^M))$, then the optimization objective can be written as

$$
\frac{1}{M} (c^T K^2 c + 2ac^T Kh + a^2 h^T h) + 2(a \|\hat{\zeta}\|_{\mathcal{H}}^2 + h^T c) + \lambda (c^T Kc + 2ac^T h + a^2 \|\hat{\zeta}\|_{\mathcal{H}}^2).
$$

Taking the derivative, we need to solve the following linear system

$$
\frac{1}{M} (K^2 c + a Kh) + h + \lambda (Kc + ah) = 0,
$$

$$
\frac{1}{M} (ah^T h + c^T Kh) + (1 + \lambda a) \|\hat{\zeta}\|_{\mathcal{H}}^2 + \lambda c^T h = 0.
$$

By some calculations, this system is equivalent to $a = -1/\lambda$ and $(K + M\lambda I)c = h/\lambda$. \qed
C.2.2. Spectral Cut-Off Regularization

Proof of Lemma 3.2. Let $\mathcal{H}_0$ be the subspace of $\mathcal{H}_K$ generated by $\{K_x c : c \in \mathbb{R}^d, m \in [M]\}$. Note that $f(x^m)^T c = (K(\cdot, x^m)c, f)_{\mathcal{H}} = 0$ for any $f \in \mathcal{H}_0^\perp$ and $c \in \mathbb{R}^d$. We know $\hat{L}_K = 0$ on $\mathcal{H}_0^\perp$. Also note $L_K v \in \mathcal{H}_0$ and $v(x^m) = u^{(m)}\sqrt{M}\sigma$, then

$$\hat{L}_K v(x^k) = \frac{1}{M} \sum_{m=1}^M K(x^k, x^m) v(x^m) = \frac{1}{\sqrt{M}} \sum_{m=1}^M K(x^k, x^m) v(x^m),$$

and we conclude that $\hat{L}_K v = \sigma v$. The following equation shows $v$ is normalized:

$$\|v\|^2_{\mathcal{H}} = \frac{1}{\sqrt{M}} \sum_{m=1}^M \left\langle K(\cdot, x^m)u^{(m)}, v \right\rangle_{\mathcal{H}} = \frac{1}{\sqrt{M}} \sum_{m=1}^M \left\langle u^{(m)}, v(x^m) \right\rangle_{\mathbb{R}^d} = \sum_{m=1}^M (u^{(m)})^T u^{(m)} = 1.$$ 



Theorem 3.3 is a corollary of the following lemma, which provides a general form for the regularizer $g(\lambda)$ with $g(\lambda)(0) = 0$.

Lemma C.1. Let $g(\lambda) : [0, \kappa^2] \rightarrow \mathbb{R}$ be a regularizer such that $g(\lambda)(0) = 0$. Let $(\sigma_j, u_j)_{j \geq 1}$ be the non-zero eigenvalue and eigenvector pairs that satisfy $\frac{1}{M} K u_j = \sigma_j u_j$. Then we have

$$g(\lambda)(\hat{L}_K) \hat{\zeta} = K_{xx} \left( \sum \frac{g(\sigma_i)}{M \sigma_i} u_i u_i^T \right) h,$$

where $K_{xx}$ and $h$ are defined as in Theorem 3.1.

Proof. Let $\{(\mu_i, v_i)\}$ be the pairs of non-zero eigenvalues and eigenfunctions of $\hat{L}_K : \mathcal{H} \rightarrow \mathcal{H}$, then by Lemma 3.2 we have $\sigma_i = \mu_i$. Note that

$$\hat{L}_K = \sum \mu_i \langle v_i, \cdot \rangle_{\mathcal{H}} v_i$$

and $g(\lambda)(\hat{L}_K) = \sum g(\lambda)(\mu_i) \langle v_i, \cdot \rangle_{\mathcal{H}} v_i$.

From Lemma 3.2, we have

$$g(\lambda)(\hat{L}_K) \hat{\zeta} = \sum g(\lambda)(\mu_i) \langle v_i, \hat{\zeta} \rangle_{\mathcal{H}} v_i$$

$$= \sum \left\{ g(\lambda)(\sigma_i) \left( \frac{1}{\sqrt{M \sigma_i}} \sum_{j=1}^M K_{x^i} u_j^{(j)} \hat{\zeta} \right) \frac{1}{\sqrt{M \sigma_i}} \sum_{k=1}^M K_{x^i} u_k^{(k)} \right\}$$

$$= \frac{1}{M} \sum_{j,k=1}^M g(\lambda)(\sigma_i) \sigma_i^{-1} \langle K_{x^j} u_j^{(j)}, \hat{\zeta} \rangle_{\mathcal{H}} K_{x^k} u_k^{(k)}$$

$$= \frac{1}{M} \sum_{j,k=1}^M g(\lambda)(\sigma_i) \sigma_i^{-1} \hat{\zeta}(x^j)^T u_j^{(j)} K_{x^k} u_k^{(k)}$$

$$= K_{xx} \left( \sum \frac{g(\lambda)(\sigma_i)}{M \sigma_i} u_i u_i^T \right) h.$$



C.2.3. Iterative Regularization

Theorem C.2 (Landweber iteration). Let $s_{p,\lambda}^\eta$ be defined as in (8), and $g(\sigma) = \eta \sum_{i=0}^t (1 - \eta \sigma)^i$. Then we have

$$s_{p,\lambda}^\eta(x) = -t \eta \hat{\zeta}(x) + K_{xx} c_t,$$

where $c_0 = 0$ and $c_{t+1} = (I_d - \eta K/M) c_t - t \eta^2 h/M$, and $K_{xx}$ and $h$ are defined as in Theorem 3.1.
Proof. We note that the iteration process is

\[
\hat{s}_p^{(1)} = -\eta \hat{\zeta}, \\
\hat{s}_p^{(t)} = -\eta \hat{\zeta} + (I - \eta \hat{L}_K)\hat{s}_p^{(t-1)} = \hat{s}_p^{(t-1)} + \eta(-\hat{\zeta} - \hat{L}_K \hat{s}_p^{(t-1)}),
\]

where we define \(\hat{s}_p^{(t)} := \hat{s}_{p,1/t}\). We can assume

\[
\hat{s}_p^{(t)} = a_t \hat{\zeta} + K_{\Sigma} c_t.
\]

Then, by induction,

\[
\hat{s}_p^{(t)} = -\eta \hat{\zeta} + (I - \eta \hat{L}_K)(a_{t-1} \hat{\zeta} + K_{\Sigma} c_{t-1}) = (a_{t-1} - \eta) \hat{\zeta} + K_{\Sigma} (c_{t-1} + \eta a_{t-1} h/M - \eta K c_{t-1}/M).
\]

Thus, we have \(a_t = -t\eta\) and \(c_t = (I - \eta K/M)c_{t-1} - (t - 1)\eta^2 h/M\), and \(c_1 = 0\).

Example C.3 (\(\nu\)-method). The \(\nu\)-method (Engl et al., 1996) is an accelerated version of the Landweber iteration, which corresponds to the following iteration and requires less iteration steps than the Landweber iteration, where \(\lambda\) is identified with \(1/t^2\) and \(\hat{s}_p^{(t)} := \hat{s}_{p,1/t^2}\).

\[
\hat{s}_p^{(0)} = 0, \quad \hat{s}_p^{(1)} = -\omega_1 \hat{\zeta}, \\
\hat{s}_p^{(t)} = \hat{s}_p^{(t-1)} + u_t(\hat{s}_p^{(t-1)} - \hat{s}_p^{(t-2)}) + \omega_t(-\hat{\zeta} - \hat{L}_K \hat{s}_p^{(t-1)}),
\]

where

\[
u_t = \frac{(t - 1)(2t - 3)(2t + 2\nu - 1)}{(t + 2\nu - 1)(2t + 4\nu - 1)(2t + 2\nu - 3)},
\]

\[
\omega_t = \frac{4(2t + 2\nu - 1)(t + \nu - 1)}{(t + 2\nu - 1)(2t + 4\nu - 1)}.
\]

Similarly, we can assume

\[
\hat{s}_p^{(t)} = a_t \hat{\zeta} + K_{\Sigma} c_t.
\]

Then, by induction,

\[
\hat{s}_p^{(t)} = \left(1 + u_t - \omega_t \hat{L}_K\right)\hat{s}_p^{(t-1)} - u_t \hat{s}_p^{(t-2)} - \omega_t \hat{\zeta}, \\
= \left(1 + u_t - \omega_t \hat{L}_K\right)\left(a_{t-1} \hat{\zeta} + K_{\Sigma} c_{t-1}\right) - u_t(a_{t-2} \hat{\zeta} + K_{\Sigma} c_{t-2}) - \omega_t \hat{\zeta}, \\
= \left(1 + u_t\right)a_{t-1} - u_t a_{t-2} - \omega_t \hat{\zeta}, \\
+ K_{\Sigma} \left((1 + u_t)c_{t-1} - \frac{\omega_t}{M}(a_{t-1} h + K c_{t-1}) - u_t c_{t-2}\right).
\]

Thus, we obtain the iteration formula for \(a_t\) and \(c_t\) as follows:

\[
a_t := (1 + u_t)a_{t-1} - u_t a_{t-2} - \omega_t, \\
c_t := (1 + u_t)c_{t-1} - \frac{\omega_t}{M}(a_{t-1} h + K c_{t-1}) - u_t c_{t-2},
\]

and \(c_0 = c_1 = 0, a_0 = 0, a_1 = -\omega_1\).
D. Technical Results

Lemma D.1. Suppose Assumption B.5 holds, then $L_{K^c}, \hat{L}_{K^c} : \mathcal{H}_K \to \mathcal{H}_{K^c}$ are positive, self-adjoint, trace class operators. Moreover, $\text{tr} \ L_{K^c} \leq \kappa^2$ and $\text{tr} \ \hat{L}_{K^c} \leq \kappa^2$.

Proof. The result follows from a simple calculation. It is easy to see $L_{K^c}$ and $\hat{L}_{K^c}$ are positive and self-adjoint. We prove they are in trace class. Let $\{\varphi_i\}$ be a orthonormal basis of $\mathcal{H}_{K^c}$ and $\{e_i\}$ be the standard basis of $\mathbb{R}^d$, then

$$
\text{tr} \ L_{K^c} = \sum_{i} \langle L_{K^c} \varphi_i, \varphi_i \rangle_{\mathcal{H}} = \int_{\mathcal{X}} \sum_{i} \langle K(x) \varphi_i, \varphi_i \rangle_{\mathcal{H}} d\rho = \sum_{i} \int_{\mathcal{X}} \langle (K(x) e_i, \varphi_i)_{\mathcal{H}} K(x) e_i, \varphi_i \rangle_{\mathcal{H}} d\rho
$$

$$
= \sum_{i} \int_{\mathcal{X}} \sum_{i} \langle (K(x) e_i, \varphi_i)_{\mathcal{H}} \rangle d\rho = \sum_{i} \int_{\mathcal{X}} \langle K(x) e_i \rangle_{\mathcal{H}}^2 d\rho = \int_{\mathcal{X}} \text{tr} K(x) d\rho \leq \kappa^2.
$$

Similarly, we have $\text{tr} \ \hat{L}_{K^c} \leq \kappa^2$.

We need the following concentration inequality in Hilbert spaces used in Bauer et al. (2007).

Lemma D.2 (Bauer et al. (2007), Proposition 23). Let $\xi$ be a random variable with values in a real Hilbert space $H$. Assume there are two constants $\sigma, H$, such that

$$
\mathbb{E}[\|\xi - \mathbb{E}[\xi]\|_H] \leq \frac{1}{2} m! \sigma^2 H^{m-2}, \quad \forall m \geq 2.
$$

Then, for all $n \in \mathbb{N}, 0 < \delta < 1$, the following inequality holds with probability at least $1 - \delta$

$$
\|\hat{\xi} - \mathbb{E}_{\xi}\|_H \leq 2 \left( \frac{H}{n} + \frac{\sigma}{\sqrt{n}} \right) \log \frac{2}{\delta},
$$

where $\hat{\xi} = \frac{1}{n} \sum_{i=1}^{n} \xi_i$ and $\{\xi_i\}$ are independent copies of $\xi$.

Lemma D.3. Under Assumption B.4, we have for all $M \in \mathbb{N}, 0 < \delta < 1$, the following inequality holds with probability at least $1 - \delta$

$$
\|\hat{\xi} - \xi\|_H \leq 2 \left( \frac{K}{M} + \frac{\sum}{\sqrt{M}} \right) \log \frac{2}{\delta},
$$

where $\hat{\xi} = \frac{1}{M} \sum_{m=1}^{M} \text{div}_{\nu_x} K_{x^n}^m$ and $\{x^n\}$ is the set of i.i.d. samples from $\nu$.

Proof. Define an $\mathcal{H}_K$-valued random variable $\xi_x := \text{div}_{\nu_x} K_{x^n}^m$. It is easy to see $\mathbb{E}_{x_i \sim \nu}[\xi_x] = -L_{K^c} \nu =: \xi$. From Assumption B.4, we have for $m \geq 2$,

$$
\mathbb{E}_{\nu}[\|\xi_x - \xi\|_H] \leq m! K^m \mathbb{E}_{\nu} \left[ \exp \left( \frac{\|\xi_x - \xi\|_H}{K} \right) \right] \right] \leq \frac{1}{2} m! \exp K^m.
$$

Note that $\hat{\xi} = \frac{1}{M} \sum_{m=1}^{M} \xi_x^m$ and $\mathbb{E}_{\nu} \hat{\xi} = \xi$. Then (17) follows from Lemma D.2.

Lemma D.4. Under Assumption B.5, we have for all $M \in \mathbb{N}, 0 < \delta < 1$, the following inequality holds with probability at least $1 - \delta$

$$
\|\hat{L}_{K^c} - L_{K^c}\|_H \leq 2 \sqrt{2} K^2 \sqrt{\log \frac{2}{\delta}}.
$$

Proof. This is a direct consequence of Vito et al. (2005, Lemma 8) and Lemma D.1.

The following useful lemma is from De Vito et al. (2014, Lemma 7) and Sriperumbudur et al. (2017, Lemma 15)

Lemma D.5. Suppose $S$ and $T$ are two self-adjoint Hilbert-Schmidt operators on a separable Hilbert space $H$ with spectrum contained in the interval $[a, b]$. Given a Lipschitz function $r : [a, b] \to \mathbb{R}$ with Lipschitz constant $L_r$, we have

$$
\|r(S) - r(T)\|_{HS} \leq L_r \|S - T\|_{HS}.
$$
E. Samples

| Method   | $d = 8$ | $d = 32$ | $d = 64$ | $d = 128$ |
|----------|---------|----------|----------|-----------|
| Stein    | ![Images](image1.png) | ![Images](image2.png) | ![Images](image3.png) | ![Images](image4.png) |
| SSGE     | ![Images](image5.png) | ![Images](image6.png) | ![Images](image7.png) | ![Images](image8.png) |
| SSM      | ![Images](image9.png) | ![Images](image10.png) | ![Images](image11.png) | ![Images](image12.png) |
| NKEF$_2$ | ![Images](image13.png) | ![Images](image14.png) | ![Images](image15.png) | ![Images](image16.png) |
| $\nu$-method | ![Images](image17.png) | ![Images](image18.png) | ![Images](image19.png) | ![Images](image20.png) |
| KEF-CG   | ![Images](image21.png) | ![Images](image22.png) | ![Images](image23.png) | ![Images](image24.png) |
Table 6. WAE samples on CelebA.

| Method      | $d = 8$ | $d = 32$ | $d = 64$ | $d = 128$ |
|-------------|---------|----------|----------|-----------|
| Stein       | ![Image](image1) | ![Image](image2) | ![Image](image3) | ![Image](image4) |
| SSGE        | ![Image](image5) | ![Image](image6) | ![Image](image7) | ![Image](image8) |
| SSM         | ![Image](image9) | ![Image](image10) | ![Image](image11) | ![Image](image12) |
| NKEF$^2$    | ![Image](image13) | ![Image](image14) | ![Image](image15) | ![Image](image16) |
| $d$-method  | ![Image](image17) | ![Image](image18) | ![Image](image19) | ![Image](image20) |
| KEF-CG      | ![Image](image21) | ![Image](image22) | ![Image](image23) | ![Image](image24) |