DEEP IMPORTANCE SAMPLING USING TENSOR TRAINS WITH
APPLICATION TO A PRIORI AND A POSTERIORI RARE EVENTS

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Abstract. We propose a deep importance sampling method that is suitable for estimating rare event probabilities in high-dimensional problems. We approximate the optimal importance distribution in a general importance sampling problem as the pushforward of a reference distribution under a composition of order-preserving transformations, in which each transformation is formed by a squared tensor-train decomposition. The squared tensor-train decomposition provides a scalable ansatz for building order-preserving high-dimensional transformations via density approximations. The use of composition of maps moving along a sequence of intermediate densities alleviates the difficulty of directly approximating concentrated density functions. To compute expectations over unnormalized probability distributions, we design a ratio estimator that estimates the normalizing constant using a separate importance distribution, again constructed via a composition of transformations in tensor-train format. This offers better theoretical variance reduction compared with self-normalized importance sampling, and thus opens the door to efficient computation of rare event probabilities in Bayesian inference problems. Numerical experiments on problems constrained by differential equations show little to no increase in the computational complexity with the event probability going to zero, and allow to compute hitherto unattainable estimates of rare event probabilities for complex, high-dimensional posterior densities.

Key words. Rare events, Bayesian inference, inverse problems, tensor train, transport maps

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1. Introduction. In the analysis of many scientific and engineering systems, practitioners often assess the performance and the inherent uncertainty using expectations of functions of random variables or random processes. As a starting point, the potential sources of input uncertainty in the system are parametrized by some random variable and equipped with a prior distribution. Then, given some model that maps the uncertain parameters to observables, the a priori uncertainty can be reduced to the a posteriori uncertainty by conditioning on observed data to obtain the posterior distribution under the Bayesian framework. Depending on the availability of data, accurate estimates of a priori and a posteriori expectations of some output functionals are both of interest.

Analytical or asymptotic characterizations of the abovementioned expectations are often unavailable, because of non-analytically tractable posterior distributions, nonlinear functions of interests, or a combination of both. Thus, numerical techniques such as Monte Carlo methods must be employed. Importance sampling provides a general tool to efficiently compute expectations of this sort by allocating computational resources to the “important” regions of the expectation problem. In the literature, adaptive importance sampling strategies have been developed to iteratively identify the important region and also to adaptively estimate importance distributions in some parametric family, e.g., mixture distributions [7, 24]. In general, the construction of importance distributions in high dimensions is challenging, especially when the important region localizes to the tail of the input distribution, as we may not be able to accurately approximate the optimal importance distribution using parametric families. As a result, the mean square error of an importance sampling estimator may deteriorate quickly,
sometimes exponentially, as the parameter dimension increases. This becomes more critical for rare event problems, where the rather small event probability, often on a scale of $10^{-6}$ or less, requires an accurate approximation to the optimal importance distribution, so that the relative mean square error can be controlled for a fixed computational budget.

We present a deep importance sampling method suitable for high-dimensional rare event problems. It employs the deep inverse Rosenblatt transport (IRT) developed in [22] and [13] to adaptively approximate the optimal importance density using a composition of order-preserving maps. When the optimal importance density is multi-modal and concentrated in the tails of the input distribution, the composite structure is able to adapt to those complicated features. Each of the maps in the composition is constructed using functional tensor-train (TT) decomposition and the cross algorithm [3, 32, 34, 43, 44]. It provides a non-parametric ansatz for approximating the optimal importance density. Thus, it can be significantly more accurate than alternative importance sampling densities based on mixture distributions. In addition, for problems with sufficient regularity, the accuracy of TT approximations can be independent of the parameter dimension; see [33] for details. The computational complexity of building TT decompositions and the resulting transport maps scales linearly in the dimension. The proposed importance sampling scheme is further extended to handle input probability distributions with unknown normalizing constants, so it can be applied to estimate a posteriori expectations. Crucially, it is possible to construct a significantly more effective estimator than the familiar self-normalized importance sampling scheme, by constructing an additional importance density, again based on the deep IRT framework, but now targeting the optimized importance density for the normalizing constant.

To demonstrate the power of the proposed deep importance sampling, we present non-trivial applications in risk assessment of spatial, susceptible-infectious-removed models and contaminant transport in groundwater systems in the challenging regime of rare events. Our numerical results suggest that the proposed method can accurately estimate both a priori and a posteriori expectations using several orders of magnitude smaller sample sizes compared to importance densities based on mixtures distributions. More importantly, the use of composition of maps and TT decomposition allows us to estimate rare event probabilities in high dimensions so far intractable by standard importance sampling methods.

This paper is organized as follows. Section 2 provides background of the problem of interest. Section 3 presents and analyses the deep importance sampling scheme for computing a priori and a posteriori expectations. Section 4 discusses the application to rare event estimation problems. Section 5 and 6 apply the proposed method to a spatial, susceptible-infectious-removed model and to contaminant transport in groundwater systems, respectively. Additional numerical examples and derivations are provided in Appendix.

2. Background. We consider a random variable $X$ taking values in $\mathcal{X} \subseteq \mathbb{R}^d$ and assign a prior probability density $\pi_0$ to it. Given an integrable function $f : \mathcal{X} \rightarrow \mathbb{R}$, our goal is to estimate the expectation $F = \mathbb{E}_{\pi_0}\{f(X)\}$. Importance sampling methods approach this goal by choosing a suitable importance density $p$, satisfying the sufficient condition $\text{supp}(f\pi_0) \subseteq \text{supp}(p)$, and then estimating $E_p\{f(X)\pi_0(X)/p(X)\}$ instead. Drawing $N$ independent and identically distributed (i.i.d.) samples from $p$, one can construct the unbiased importance sampling estimator of $F$:

$$
\hat{F}_{p,N} = \frac{1}{N} \sum_{i=1}^{N} \frac{f(X^i)\pi_0(X^i)}{p(X^i)}, \quad X^i \sim p.
$$

The performance of $\hat{F}_{p,N}$ is measured using the relative mean square error,

$$
\text{rmse}(\hat{F}_{p,N}, F) = \frac{E\{(\hat{F}_{p,N} - F)^2\}}{F^2} = \frac{\text{var}_p(\hat{F}_{p,N})}{F^2} + \frac{|E(\hat{F}_{p,N}) - F|^2}{F^2},
$$
where \( \text{var}_p(g) = E_p\{g(X)^2\} - E_p\{g(X)\}^2 \) gives the variance of a function \( g : \mathcal{X} \to \mathbb{R} \) with respect to the density \( p \). The relative mean square error (2.2) is minimized for any sample size \( N \) by choosing the optimal importance density \( p^* \propto |f|\pi_0 \) that minimizes \( \text{var}_p(f\pi_0/p) \) over all densities \( p \) with \( \text{supp}(f\pi_0) \subseteq \text{supp}(p) \). If the function of interest \( f(x) \) is non-negative on \( \mathcal{X} \), then we have \( \text{var}_p(f\pi_0/p^*) = 0 \), which leads to a zero-variance estimator.

Remark 2.1. The estimator of the a priori expectation in (2.1) implicitly assumes that the normalizing constants of the prior \( \pi_0 \) and of the importance distribution \( p \) are known, or at least the ratio of those two constants. This is also one of the necessary conditions to ensure unbiasedness of the resulting estimator. In situations where the normalizing constants are unknown—such as in the estimation of \( \pi \) the normalizing constants of the prior \( \pi_0 \)—we need to estimate the expectation in (2.1) implicitly assumes that \( \pi \) the normalizing constant. Conditioned on observed data, the central goal of the paper is to estimate the a posteriori expectation

\[
R = E_{\pi_0}\{f(X)\} = \frac{1}{Z} \int_{\mathcal{X}} f(x) L^\pi(x)\pi_0(x) \, dx.
\]

The a posteriori setting adds additional challenges. In particular, simulating i.i.d. random variables from the posterior is often impossible and the normalizing constant \( Z \) is typically unknown. Since the posterior expectation can be written as the ratio

\[
R = \frac{E_{\pi_0}\{f(X)L^\pi(X)\}}{E_{\pi_0}\{L^\pi(X)\}},
\]

an alternative importance sampling estimator can be constructed by carefully selecting two importance densities \( p \) and \( q \) such that \( \text{supp}(f\pi) \subseteq \text{supp}(p) \) and \( \text{supp}(\pi) \subseteq \text{supp}(q) \) to estimate the numerator and the denominator of (2.5), which now can be equivalently written as

\[
Q = E_p\left\{ f(X)\frac{L^\pi(X)\pi_0(X)}{p(X)} \right\}, \quad Z = E_q\left\{ \frac{L^\pi(X)\pi_0(X)}{q(X)} \right\},
\]

respectively. Drawing i.i.d. samples \( X^i_p \sim p \) and \( X^i_q \sim q \), we can construct unbiased importance sampling estimators

\[
\hat{Q}_{p,N} = \frac{1}{N} \sum_{i=1}^{N} f(X^i_p)\frac{L^\pi(X^i_p)\pi_0(X^i_p)}{p(X^i_p)}, \quad \hat{Z}_{q,N} = \frac{1}{N} \sum_{i=1}^{N} \frac{L^\pi(X^i_q)\pi_0(X^i_q)}{q(X^i_q)},
\]

to estimate \( Q \) and \( Z \), respectively. This leads to the ratio estimator

\[
\hat{R}_{p,q,N} := \frac{\hat{Q}_{p,N}}{\hat{Z}_{q,N}},
\]

for the a posteriori expectation. Although \( \hat{Q}_{p,N} \) and \( \hat{Z}_{q,N} \) are unbiased, the ratio estimator \( \hat{R}_{p,q,N} \) is biased. We will discuss the impact of this bias in later sections.

A computationally convenient choice is the so-called self-normalized importance sampling estimator with \( p = q \). However, the respective optimal importance densities \( p^* \propto |f|L^\pi\pi_0 \) and
$q^* = \pi^y$ for $Q$ and $Z$ may differ significantly, e.g., when the function of interest $f$ only takes significant values in the tail of the posterior density $\pi^y$. We propose to construct separate, near-optimal importance densities $p$ and $q$ to reduce the overall relative mean square error of the ratio estimator (2.8).

A particular application is the estimation of failure probabilities of physical or engineering systems to assess their reliability or to inform policy makers. Given a response function $h : \mathcal{X} \mapsto \mathbb{R}$, system failure is characterized by determining whether the output of $h$ falls inside of a set $\mathcal{A} \subset \mathbb{R}$. Thus, the function of interest representing a system failure becomes

\begin{equation}
    f(x) = 1_{\mathcal{A}}\{h(x)\}
\end{equation}

where $1_{\mathcal{A}}(\cdot)$ denotes the indicator function of the set $\mathcal{A}$. Depending on the availability of data, both the $a$ priori and the $a$ posteriori failure probabilities,

\begin{equation}
    \text{pr}_{\pi_0}\{h(X) \in \mathcal{A}\} = E_{\pi_0}\{f(X)\}, \quad \text{pr}_{\pi^*}\{h(X) \in \mathcal{A}\} = E_{\pi^*}\{f(X)\},
\end{equation}

provide risk assessment criteria associated with the response function $h$. Estimating those probabilities is particularly challenging when the failure set $\mathcal{X}_F := \{x \in \mathcal{X} : f(x) = 1\}$ has a very small probability mass, also referred to as a rare event.

Most of the existing literature for complex high-dimensional applications focuses on estimating $a$ priori failure probabilities, e.g., [21, 28, 47, 48, 55, 56, 57], while our approach applies equally to $a$ posteriori failure probabilities and clearly outperforms the classical cross entropy method [4]; see Sections 4–6 for numerical examples.

3. Deep importance sampling using TT.

3.1. Problem setup. To encompass both $a$ priori and $a$ posteriori expectations the optimal importance density is presented in the general form of

\begin{equation}
    p^*(x) = \frac{1}{\zeta^*} \rho^*(x), \quad \zeta^* = \int_{\mathcal{X}} \rho^*(x)dx,
\end{equation}

where $\rho^*(x)$ is the unnormalized optimal importance density and $\zeta^*$ is the normalizing constant. This includes $a$ priori expectations, where $\rho^* = |f|\pi_0$, as well as the numerator and the denominator of the ratio estimator (2.8) for $a$ posteriori expectations, where $\rho^* = |f|\mathcal{L}^y\pi_0$ and $\rho^* = \mathcal{L}^y\pi_0$, respectively. For the remainder we assume that $\zeta^*$ is unknown and that we can only evaluate the unnormalized density $\rho^*$.

Our ultimate goal is to build a normalized approximation to the optimal $p^*$ as the pushforward of an analytically tractable and product-form reference density $\lambda(x) = \prod_{k=1}^d \lambda_k(x_k)$ under an order-preserving map $T : \mathbb{R}^d \rightarrow \mathbb{R}^d$. Then, the resulting transformation can be used to generate i.i.d. random variables for importance sampling. We make the following assumptions about the importance sampling problem:

**Assumption 3.1.** The function of interest $f$ is non-negative.

**Assumption 3.2.** The ratio $\rho^*/\pi_0$ has finite mean and finite second moment with respect to $\pi_0$.

**Assumption 3.3.** The reference density $\lambda$ satisfies $\sup_{x \in \mathcal{X}} \pi_0(x)/\lambda(x) < \infty$.

Assumption 3.1 holds for the failure probability problem, which is our main application. By focusing on non-negative $f$, the optimal importance density leads to a zero-variance estimator. Thus, our goal is to design importance densities that closely approximate the optimal density to provide near zero-variance estimators. However, our discussion can easily be extended to general functions. One can decompose any function $f$ as the difference of two non-negative functions $f(x) = f_+(x) - f_-(x)$, where $f_+(x) = f(x)1_{\{f(x) > 0\}}(x)$ and $f_-(x) = -f(x)1_{\{f(x) < 0\}}(x)$. The original expectation $E_{\pi_0}\{f(X)\}$ can then be computed from $E_{\pi_0}\{f_+(X)\} - E_{\pi_0}\{f_-(X)\}$, if both $f_+$ and $f_-$ are integrable.
3.3 is introduced to ensure support of the importance density, satisfies the assumptions of the central limit theorem. We adopt this assumption to analyse the relative mean square error of our proposed estimators. Assumption 3.2 guarantees that the nominal estimator, which uses the prior density \( \pi_0 \) as the importance density, satisfies the assumptions of the central limit theorem. We adopt this assumption to analyse the relative mean square error of our proposed estimators.

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\[
\sqrt{\rho^*}(x) \approx \tilde{g}(x) = G_1(x_1) \cdots G_k(x_k) \cdots G_d(x_d),
\]

where each of the \( G_k(x_k) \) is a matrix-valued function of size \( r_{k-1} \times r_k \), with \( r_0 = r_d = 1 \). Using a representation of \( \sqrt{\rho^*} \) in tensor product form with \( n_k \) basis functions in the \( k \)th coordinate, such a TT decomposition can be computed very efficiently without incurring the curse of dimensionality for a wide range of densities via alternating linear schemes together with cross approximation [3, 32, 43]. We employ the functional extension of the alternating minimal energy method with residual-based rank adaptation of [23]. It requires only \( \mathcal{O}(dnr^2) \) evaluations of the density \( \rho^* \) and \( \mathcal{O}(dnr^3) \) floating point operations, where \( n = \max_k n_k \) and \( r = \max_k r_k \). For more details see [13, 22]. In general, the maximal rank \( r \) depends on the dimension \( d \) and can be large when the density \( \rho^* \) concentrates in some part of its domain, but some theoretical results exist that provide rank bounds. While [49] establish specific bounds for certain multivariate Gaussian densities that depend poly-logarithmically on \( d \), [33] prove dimension-independent bounds for general functions in weighted spaces with dominating mixed smoothness.

Starting with a TT decomposition of \( \sqrt{\rho^*} \), we construct the following approximation to the normalized optimal importance density,

\[
p(x) = \frac{1}{\zeta} \rho(x), \quad \rho(x) = \tilde{g}(x)^2 + \tau \lambda(x), \quad \zeta = \int_{\mathcal{X}} \{ \tilde{g}(x)^2 + \tau \lambda(x) \} \, dx,
\]

for some \( \tau > 0 \). The additional term \( \tau \lambda(x) \) guarantees that \( \text{supp}(\rho^*) \subseteq \text{supp}(p) \), and thus the importance sampling estimator defined by the approximate density \( p \) is unbiased. The following lemma, whose original proof is given in [13], shows how to choose \( \tau \) as a function of the error in \( \tilde{g} \) in the \( L^2 \)-norm, to be able to control the overall error of the approximate density \( p \) in the Hellinger distance.

**Lemma 3.4.** Suppose \( ||\sqrt{\rho^*} - \tilde{g}||_2 \leq \epsilon \) and \( \tau \leq \epsilon^2 \). Then, the exact normalizing constant \( \zeta^* \) in (3.1) and its approximation \( \zeta \) in (3.3) satisfy \( ||\zeta^* - \zeta|| \leq 2\epsilon \) and the Hellinger distance between \( \rho^* \) and its normalized approximation \( p \) defined in (3.3) can be bounded by \( D_H(p^*, p) \leq 2\epsilon/\sqrt{\zeta^*} \).

**Definition 3.5.** For any vector \( x \in \mathbb{R}^d \) and any index \( k \in \{1, \ldots, d\} \), the first \( k-1 \) coordinates and the last \( d-k \) coordinates of \( x \) are expressed as \( x_{\leq k} = [x_1, \ldots, x_{k-1}]^T \) and \( x_{>k} = [x_{k+1}, \ldots, x_d]^T \), respectively. Similarly, we write \( x_{\leq k} = (x_{<k}, x_k) \), \( x_{\geq k} = (x_k, x_{>k}) \), \( x_{\leq 1} = x_1 \), \( x_{\geq d} = x_d \), and \( x_{\leq d} = x \).

Following [13], to build an efficient sampling method based on this density approximation we now build an order-preserving map \( \mathcal{Q} : \mathbb{R}^d \to \mathcal{X} \), the *generalized IRT*, such that the pushforward of the reference density \( \lambda \) under the map \( \mathcal{Q} \) is the normalized approximate density \( p \), i.e., \( \mathcal{Q}_\sharp \lambda = p \). Exploiting the separable structure of the TT approximation \( \tilde{g} \), the unnormalized marginal densities

\[
\rho_{\leq k}(x_{\leq k}) = \int_{\mathcal{X}_{>k}} \rho(x_{\leq k}, x_{>k}) \, dx_{>k} = \int_{\mathcal{X}_{>k}} \tilde{g}(x_{\leq k}, x_{>k})^2 \, dx_{>k} + \tau \lambda_{\leq k}(x_{\leq k}),
\]

with \( \lambda_{\leq k}(x_{\leq k}) = \prod_{j=1}^{k} \lambda_j(x_j) \) for \( 1 \leq k < d \), can be computed analytically via a sequence of one-dimensional integrations. Finally, by integrating the univariate unnormalized marginal density
\[ \rho_{\leq 1}(x_1), \] we obtain the normalizing constant \( \zeta \). We provide the implementation detail of the marginalization procedure in Appendix.

Thus, the normalized densities for the marginal random variables \( X_{\leq k} \) are

\[ p_{\leq k}(x_{\leq k}) = \frac{1}{\zeta} \rho_{\leq k}(x_{\leq k}). \]

Now, the joint random variable \( \rho \) with distribution functions and a sequence of \( d-1 \) one-dimensional conditional random variables, \( X_1, X_2|X_{\leq 2}, \cdots, X_d|X_{\leq d} \), with distribution functions

\[ \mathcal{F}_{\leq 1}(x_1) = \int_{-\infty}^{x_1} p_{\leq 1}(x_1) \, dx_1, \quad \mathcal{F}_{k|\leq k}(x_k|x_{\leq k}) = \int_{-\infty}^{x_k} \frac{p_{\leq k}(x_{\leq k}, x_k)}{p_{\leq k}(x_{\leq k})} \, dx_k, \]

respectively. This defines the Rosenblatt transport according to \([50]\),

\[ \xi = \begin{bmatrix} \xi_1 \\ \vdots \\ \xi_d \end{bmatrix} = \begin{bmatrix} \mathcal{F}_{\leq 1}(x_1) \\ \vdots \\ \mathcal{F}_{d|\leq d}(x_d|x_{\leq d}) \end{bmatrix} = \mathcal{F}(x). \]

Given \( X \sim p \), the random variable \( \Xi = \mathcal{F}(X) \) is distributed uniformly in the unit hypercube \([0, 1]^d\). Since the \( k \)-th component of \( \mathcal{F} \) is a scalar valued function \( \mathcal{F}_{k|\leq k} : \mathbb{R}^k \to \mathbb{R} \), depending on the first \( k \) variables only, the map \( \mathcal{F} \) is lower-triangular.

The reason for decomposing the square root \( \sqrt{\rho^*} \) of the unnormalized importance density instead of \( \rho^* \) becomes apparent here. Directly decomposing the density \( \rho^* \) using TTs, the non-negativity of the approximated density function can not be guaranteed due to rank truncation. Approximating \( \sqrt{\rho^*} \) preserves non-negativity without any loss of smoothness in the resulting approximate density \( p \) and in all marginal densities \( \rho_{\leq k}, 1 \leq k < d \). Crucially, it also guarantees that all one-dimensional distribution functions in (3.5) are monotonically increasing and that the map \( \mathcal{F} \), as well as its inverse are order-preserving and almost surely differentiable. For a wide range of basis functions—including piecewise Lagrange polynomials, (weighted) spectral polynomials such as Chebyshev and Hermite polynomials, and Fourier series—closed-form, analytical expressions of the marginal densities in (3.4), of the conditional distribution functions in (3.5), and of the resulting Rosenblatt transport in (3.6) are available. We refer the reader to the appendix of \([15]\) for details.

Denoting the uniform density on \([0, 1]^d\) by \( \mu \), the pullback of \( \mu \) under \( \mathcal{F} \) satisfies

\[ \mathcal{F}^\dagger \mu(x) = \mu(\mathcal{F}(x)) |\nabla_x \mathcal{F}(x)| = |\nabla_x \mathcal{F}(x)| = p(x). \]

The product-form reference density \( \lambda(u) \) is naturally equipped with the diagonal map

\[ \xi = \mathcal{R}(u) = [\mathcal{R}_1(u_1), \ldots, \mathcal{R}_k(u_k), \ldots, \mathcal{R}_d(u_d)]^\top, \quad \mathcal{R}_k(u_k) = \int_{-\infty}^{u_k} \lambda_k(u'_k) \, du'_k, \]

such that \( \mathcal{R} \lambda = \mu \). Thus, the composite map \( Q = \mathcal{F}^{-1} \circ \mathcal{R} \) also has the lower-triangular structure and satisfies \( Q \lambda = p \). Thus, one can first generate random variables \( U \sim \lambda \), distributed according to the reference density \( \lambda \), and then apply the general IRT \( X = Q(U) \) to obtain a random variable \( X \sim p \). The map \( Q : \mathbb{R}^d \to \mathcal{X} \) is again lower-triangular and can be evaluated successively as

\[ x = \begin{bmatrix} \mathcal{F}_{\leq 1}^{-1}(R_1(u_1)), \ldots, \mathcal{F}_{d|\leq d}^{-1}(R_d(u_d)|x_{\leq d}) \end{bmatrix}^\top. \]

Thus defined squared IRT can be also used as an efficient conditional distribution method in the classical sense, see, e.g., \([35]\).
We want to highlight some relevant work. In the Bayesian context, the work of [26, 27] employs TT to approximate elements of the posterior density, such as the log-likelihood function, to compute posterior statistics. In comparison, our method approximates the optimal importance density and the expectation to be estimated for general problems using TT, while naturally devising an IRT to remove potential approximation bias via sampling.

Practical implementations of the general Rosenblatt transport in high-dimensions were previously investigated within a variational framework. One such class of methods, cf. [2, 46, 58], adopts a map-from-samples approach that estimates the map \( Q \) by minimizing the Kullback–Leibler divergence of the target density from the pushforward of the reference density under \( Q \). In particular, the work of [58] learns the map \( Q \) using reduced order models to accelerate importance sampling estimators. The map-from-samples approach is flexible to implement, as it only requires a set of samples drawn from the target density. However, it comes with an \( O(N^{-1/2}) \) error rate, where \( N \) is the sample size, due to the Monte Carlo estimate of the KL divergence. See [59] and references therein for the analysis. Another related approach is the variational density estimation in the TT format [42], in which it is possible to derive the Rosenblatt transport in TT format after the density estimation.

When samples from the target density are hard to obtain—e.g., the computation of a posteriori expectations and rare event estimations considered in this work—one may employ an alternative class of methods that adopts a map-from-density approach. The map-from-density approach builds the Rosenblatt transport \( Q \) by minimizing the Kullback–Leibler divergence of the pushforward of the reference density under \( Q \) from the target density, cf. [5, 41, 53]. The training of this class of methods is often quite involved in practice—the objective function presents many local minima and each optimization iteration requires many evaluations of the unnormalized target density at transformed reference variables under the candidate map. Our method also uses pointwise evaluation of the target density, and thus can be considered as a map-from-density approach. Instead of the computationally demanding iterative minimization of the Kullback–Leibler divergence, our method builds the TT-Cross approximation of the square root of an unnormalized density function, which naturally relates to the Hellinger distance (cf. Lemma 3.4). Under our construction, the resulting Rosenblatt transport maps exactly to the approximated target density built by TT-Cross.

3.3. From IRT to deep importance sampling. For problems such as rare event estimation, the optimal importance density can concentrate to a small region of the parameter space, or even to a sub-manifold, due to complex nonlinear interactions. In this situation, constructing in one step a TT approximation of \( \sqrt{\rho^*} \) may result in rather high tensor ranks. It is also challenging to find an appropriate basis to efficiently discretize \( \sqrt{\rho^*} \) that can adapt to high-probability regions of the optimal importance density. As a consequence, both \( r \) and \( n \) can become very large.

We overcome this difficulty by building a composition of maps \( T^{(L)} = Q^{(1)} \circ Q^{(2)} \circ \cdots \circ Q^{(L)} \), that can adapt to a concentrated optimal importance density layer-by-layer. The adaptive construction is guided by a sequence of unnormalized intermediate densities \( \phi^{(1)}, \phi^{(2)}, \ldots, \phi^{(L)} \equiv \rho^* \) with increasing complexity. To specify the adaptation, we denote the \( \ell \)th normalized intermediate density as

\[
\phi^{(\ell)}(x) = \frac{1}{\omega^{(\ell)}} \varphi^{(\ell)}(x), \quad \omega^{(\ell)} = \int_X \varphi^{(\ell)}(x) dx.
\]

At any layer \( \ell \), the pushforward of the reference density \( \lambda \) under the partial composition \( T^{(\ell)} \) is constructed such that it approximates the \( \ell \)th normalized intermediate density, i.e., \( \{T^{(\ell)}\}_2 \lambda \approx \varphi^{(\ell)} \), with a controlled error. This leads to a recursive construction procedure. Given \( T^{(\ell)} \), we need to add a new layer \( Q^{(\ell+1)} \) so that the new composition \( T^{(\ell+1)} = T^{(\ell)} \circ Q^{(\ell+1)} \) yields

\[
\{T^{(\ell)} \circ Q^{(\ell+1)}\}_2 \lambda \approx \varphi^{(\ell+1)}.
\]

This is equivalent to finding \( Q^{(\ell+1)} \) such that \( \{Q^{(\ell+1)}\}_2 \lambda \approx \{T^{(\ell)}\}_2 \varphi^{(\ell+1)} \). Thus, we can build...
\( Q^{(\ell+1)} \) as a squared IRT that pushes forward the reference density \( \lambda \) to the pullback density \( \{ T^{(\ell)} \}^2 \phi^{(\ell+1)} \). Since the pushforward of \( \lambda \) under \( T^{(\ell)} \) approximates \( \phi^{(\ell)} \), the pullback of the normalized density \( \phi^{(\ell)} \) under \( T^{(\ell)} \) satisfies

\[
\{ T^{(\ell)} \}^2 \phi^{(\ell+1)}(u) = \phi^{(\ell)} \{ T^{(\ell)}(u) \} \nabla T^{(\ell)}(u) \approx \lambda(u).
\]

Similarly, we can see that

\[
\{ T^{(\ell)} \}^2 \phi^{(\ell+1)}(u) = \phi^{(\ell+1)} \{ T^{(\ell)}(u) \} \nabla T^{(\ell)}(u) \approx \frac{\phi^{(\ell+1)} \{ T^{(\ell)}(u) \}}{\phi^{(\ell)} \{ T^{(\ell)}(u) \}} \lambda(u).
\]

With suitable intermediate densities, the ratio \( \phi^{(\ell+1)}/\phi^{(\ell)} \) is significantly less concentrated than the optimal importance density \( \rho^* \). As a result, it will be much easier to approximate the map \( Q^{(\ell+1)} \) rather than directly attempting to approximate the pullback of \( \rho^* \).

Although the normalizing constant of \( \phi^{(\ell+1)} \) is unknown, it is possible to recursively decompose the square root of the unnormalized pullback density \( \{ T^{(\ell)} \}^2 \phi^{(\ell+1)} \) in TT format using the construction outlined in Section 3.2. This procedure is summarized in Alg. 3.1.

**Algorithm 3.1** Construction of deep importance density.

Input: reference density \( \lambda \) and unnormalized intermediate densities \( \phi^{(1)}, \ldots, \phi^{(L)} \)

Initialize the map as \( T^{(0)}(x) = x \).

For \( \ell = 1, \ldots, L \), apply all steps as outlined in Section 3.2:

1. Factorize the square root of \( \{ T^{(\ell-1)} \}^2 \phi^{(\ell)}(x) \) in a TT format \( \tilde{g}^{(\ell)}(x) \).
2. Choose appropriate \( \tau^{(\ell)} \).
3. Construct the approximation \( \{ T^{(\ell-1)} \}^2 \phi^{(\ell)}(x) \approx \rho^{(\ell)}(x) = \tilde{g}^{(\ell)}(x)^2 + \tau^{(\ell)} \lambda(x) \).
4. Compute the normalizing constant \( \zeta^{(\ell)} \).
5. Compute the IRT \( Q^{(\ell)} \) associated with \( \rho^{(\ell)} \) as in (3.7).
6. Update the composition as \( T^{(\ell)} = T^{(\ell-1)} \circ Q^{(\ell)} \).

Return \( \{ \tilde{g}^{(\ell)}, \tau^{(\ell)}, \zeta^{(\ell)} \}_{\ell=1}^L \) and the composite map \( T^{(L)} \).

Given the output of Alg. 3.1, the pushforward of the reference density \( \lambda \) under the composite map \( T^{(L)} \) has the normalized density \( \bar{\rho} = \{ T^{(L)} \}_\sharp \lambda \) with

\[
\bar{\rho}(x) = \left\{ \prod_{\ell=1}^L \zeta^{(\ell)} \right\}^{-1} \left( \tilde{g}^{(1)}(x)^2 + \tau^{(1)} \lambda(x) \right) \prod_{\ell=2}^L \left( \frac{\tilde{g}^{(\ell)}(x)^2}{\lambda(x)} \right) + \tau^{(\ell)}.
\]

Since the Hellinger distance is invariant to change of measure, the composition map satisfies

\[
D_H \left[ \{ T^{(\ell-1)} \circ Q^{(\ell)} \}_\sharp \lambda, \phi^{(\ell)} \right] = D_H \left[ \{ Q^{(\ell)} \}_\sharp \lambda, \{ T^{(\ell-1)} \}^2 \phi^{(\ell)} \right], \quad \text{for } 1 \leq \ell \leq L.
\]

As a consequence, the total Hellinger error of the approximate optimal importance density \( \bar{\rho} = \{ T^{(L)} \}_\sharp \lambda \) is equivalent to the Hellinger error in the final iteration, \( D_H \left[ \{ Q^{(L)} \}_\sharp \lambda, \{ T^{(L-1)} \}^2 \phi^{(L)} \right] \), which can be controlled by the \( L^2 \)-error of the TT approximation, as shown in Lemma 3.4.

Assuming that the function of interest \( f \) is non-negative, the goal of deep importance sampling is to estimate the normalizing constant \( \zeta^* = E_\bar{\rho} \rho^* T^{(L)} / \bar{\rho} T^{(L)} \) as an expectation with respect to the reference density \( \lambda \) such that

\[
\zeta^* = E_\lambda \left[ \rho^* T^{(L)} / \bar{\rho} T^{(L)} \right].
\]

This leads to the deep importance sampling estimator

\[
\hat{\zeta}_{\bar{\rho}, N} = \frac{1}{N} \sum_{i=1}^N \rho^* \{ T^{(L)}(U^i) \} / \bar{\rho} \{ T^{(L)}(U^i) \}, \quad U^i \sim \lambda.
\]

Its properties are established in the following lemma.
LEMMA 3.6. Suppose Assumptions 3.1–3.3 holds, and let $p^* = \rho^*/\zeta^*$ and $\bar{p}$ be the exact optimal importance density (3.1) and its approximation in (3.9), respectively. Then, we have $E_{\bar{p}}(p^*) \subseteq \supp(\bar{p})$, $E_{\bar{p}}(p^*/\bar{p}) = \zeta^*$ and $\text{var}_{\bar{p}}(p^*/\bar{p}) < \infty$.

1. Assuming furthermore $\{\rho^*(x)/\pi_0(x)\}^2\pi_0(x)dx < \infty$, then

$$\text{var}_{\bar{p}}(p^*/\bar{p}) \leq C_pD_H(p^*, \bar{p}), \quad \text{where} \quad C_p = 2 \left[ E_{p^*}\{(p^*/\bar{p})^2\} - E_{\bar{p}}\{(p^*/\bar{p})^2\} \right]^{1/2}. $$

3. Assuming instead that $\sup_{x \in \mathcal{X}} p^*(x)/\bar{p}(x) = M_{p^*/\bar{p}} < \infty$, then

$$\text{var}_{\bar{p}}(p^*/\bar{p}) \leq C_mD_H(p^*, \bar{p})^2, \quad \text{where} \quad C_m = 4 + 4M_{p^*/\bar{p}}. $$

Proof. Because $\bar{g}^{(t)}(x)^2 \geq 0$ and $\lambda(x) \geq 0$ for all $x \in \mathcal{X}$, the density $\bar{p}(x)$ satisfies

$$\bar{p}(x) \geq \lambda(x) \left\{ \prod_{t=1}^L \frac{\tau^{(t)}}{\zeta^{(t)}} \right\} \quad \text{(3.11)}$$

for all $x \in \mathcal{X}$, which leads to $\supp(\lambda) \subseteq \supp(\bar{p})$. Under Assumption 3.3, we have $\supp(\rho^*) \subseteq \supp(\lambda) \subseteq \supp(\bar{p})$, and thus we can express $\zeta^*$ as

$$\zeta^* = \int_{\mathcal{X}} \frac{\rho^*(x)}{\pi_0(x)}\pi_0(x) dx = \int_{\mathcal{X}} \frac{\rho^*(x)}{\bar{p}(x)}\bar{p}(x) dx.$$

Furthermore, the identity in (3.11) also leads to

$$\frac{\pi_0(x)}{\bar{p}(x)} \leq \frac{\pi_0(x)}{\lambda(x)} \left\{ \prod_{t=1}^L \frac{\zeta^{(t)}}{\tau^{(t)}} \right\}. $$

Together with Assumption 3.3, we also have $\sup_{x \in \mathcal{X}} \pi_0(x)/\bar{p}(x) < \infty$. This way, the second moment $E_{\bar{p}}[(p^*/\bar{p})^2]$ satisfies

$$E_{\bar{p}}\left\{ \left( \frac{\rho^*}{\bar{p}} \right)^2 \right\} = \int_{\mathcal{X}} \left\{ \frac{\rho^*(x)}{\pi_0(x)} \right\}^2 \frac{\pi_0(x)}{\bar{p}(x)}\pi_0(x) dx \leq E_{\pi_0} \left\{ \left( \frac{\rho^*}{\pi_0} \right)^2 \right\} \sup_{x \in \mathcal{X}} \frac{\pi_0(x)}{\bar{p}(x)}. $$

Then, we have $E_{\bar{p}}[(p^*/\bar{p})^2] < \infty$ by Assumption 3.2 and thus the first result follows.

Recall that the relative variance takes the form

$$\text{var}_{\bar{p}}(p^*/\bar{p}) = E_{\bar{p}}\{(p^*/\bar{p})^2\} - E_{\bar{p}}(p^*/\bar{p})^2, $$

where $E_{\bar{p}}(p^*/\bar{p}) = 1$. Together with $\supp(p^*) \subseteq \supp(\bar{p})$ in the first result, the relative variance can be expressed as

$$\text{var}_{\bar{p}}(p^*/\bar{p}) = E_{\bar{p}}\{(p^*/\bar{p})^2\} - 1$$

$$\begin{align*}
= & E_{p^*}(p^*/\bar{p}) - E_{\bar{p}}(p^*/\bar{p}) \\
= & \int_{\mathcal{X}} \frac{p^*(x)}{\bar{p}(x)}p^*(x) dx - \int_{\mathcal{X}} \frac{p^*(x)}{\bar{p}(x)}\bar{p}(x) dx - \int_{\mathcal{X}} p^*(x) dx + \int_{\mathcal{X}} \bar{p}(x) dx \\
= & \int_{\mathcal{X}} \left\{ \frac{p^*(x)}{\bar{p}(x)} - 1 \right\}p^*(x) dx - \int_{\mathcal{X}} \left\{ \frac{p^*(x)}{\bar{p}(x)} - 1 \right\}\bar{p}(x) dx \\
= & \int_{\mathcal{X}} \left\{ \frac{p^*(x)}{\bar{p}(x)} - 1 \right\}\{p^*(x) - \bar{p}(x)\} dx \\
= & \int_{\mathcal{X}} \left\{ \frac{p^*(x)}{\bar{p}(x)} - 1 \right\}\{\sqrt{p^*(x)} + \sqrt{\bar{p}(x)}\} \{\sqrt{p^*(x)} - \sqrt{\bar{p}(x)}\} dx. \quad \text{(3.12)}
\end{align*}$$
Apply the Cauchy-Schwartz inequality to (3.12), the relative variance has the bound

$$\text{var}_\tilde{p}(p^*/\tilde{p}) \leq \left[ \int_X \left\{ \frac{p^*(x)}{\tilde{p}(x)} - 1 \right\} \left\{ \sqrt{p^*(x)} + \sqrt{\tilde{p}(x)} \right\}^2 dx \right]^{\frac{1}{2}} \left[ \int_X \{ \sqrt{p^*(x)} - \sqrt{\tilde{p}(x)} \}^2 dx \right]^{\frac{1}{2}}$$

(3.13)

$$= \left[ \int_X \left\{ \frac{p^*(x)}{\tilde{p}(x)} - 1 \right\} \left\{ \sqrt{p^*(x)} + \sqrt{\tilde{p}(x)} \right\}^2 dx \right]^{\frac{1}{2}} \sqrt{2D_H(p^*, \tilde{p})}.$$  

Depending on the assumption imposed on $p^*/\tilde{p}$, the upper bound of $\text{var}_\tilde{p}(p^*/\tilde{p})$ depends differently on the Hellinger error. We note that

$$\left[ \int_X \left\{ \frac{p^*(x)}{\tilde{p}(x)} - 1 \right\} \left\{ \sqrt{p^*(x)} + \sqrt{\tilde{p}(x)} \right\}^2 dx \right]^{\frac{1}{2}}$$

$$\leq \sqrt{2} \left[ \int_X \left\{ \frac{p^*(x)}{\tilde{p}(x)} - 1 \right\} p^*(x) dx + \int_X \left\{ \frac{p^*(x)}{\tilde{p}(x)} - 1 \right\} \tilde{p}(x) dx \right]^{\frac{1}{2}}$$

$$= \sqrt{2} \left[ \int_X \left\{ \frac{p^*(x)}{\tilde{p}(x)} \right\} p^*(x) dx - \int_X \left\{ \frac{p^*(x)}{\tilde{p}(x)} \right\} \tilde{p}(x) dx \right]^{\frac{1}{2}}$$

(3.14)

$$= \sqrt{2} \left[ E_{p^*}(p^*/\tilde{p})^2 - E_{\tilde{p}}(p^*/\tilde{p})^2 \right]^{\frac{1}{2}}.$$  

Note that $E_{p^*}(p^*/\tilde{p})^2 \geq \{ E_{p^*}(p^*/\tilde{p}) \}^2$ and $E_{\tilde{p}}(p^*/\tilde{p})^2 \geq \{ E_{\tilde{p}}(p^*/\tilde{p}) \}^2 = 1$ by Jensen’s inequality. Together with $E_{p^*}(p^*/\tilde{p}) = E_{\tilde{p}}(p^*/\tilde{p})^2$, the difference on the right hand side of (3.14) is non-negative. In addition, we have

$$E_{p^*}(p^*/\tilde{p})^2 = E_{\tilde{p}}(p^*/\tilde{p})^3 = \frac{1}{(\zeta^*)^3} E_{\tilde{p}}(p^*/\tilde{p})^3 < \infty,$$

which can be obtained using a similar derivation as in the proof of the first result and the assumption that the ratio $\rho^*/\pi_0$ has finite third moment with respect to $\pi_0$. Thus, we have the upper bound

$$\text{var}_\tilde{p}(p^*/\tilde{p}) \leq 2 \left[ E_{p^*}(p^*/\tilde{p})^2 - E_{\tilde{p}}(p^*/\tilde{p})^2 \right]^{\frac{1}{2}} D_H(p^*, \tilde{p}),$$

which concludes the second result of this Lemma.

With a more restrictive assumption $\sup_{x \in X} p^*(x)/\tilde{p}(x) = M_{p^*, \tilde{p}} < \infty$, we can also use the identity

$$\left[ \int_X \left\{ \frac{p^*(x)}{\tilde{p}(x)} - 1 \right\} \left\{ \sqrt{p^*(x)} + \sqrt{\tilde{p}(x)} \right\}^2 dx \right]^{\frac{1}{2}}$$

$$= \left[ \int_X \left\{ \frac{\sqrt{p^*(x)}}{\sqrt{\tilde{p}(x)}} + 1 \right\} \left\{ \sqrt{p^*(x)} - \sqrt{\tilde{p}(x)} \right\}^2 dx \right]^{\frac{1}{2}}$$

$$\leq \left[ \sup_{x \in X} \left\{ \frac{\sqrt{p^*(x)}}{\sqrt{\tilde{p}(x)}} + 1 \right\} 2 D_H(p^*, \tilde{p}) \right]^{\frac{1}{2}}$$

$$= \sqrt{2(1 + M_{p^*, \tilde{p}})^2} D_H(p^*, \tilde{p})$$

(3.15)

$$\leq 2\sqrt{2(1 + M_{p^*, \tilde{p}})} D_H(p^*, \tilde{p})$$

Plugging the above identity into (3.13), we obtain the upper bound

$$\text{var}_\tilde{p}(p^*/\tilde{p}) \leq (4 + 4 M_{p^*, \tilde{p}}) D_H(p^*, \tilde{p}).$$

This concludes the third result of this Lemma.

The first condition of Lemma 3.6 establishes that the estimator $\hat{\zeta}_{p,N}$ is unbiased and satisfies the central limited theorem, i.e., $\sqrt{N} \hat{\zeta}_{p,N} \xrightarrow{d} N(\zeta^*, \text{var}_\tilde{p}(p^*/\tilde{p}))$, where $\xrightarrow{d}$ denotes convergence in distribution. Since $p^* = \rho^*/\zeta^*$, and thus $E_{\tilde{p}}(p^*/\tilde{p}) = 1$, the variance $\text{var}_\tilde{p}(p^*/\tilde{p})$ can be
interpreted as the relative variance of the importance ratio \( \rho^*/\bar{p} \), i.e., \( (\zeta^*)^{-2} \text{var}_p(\rho^*/\bar{p}) = \text{var}_p(\rho^*/\bar{p}) \). In this way, the relative mean square error of the estimator \( \hat{\zeta}_{p,N} \) is given by

\[
\text{rmse}(\hat{\zeta}_{p,N}, \zeta^*) = N^{-1} \{ \zeta^* \}^{-2} \text{var}_p(\rho^*/\bar{p}) = N^{-1} \text{var}_p(\rho^*/\bar{p}).
\]

Thus, to guarantee a \( \text{rmse}(\hat{\zeta}_{p,N}, \zeta^*) \leq \varepsilon \) for some error threshold \( \varepsilon > 0 \), it is sufficient to choose either \( N \geq C_p \varepsilon^{-1} D_H(\rho^*/\bar{p}, \bar{p}) \) or \( N \geq C_m \varepsilon^{-1} D_H(\rho^*/\bar{p})^2 \), depending on whether the assumption in Part 2 or Part 3 of Lemma 3.6 holds, respectively.

3.4. The ratio estimator: from a priori to a posteriori expectations. Finally, we want to extend the concept of deep importance sampling just introduced to the case of a posteriori expectations using the ratio estimator in (2.8). The optimal importance densities for estimating the numerator and the denominator in (2.8) are \( p^* \propto \int L^y \pi_0 \) and \( q^* \propto \int L^y \pi_0 \), respectively. We can apply Alg. 3.1 to construct two composite maps \( T_p^{(L)} \) and \( T_q^{(L)} \) to approximately push forward the reference density \( \tilde{p} \) building a normalized posterior approximation. In general, we can choose different numbers of layers for \( T_p^{(L)} \) and \( T_q^{(L)} \) to adapt to the structures of two optimal densities.

We are now ready to define the ratio estimator based on deep importance sampling

\[
\hat{R}_{p,q,N} = \frac{\hat{Q}_{p,N}}{\hat{Z}_{q,N}}, \quad \hat{Q}_{p,N} = \frac{1}{N} \sum_{i=1}^{N} w_Q(U_{p}^i), \quad \hat{Z}_{q,N} = \frac{1}{N} \sum_{i=1}^{N} w_Z(U_{q}^i), \quad U_{p}^i, U_{q}^i \sim \lambda,
\]

where

\[
w_Q(U) = \frac{f(T_p^{(L)}(U))L^y(T_p^{(L)}(U))\pi_0(T_p^{(L)}(U))}{\tilde{p}(T_p^{(L)}(U))}, \quad w_Z(U) = \frac{L^y(T_q^{(L)}(U))\pi_0(T_q^{(L)}(U))}{\tilde{q}(T_q^{(L)}(U))}.
\]

For variance reduction, we consider that each pair of random variables \( (U_{p}^i, U_{q}^i) \) follows some joint distribution but their marginal laws have the reference density \( \lambda \).

To simplify notation, we define random variables \( W_Q = w_Q(U_{p}) \) and \( W_Z = w_Z(U_{q}) \). Under Assumptions 3.2 and 3.3, we have \( E(W_Q) = Q \) and \( E(W_Z) = Z \), and thus \( \hat{Q}_{p,N} \) and \( \hat{Z}_{q,N} \) are unbiased estimators of \( Q \) and \( Z \), respectively. However, in general the resulting ratio estimator \( \hat{R}_{p,q,N} \) is only asymptotically unbiased. In Lemmas 3.8 and 3.9, we want to characterize the asymptotic behaviour of the relative mean square error of \( \hat{R}_{p,q,N} \) using its relative deviation from the a posteriori expectation \( R = Q/Z \). We define the relative mean square error of \( \hat{R}_{p,q,N} \) as

\[
\Delta_{R,N} = \frac{\hat{R}_{p,q,N} - R}{R} = \frac{\sum_{i=1}^{N} W_Q^i/Q}{\sum_{i=1}^{N} W_Z^i/Z} - 1,
\]

which is controlled by the laws of \( W_Q^1, ..., W_Q^N \) and \( W_Z^1, ..., W_Z^N \).

Remark 3.7. The following definitions and results are used for showing properties of \( \Delta_{R,N} \). We introduce the relative derivations of \( \hat{Q}_{p,N} \) and \( \hat{Z}_{q,N} \), which are given by

\[
\Delta_{Q,N} = \frac{\hat{Q}_{p,N} - Q}{Q} \quad \text{and} \quad \Delta_{Z,N} = \frac{\hat{Z}_{q,N} - Z}{Z},
\]

respectively. Defining random variables \( \Theta_Q := W_Q/Q - 1 \) and \( \Theta_Z := W_Z/Z - 1 \), the relative derivations \( \Delta_{Q,N} \) and \( \Delta_{Z,N} \) can be expressed as

\[
\Delta_{Q,N} = \frac{1}{N} \sum_{i=1}^{N} \Theta_Q^i, \quad \Delta_{Z,N} = \frac{1}{N} \sum_{i=1}^{N} \Theta_Z^i.
\]
Note that \( E(\Theta_Q) = E(\Theta_Z) = 0 \) as \( E(W_Q) = Q \) and \( E(W_Z) = Z \). Thus, \( E(\Delta_{Q,N}) = E(\Delta_{Z,N}) = 0 \) for any sample size \( N \). The variances and the covariance of \( \Theta_Q \) and \( \Theta_Z \) can be given as

\[
(3.19) \quad \text{var}(\Theta_Q) = \frac{\text{var}(W_Q)}{Q^2}, \quad \text{var}(\Theta_Z) = \frac{\text{var}(W_Z)}{Z^2}, \quad \text{cov}(\Theta_Q, \Theta_Z) = \frac{\text{cov}(W_Q, W_Z)}{QZ}.
\]

The relative deviation \( \Delta_{R,N} \) can be expressed as

\[
\Delta_{R,N} = R_p Q_N - R = Z \frac{\hat{Q}_N - Q}{Z} = 1 + \Delta_{Q,N} - \frac{\Delta_{Q,N} - \Delta_{Z,N}}{1 + \Delta_{Z,N}}.
\]

Applying Taylor’s theorem, there exist some \( s, t \in [0,1] \) such that

\[
(3.20) \quad (1 + \Delta_{Z,N})^{-1} = 1 - (1 + s\Delta_{Z,N})^{-1} \Delta_{Z,N},
\]

\[
(3.21) \quad (1 + \Delta_{Z,N})^{-1} = 1 - \Delta_{Z,N} - (1 + t\Delta_{Z,N})^{-1} \Delta_{Z,N}^2,
\]

where \( s \) and \( t \) depend on \( \Delta_{Z,N} \). The term \( 1 + s\Delta_{Z,N} \) (and similarly \( 1 + t\Delta_{Z,N} \)) satisfies

\[
1 + s\Delta_{Z,N} = (1 - s) + s(1 + \Delta_{Z,N}) = (1 - s) + s\hat{Z}_{q,N}/Z > 0
\]

almost surely, because the estimator \( \hat{Z}_{q,N} \) is almost surely positive by construction. Thus, the expansions in (3.20) and (3.21) are not subject to division-by-zero. □

**Lemma 3.8.** Suppose Assumptions 3.1–3.3 hold and the sequence \( \{ (W_Q, W_Z) \}_{i=1}^N \) is i.i.d., but allowing each pair \( (W_Q, W_Z) \) to be correlated. Then, we have

\[
\sqrt{N}\Delta_{R,N} \xrightarrow{d} \mathcal{N}\left(0, \frac{\text{var}(W_Q)}{Q^2} + \frac{\text{var}(W_Z)}{Z^2} - \frac{2\text{cov}(W_Q, W_Z)}{QZ} \right).
\]

**Proof.** Using the expansion (3.20), we have

\[
\sqrt{N}\Delta_{R,N} = \sqrt{N}(\Delta_{Q,N} - \Delta_{Z,N}) - \frac{\Delta_{Z,N}}{(1 + s\Delta_{Z,N})^2} \sqrt{N}(\Delta_{Q,N} - \Delta_{Z,N}).
\]

Since \( \Delta_{Q,N} - \Delta_{Z,N} = \sum_{i=1}^N \Theta_Q - \Theta_Z \), we have \( \sqrt{N}(\Delta_{Q,N} - \Delta_{Z,N}) \) converges in distribution to \( \mathcal{N}(0, \text{var}(\Theta_Q - \Theta_Z)) \) by the central limit theorem, where

\[
\text{var}(\Theta_Q - \Theta_Z) = \text{var}(\Theta_Q) + \text{var}(\Theta_Z) - 2\text{cov}(\Theta_Q, \Theta_Z).
\]

Since the sequence \( \Delta_{Z,N} \) converge to zero in probability as \( N \) tends to infinity, i.e., \( \Delta_{Z,N} = o_p(1) \), and the sequence \( \sqrt{N}(\Delta_{Q,N} - \Delta_{Z,N}) \) is tight, the result follows from Slutsky’s theorem and the identities in (3.19). □

Thus, the ratio estimator in (3.16) is asymptotically unbiased and converges at the correct rate with respect to the sample size \( N \). We also see that by correlating each pair of random variables \( (U^i_p, U^i_q) \) in (3.16) we can maximize the correlation between \( W_Q = w_Q(U_p) \) and \( W_Z = w_Z(U_q) \) to minimize the relative variance of the ratio estimator. For example, if \( \lambda \) is a zero mean Gaussian distribution, one can use the antithetic formula \( U_p = aU_q + (1 - a^2)^{1/2}\epsilon \), with \( \epsilon \sim \lambda \) and some constant \( a \) to correlate or anti-correlate the random variables. This way, the marginal distributions of \( (U_p, U_q) \) still have the same density \( \lambda \), but \( U_p \) and \( U_q \) are correlated and it is possible to maximize \( \text{cov}(W_Q, W_Z) \) as a function of \( a \).

To get a more explicit, quantitative result regarding the benefits of the deep importance sampling strategy, in the following lemma we focus only on the case of independent samples \( U^i_p, U^i_q \), for each \( i = 1, \ldots, N \).
Lemma 3.9. Under the assumptions of Lemma 3.8, but now assuming furthermore independence of \( \{W_Q^i\}_{i=1}^N \) and \( \{W_Z^i\}_{i=1}^N \), the relative bias of \( \hat{R}_{\tilde{p}, \tilde{q}, N} \) satisfies

\[
\frac{N|E(\hat{R}_{\tilde{p}, \tilde{q}, N}) - R|}{R} \rightarrow \frac{\text{var}(W_Z)}{Z^2} \quad \text{as} \quad N \rightarrow \infty,
\]

and the relative mean square error of \( \hat{R}_{\tilde{p}, \tilde{q}, N} \) satisfies

\[
\text{rmse}(\hat{R}_{\tilde{p}, \tilde{q}, N}, R) = O \left\{ \frac{C_p D_H(p^*, \bar{p}) + C_q D_H(q^*, \bar{q})}{N} + \frac{1}{N^2} \right\},
\]

where

\[
C_p = 2|E_p^* \{ (p^*/\bar{p})^2 \} - E_p \{ (p^*/\bar{p})^2 \}|^{1/2}, \quad C_q = 2|E_q^* \{ (q^*/\bar{q})^2 \} - E_q \{ (q^*/\bar{q})^2 \}|^{1/2}.
\]

Proof. Using (3.21), the expected relative deviation \( \Delta_{R,N} \) can be expressed as

\[
E(\Delta_{R,N}) = E(\Delta_{Q,N}) - E(\Delta_{Z,N}) - E(\Delta_{Q,N} \Delta_{Z,N}) + E \left[ \Delta_{Z,N}^2 \left\{ 1 + \frac{\Delta_{Q,N} - \Delta_{Z,N}}{(1 + t \Delta_{Z,N})^3} \right\} \right],
\]

where \( t \in [0, 1] \) depending on \( \Delta_{Z,N} \). Recall Remark 3.7, we have \( E(\Delta_{Q,N}) = 0 \) and \( E(\Delta_{Z,N}) = 0 \) for any given sample size \( N \). With the additional assumption that the sequences \( \{W_Q^i\}_{i=1}^N \) and \( \{W_Z^i\}_{i=1}^N \) are independent, we have that \( \{\Theta_Q^i\}_{i=1}^N \) and \( \{\Theta_Z^i\}_{i=1}^N \) are also independent. Therefore, we have mutually independent \( \Delta_{Q,N} \) and \( \Delta_{Z,N} \) for all \( N \), and hence \( E(\Delta_{Q,N} \Delta_{Z,N}) = 0 \). This leads to

\[
E(\Delta_{R,N}) = E \left[ \Delta_{Z,N}^2 \left\{ 1 + \frac{\Delta_{Q,N} - \Delta_{Z,N}}{(1 + t \Delta_{Z,N})^3} \right\} \right].
\]

Thus, we can introduce a random variable

\[
B_N = \Delta_{Z,N}^2 \left\{ 1 + \frac{\Delta_{Q,N} - \Delta_{Z,N}}{(1 + t \Delta_{Z,N})^3} \right\}
\]

such that the relative bias of \( \hat{R}_{\tilde{p}, \tilde{q}, N} \) satisfies

\[
\frac{|E(\hat{R}_{\tilde{p}, \tilde{q}, N}) - R|}{R} = |E(\Delta_{R,N})| = |E(B_N)|.
\]

We want to use Slutsky’s theorem to examine the property of the sequence

\[
\frac{NB_N}{\text{var}(\Theta_Z)} = \left\{ \frac{\sqrt{N} \Delta_{Z,N}}{\sqrt{\text{var}(\Theta_Z)}} \right\}^2 \left\{ 1 + \frac{\Delta_{Q,N} - \Delta_{Z,N}}{(1 + t \Delta_{Z,N})^3} \right\}.
\]

Since \( \sqrt{N} \Delta_{Z,N} \xrightarrow{d} N(0, \text{var}(\Theta_Z)) \), the ratio \( \sqrt{N} \Delta_{Z,N} / \sqrt{\text{var}(\Theta_Z)} \xrightarrow{d} N(0, 1) \). Then, the continuous mapping theorem implies that the term \( \{ \sqrt{N} \Delta_{Z,N} / \sqrt{\text{var}(\Theta_Z)} \}^2 \xrightarrow{d} \chi_1^2 \) converges in distribution to the random variable \( \xi^2 \), where \( \xi \sim \chi_1(0, 1) \).

Note that \( \xi^2 \) follows the chi-squared distribution with one degree of freedom, i.e., \( \xi^2 \sim \chi_1^2 \), and hence we equivalently have \( \{ \sqrt{N} \Delta_{Z,N} / \sqrt{\text{var}(\Theta_Z)} \}^2 \xrightarrow{d} \chi_1^2 \). Since \( \Delta_{Z,N} = o_p(1) \) and \( \Delta_{Q,N} = o_p(1) \), we have \( NB_N / \text{var}(\Theta_Z) \xrightarrow{d} \chi_1^2 \) by Slutsky’s theorem. Thus, by the Portmanteau lemma, we have \( E[NB_N / \text{var}(\Theta_Z)] \rightarrow 1 \) as \( N \rightarrow \infty \). Therefore, applying the identities in (3.19), as \( N \rightarrow \infty \) the asymptotic behaviour of the relative bias satisfies

\[
\frac{N|E(\hat{R}_{\tilde{p}, \tilde{q}, N}) - R|}{R} \rightarrow \frac{\text{var}(W_Z)}{Z^2}.
\]
Thus, the relative bias is asymptotically $O(N^{-1})$.

With the additional assumption that the sequences $\{W_Q^i\}_{i=1}^N$ and $\{W_Z^j\}_{j=1}^N$ are also independent, we have $\text{cov}(W_Q, W_Z) = 0$. Applying the result of Lemma 3.8, the relative mean square error of $\hat{R}_{\bar{p}, \bar{q}}$ asymptotically follows

$$\text{rmse}(\hat{R}_{\bar{p}, \bar{q}}, R) = O\left\{\frac{\text{var}(W_Q)}{NQ^2} + \frac{\text{var}(W_Z)}{NZ^2} + \frac{1}{N^2}\right\}.$$ 

Since $\text{var}(W_Q)/Q^2 = \text{var}(p^*/\bar{p})$ and $\text{var}(W_Z)/Z^2 = \text{var}(q^*/\bar{q})$, the rest of the proof directly follows from the second result of Lemma 3.6.

Lemma 3.9 suggests that the bias is negligible with a large, finite sample size. More importantly, the relative mean square error can be greatly reduced by constructing two importance densities $\bar{p}$ and $\bar{q}$ that can accurately approximate the corresponding optimal densities $p^*$ and $q^*$. In theory, the Hellinger errors on the right hand side of (3.22) can be made to go to zero by increasing the tensor ranks and the number of discretization basis functions, leading to a zero-variance estimator. In comparison, the self-normalized importance sampling method uses identical importance densities for estimating the numerator and the denominator, i.e., $\bar{p} = \bar{q}$, which is always suboptimal at least for one of the terms. This leads to a theoretical lower bound on the estimation variance for finite sample size that cannot be further reduced.

4. Application to rare event estimation. We now use deep importance sampling to devise efficient estimators for $a$ priori and $a$ posteriori failure probabilities. The failure function $f(x) = 1_{A}\{h(x)\}$ defined in (2.9) will in general have discontinuities at the boundary of the failure set $A_F := \{x \in \mathcal{X} : f(x) = 1\}$. When the boundary of $A_F$ is not aligned with the coordinate axes in the parameter domain, the resulting TT approximation of the optimal importance density may have high ranks. The discontinuities also make it challenging to choose appropriate bases to efficiently discretize the optimal importance density. To alleviate those difficulties and to provide a natural family of intermediate densities $\phi^{(1)}, ..., \phi^{(L)}$ for Alg. 3.1, we construct a smooth surrogate $g_\gamma(z; A)$ that converges to the indicator function $1_A(z) = \gamma \rightarrow \infty$, that is, $g_\gamma(z; A)$ is continuous for $\gamma < \infty$ and $\lim_{\gamma \rightarrow \infty} g_\gamma(z; A) = 1_A(z)$.

For simplicity, we assume that $A = [a, b]$ for some $a < b$. In fact, since the indicator function satisfies $1_{[a,b]}(z) = 1_{[a,\infty)}(z) - 1_{[b,\infty)}(z)$ and $1_{(-\infty,a]}(z) = 1 - 1_{(a,\infty)}(z)$ for any finite $a$ and $b$, without loss of generality, it suffices to consider the case $A = [a, \infty)$ with $a < \infty$. Since the weak derivative of $1_{[a,\infty)}(z)$ is the Dirac delta $\delta(z-a)$, one can employ a probability density function $p_\gamma(z-a)$ such that $\lim_{\gamma \rightarrow \infty} p_\gamma(z-a)$ has the same distributional properties as $\delta(z-a)$, and then constructs the surrogate function via the corresponding distribution function $g_\gamma(z; [a, \infty)) = \int_{\infty}^z p_\gamma(z' - a)dz'$. In this work, we consider to use the density $p_\gamma(z-a) = [1 - \tanh((z-a)/\gamma/2)]^2/\gamma/4$, which leads to the sigmoid function

$$g_\gamma(z; [a, \infty)) = [1 + \exp(\gamma(a-z))]^{-1}.$$

This defines a smoothed failure function $f_\gamma(x) = g_\gamma(h(x); [a, \infty))$. Instead of directly approximating the optimal importance density $\rho^* = f\pi_0$ for estimating $E_{\pi_0}\{f(X)\}$, we choose a sufficiently large $\gamma^*$ and approximate the smoothed version $f_{\gamma^*}\pi_0$ to avoid potential discontinuities. This smoothing strategy is also used in [45, 55] for applying gradient-based dimension reduction methods in estimating $a$ priori failure probability.

For the $a$ priori rare event, we can now directly apply Alg. 3.1 to build a TT approximation of $f_{\gamma^*}\pi_0$. The smoothed failure function $f_{\gamma^*}(x)$ may still have a large gradient near the boundary of the failure set $A_F$ and it can concentrate in the tail of $\pi_0$. Thus, we use an increasing sequence of smoothing variables $\gamma_1 < \cdots < \gamma_L = \gamma^*$ to define the unnormalized intermediate densities

$$\phi^{(\ell)}(x) = f_{\gamma_\ell}(x)\pi_0(x), \quad \ell = 1, ..., L.$$
for Alg. 3.1. The computed composite map \( T^{(L)} \) then provides an importance density \( \tilde{p} = \{ T^{(L)} \}_y \lambda \) that is close to the smoothed optimal importance density \( f_{\gamma} \pi_0 \), and for \( \gamma^* \) sufficiently large, also close to the optimal importance density \( p^* \). Finally, to estimate the \textit{a priori} rare event probability, we can use the deep importance sampling estimator (3.10) with \( \rho^* = f \pi_0 \).

To estimate the \textit{a posteriori} rare event probability, the ratio estimator based on deep importance sampling defined in (3.16) can be used. Using a tempering approach as in [20, 31], the intermediate densities for the denominator \( E_{\pi_0} \{ L^y \} \) of the ratio estimator in Alg. 3.1 are chosen to be

\[
\phi^{(\ell)}_d(x) = \{ L^y(x) \}^{\alpha_\ell} \pi_0(x), \quad 1 \leq \ell \leq L,
\]

where \( \alpha_1 < \cdots < \alpha_L = 1 \). For \( \alpha_\ell < 1 \), the unnormalized density \( \{ L^y(x) \}^{\alpha_\ell} \pi_0(x) \) is significantly less concentrated compared to the unnormalized posterior \( L^y(x) \pi_0(x) \) and can be approximated more easily using TTs. The resulting composite map \( T^{(L)}_q \) defines a density \( \tilde{q} = \{ T^{(L)}_q \}_y \lambda \) that approximates the optimal importance density \( q^* \equiv \pi^y \). For the numerator \( E_{\pi_0} \{ f L^y \} \) of the ratio estimator in (3.16), we smooth the failure function, as in the \textit{a priori} case, and temper the likelihood to define intermediate densities

\[
\phi^{(\ell)}_n(x) = f_{\gamma\ell}(x) \{ L^y(x) \}^{\beta_\ell} \pi_0(x), \quad 1 \leq \ell \leq L,
\]

for Alg. 3.1, where \( \gamma_1 < \cdots < \gamma_L = \gamma^* \) and \( \beta_1 < \cdots < \beta_L = 1 \). This leads to the second composite map \( T^{(L)}_p \), which defines a density \( \tilde{p} = \{ T^{(L)}_p \}_y \lambda \) approximating the optimal importance density \( p^* \propto f L^y \pi_0 \). Finally, the two importance densities \( \tilde{p} \) and \( \tilde{q} \) can be used in (3.16) to evaluate the ratio estimator for the \textit{a posteriori} rare event probability.

5. Example 1: susceptible-infectious-removed model.

5.1. Problem setup. We consider a Bayesian parameter estimation problem for a compartmental susceptible-infectious-removed model, a simplified version of the model considered in [25]. Given a spatially dependent demographic model consisting of \( K \in \mathbb{N} \) compartments, we denote the numbers of susceptible, infectious and removed individuals in the \( k \)th compartment at a given time \( t \) by \( S_k(t) \), \( I_k(t) \) and \( R_k(t) \), respectively. The interaction among the individuals within and across the different compartments is modelled by the following system of differential equations

\[
\begin{align*}
\frac{dS_k}{dt} &= -\theta_k S_k I_k + \frac{1}{2} \sum_{j \in J_k} (S_j - S_k), \\
\frac{dI_k}{dt} &= \theta_k S_k I_k - \nu_k I_k + \frac{1}{2} \sum_{j \in J_k} (I_j - I_k), \\
\frac{dR_k}{dt} &= \nu_k I_k + \frac{1}{2} \sum_{j \in J_k} (R_j - R_k),
\end{align*}
\]

(5.1)

where \( J_k \) is the index set containing all neighbours of the \( k \)th compartment. See Fig. 1 for an example of the demographic connectivity graph of the states in Austria. The system of differential equations is parameterized by \( \theta_k \in \mathbb{R} \) and \( \nu_k \in \mathbb{R} \), representing the infection and recovery rate in the \( k \)th compartment, respectively. We aim to estimate the unknown parameters \( x = (\theta_1, \nu_1, \ldots, \theta_K, \nu_K) \in \mathbb{R}^{2K} \) from noisy observations of \( I_k(t) \) at discrete times. We also aim to estimate the \textit{a posteriori} risk, which is the probability of the number of infected individuals exceeding a chosen threshold.

5.2. Experiments on a one-dimensional lattice. We first consider a compartment model defined on a one-dimensional lattice, in which the \( k \)th compartment is only connected to compartments with adjacent indices \( k - 1 \) and \( k + 1 \). By changing the number of compartments, \( K \), we can vary the parameter dimension to test the scalability of deep importance sampling. We impose periodic boundary conditions, such that \( Z_{K+1} = Z_1 \) and \( Z_0 = Z_K \) for \( Z \in \{ S, I, R \} \). The differential equations in (5.1) are solved for the time interval \( t \in [0, 5] \) with
fixed inhomogeneous initial states $S_k(0) = 99 - K + k$, $I_k(0) = K + 1 - k$, and $R_k(0) = 0$ for $k = 1, ..., K$.

For parameter estimation, synthetic observations are generated from noisy measurements of infected population in each of compartments at 6 equidistant time points,

$$y_{k,j} = I_k \left( \frac{5j}{6}; x_{\text{true}} \right) + \eta_{k,j}, \quad \eta_{k,j} \sim \mathcal{N}(0, 1), \quad k = 1, ..., K, \quad j = 1, ..., 6,$$

where the “true” parameter $x_{\text{true}} = [0, 1, 1, ..., 0, 1, 1]$, is used for simulating the synthetic observations. This leads to the likelihood function

$$(5.2) \quad \mathcal{L}^y(x) \propto \exp \left[ -\frac{1}{2} \sum_{k=1}^{K} \sum_{j=1}^{6} \left( I_k \left( \frac{5j}{6}; x \right) - y_{k,j} \right)^2 \right].$$

The differential equations are solved by the explicit Runge–Kutta method with adaptive time steps that control both absolute and relative errors to be within $10^{-6}$. We specify a uniform prior on the domain $[0, 2]$ for each of $\theta_k$ and $\nu_k$, which leads to $\pi_0(x) = \prod_{k=1}^{2K} 1_{[0,2]}(x_k)$. The \textit{a posteriori} risk is defined as the posterior probability of the number of infected individuals in the last compartment at any time $t \in [0, 5]$ exceeding a threshold $I_{\text{max}} > 0$,

$$\text{pr}_{\pi^y} \left\{ \max_{t \in [0,5]} I_K(t; X) > I_{\text{max}} \right\}.$$ 

To apply deep importance sampling within the ratio estimator (3.16), we use a sequence of intermediate densities $\phi_{d}^{(\ell)}(x) = \left( \mathcal{L}^y(x) \right)^{\alpha_\ell} \pi_0(x)$, $\ell = 1, ..., L$, with tempered likelihood functions to guide Alg. 3.1 for the denominator. The tempering parameters start from $\alpha_1 = 10^{-4}$ and are incremented such that $\alpha_{\ell+1} = 10^{1/3} \alpha_\ell$ until $\alpha_L = 1$. Thus, $L = 13$. For the numerator of the ratio estimator (3.16), we use another sequence of intermediate densities with the sigmoid smoothing

$$(5.3) \quad \phi_{n}^{(\ell)}(x) = \left( \mathcal{L}^y(x) \right)^{\beta_\ell} \pi_0(x) \left( 1 + \exp \left[ \gamma_\ell \left( I_{\text{max}} - \max_{t \in [0,5]} I_K(t; x) \right) \right] \right)^{-1}, \quad \ell = 1, ..., L.$$

Here, we let $\beta_\ell = \alpha_\ell$. The smoothing widths are chosen such that $\gamma_\ell = \beta_\ell \gamma^*$, where $\gamma^*$ will be varied in different experiments. In the construction of the tensor-train approximations, $\lambda(x)$ is a truncated normal reference distribution on $[-3, 3]$, and we use piecewise linear basis functions on a uniform grid with $n_k = n = 17$ points to discretize the densities in each coordinate direction.

\textbf{Scalability and accuracy.} We vary the compartment number $K = \{3, 5, ..., 15\}$ and take the threshold $I_{\text{max}} = 88$. The threshold yields challenging values of the \textit{a posteriori} risk below $10^{-6}$ for all numbers of compartments in this set of experiments. We use a sample size of $N = 2^{14}$ in the ratio estimator.

We first fix the TT rank to $r_k = r = 7$ and the smoothing width to $\gamma^* = 10^4 / I_{\text{max}}$. The Hellinger errors of the deep importance densities, the estimated \textit{a posteriori} risks, and the number of density evaluations needed are shown in Fig. 2. We observe that the computational
positively correlated seed samples U

Alg. 3.1 appears to depend quadratically on r with true optimal biasing density p to approximate for Alg. 3.1. In contrast, the Hellinger distance of the approximation to the rank r deviation over 10 runs.

Example 1. In all figures, points denote average values, and error bars denote one standard number of function evaluations in Alg. 3.1 (right) for different numbers of compartments r (middle) for different TT ranks (right) in Example 1.

Variance reduction via sample correlation. To benchmark our deep importance sampling ap-

complexity, measured in the number of density evaluations, depends linearly on the dimension, while the Hellinger error increases only moderately for fixed TT ranks, roughly logarithmically in the probability value itself.

Then, we fix the number of compartments to K = 5, and investigate the impact of the TT rank r and the smoothing width γ* on the accuracy of deep importance sampling. Firstly, we set γ* = 10^r/I_{max} and vary r. As shown in Fig. 3, the errors in all approximate densities decay with r until the discretization error is reached, whereas the number of function evaluations in Alg. 3.1 appears to depend quadratically on r. Secondly, we fix the TT rank to r = 7 and vary the smoothing width γ*. As shown in the right plot of Fig. 3, the error in approximating the smoothed optimal importance density depends monotonically on γ*. This is expected, since a larger γ* leads to a less smooth final biasing density ϕ_{n}^{(L)}(x) that is more difficult to approximate for Alg. 3.1. In contrast, the Hellinger distance of the approximation to the true optimal biasing density p*(x) grows strongly as γ* decreases. The optimal value of γ* is therefore an intermediate one, achieved for this example between 10^3/I_{max} and 10^4/I_{max}.

Variance reduction via sample correlation. To confirm the variance reduction suggested by Lemma 3.8 we let K = 5, I_{max} = 88, γ* = 3000/I_{max} and r = 7. We consider positively correlated seed samples U_p = U_q ∼ λ with a = 1, uncorrelated samples U_p ∼ λ and U_q ∼ λ with a = 0, and negatively correlated samples with a = -2/3 and produce 20 batches of ratio estimators with N = 2^{12} samples each. The relative standard deviations of the estimated a posteriori risk are 1.2e-2, 1.4e-2 and 2.4e-2 for positively correlated, uncorrelated, and negatively correlated samples, respectively. Thus, the error is indeed reduced by making the correlation corr(Θ_Q, Θ_Z) > 0 positive, which confirms the result of Lemma 3.8.

Comparison with cross entropy. To benchmark our deep importance sampling ap-

Fig. 2: Hellinger errors in the densities (left), estimated a posteriori risk (middle) and total number of function evaluations in Alg. 3.1 (right) for different numbers of compartments K in Example 1.
Table 1: Average value of the a posteriori risk in Example 1 over 10 runs, ± 1 standard deviation, using the cross entropy method and deep importance sampling, as well as N/ESS (in brackets).

| $K$ | Cross entropy | Deep importance sampling |
|-----|---------------|--------------------------|
|     | $N = 10^5$   | $N = 10^6$               | $N \approx 2 \cdot 10^4$ |
| 1   | 4.731e-5 ± 9.58e-8 | 4.724e-5 ± 3.92e-8 | 4.726e-5 ± 9.22e-8 |
|     | (1.753 ± 3e-3)     | (1.721 ± 5.4e-2)       | (1.096 ± 3e-3)       |
| 2   | 3.911e-4 ± 9.11e-4 | 6.292e-5 ± 3.33e-5     | 8.270e-5 ± 2.03e-7   |
|     | (3689 ± 5197)      | (89259 ± 2e+4)         | (1.113 ± 6e-3)       |
| 3   | —              | —                        | 3.378e-4 ± 1.10e-6   |
|     |                |                           | (1.150 ± 5.5e-2)     |

proach we compare it to the cross entropy method of [4]. We vary the number of compartments, $K$, and compare the estimation accuracy of the cross entropy method and deep importance sampling. The cross entropy method has difficulties in estimating the rather small a posteriori risk in the above experiments. Therefore we reduce the threshold to $I_{\text{max}}=80$ in this experiment. For cross entropy, we use an importance density with a mixture of 4 Gaussian distributions. For our deep importance sampling method we use a TT rank of 3000/$I_{\text{max}}$. The estimated risks and their empirical standard deviations, which are computed over 10 replications, are summarized in Table 1, together with N/ESS estimates, where ESS denotes the effective sample size (see [29, 36] for details). We observe that the accuracy of the cross entropy method deteriorates drastically with the dimension, making $K=3$ compartments intractable even with a million samples per iteration. Increasing the number of mixture distributions gives similar results, while reducing it makes the results worse. In comparison, Alg. 3.1 is able to estimate the probability with less than 1% relative error in a fraction of the number of samples needed for the cross entropy method.

5.3. Experiments on the Austria model. Finally, we consider a more realistic setting where the model has $K=9$ compartments following the Austrian state adjacency map shown in Fig. 1. The initial condition is given as $S_1(0) = 99$, $I_1(0) = 1$, $R_1(0) = 0$ (in Vorarlberg), and $S_k(0) = 100$, $I_k(0) = R_k(0) = 0$ elsewhere. We estimate parameters $x \in \mathbb{R}^{18}$ from synthetic noisy observation of $\{I_k(5j/12; x_{\text{true}})\}$, $k = 1, ..., 9$, $j = 1, ..., 12$, with the same “true” parameter and likelihood model specified in the first experiment. The risk is defined as the number of infected individuals in Burgenland, indexed by $k = 9$, at any time $t \in [0, 5]$ exceeding a threshold $I_{\text{max}} = 69$. This value of $I_{\text{max}}$ corresponds to a dimensionless ratio of the highest number of hospitalizations (20000) and the expected initial number of infected individuals (290) employed in the modeling of lockdown strategies in England by [25].

To apply Alg. 3.1, we use the intermediate densities defined above, with different starting tempering parameters $\alpha_1=10^{-5}$ and $L=16$. The final smoothing width is fixed to $\gamma^*=10^2/I_{\text{max}}$. The TT ranks in each layer are adaptively chosen, with the maximum rank set to $r=7$. To estimate the performance we use again 10 replicated experiments. The performance is as in the previous experiments. Both importance densities used in the ratio estimator can be accurately estimated using the layered transport maps. For the denominator and the numerator, the estimated Hellinger errors of the approximate importance densities are $D_H(p^*, \bar{p})=0.135\pm 0.005$ and $D_H(p^*, \bar{p})=0.282 \pm 0.008$, respectively, using a total of 314371 $\pm$ 11727 density evaluations. The estimated a posteriori risk is $4.370 \times 10^{-10}$ with estimated standard derivation $1.05 \times 10^{-12}$.

6. Example 2: contaminant transport in groundwater.

6.1. Problem setup. We aim to estimate the risk of contaminant transport in a steady-state groundwater system; see [9] and the references therein. Here, the physical system is driven by some unknown random diffusivity field $\kappa(s, X)$ that cannot be directly observed, where $s \in D = [0, 1]^2$ is the spatial coordinate in the physical domain $D$ and $X$, taking values in $\mathbb{R}^d$, is some parameter describing the randomness of the diffusivity. The observable state of the system is the water table $u(s, X)$, which is a function that satisfies the partial differential
Fig. 4: Two groundwater experiments with a low diffusivity barrier (top row) and a high diffusivity channel (bottom row). First column: true diffusivity fields \( \kappa \). Second column: water tables \( u \) generated by true \( \kappa \) with observation locations (black dots). Third column: maximum \textit{a posteriori} estimates of diffusivity fields \( \kappa \). Fourth column: flow fields (blue arrows) and particle trajectories (red) computed using \( \kappa \) in the third column. The maximum \textit{a posteriori} particle breakthrough times of the top row and the bottom row are \( \tau = 0.1886 \) and \( \tau = 0.0929 \), respectively.

The advection equation

\[
- \nabla \cdot \{ \kappa(s, X) \nabla u(s, X) \} = 0, \quad s \in (0,1)^2,
\]

with Dirichlet boundary conditions \( u|_{s_1=0} = 1 + s_2/2 \) and \( u|_{s_1=1} = -\sin(2\pi s_2) - 1 \) imposed horizontally and no-flux boundary conditions \( \partial u/\partial s_2|_{s_2=0} = \partial u/\partial s_2|_{s_2=1} = 0 \) imposed vertically. The Dirichlet boundary conditions generate an inhomogeneous horizontal Darcy flow field \( \kappa(s, X) \nabla u(s, X) \). Figure 4 shows examples of flow fields and water tables generated by two different synthetic diffusivity fields. Contaminant particles released at a fixed location \( s^0 = (0,0.5) \) on the left boundary are transported by the flow field according to the advection equation

\[
\frac{ds(t, X)}{dt} = \kappa(s, X) \nabla u(s, X), \quad s(0, X) = s^0,
\]

to arrive at the right boundary after some time \( \tau \). The particle paths are shown in the right column of Fig. 4. The risk in this scenario is defined as the probability, subject to the random diffusivity \( \kappa(s, X) \), that the breakthrough time of contaminant particles, denoted by \( \tau(X) \), is below some threshold \( \tau_\ast \). This way, the \textit{a priori} risk and the \textit{a posteriori} risk are given by \( \text{pr}_{\pi_0}\{\tau(X) < \tau_\ast\} \) and \( \text{pr}_{\pi_T}\{\tau(X) < \tau_\ast\} \), respectively.

For each realization of \( X \), we first apply the Galerkin method with continuous, bilinear finite elements to numerically solve (6.1). The finite element solution \( u_h \) is computed on a uniform rectangular grid on \( D \) with a mesh size \( h = 1/64 \) along each of the coordinates of \( D \). The inhomogeneous horizontal Darcy flow field \( \kappa(s, X) \nabla u_h(s, X) \) is also calculated in the same finite element space. Then, the advection equation (6.2) with the discretized flow field is numerically solved by an explicit Runge-Kutta method with adaptive time stepping (\texttt{ode45} in MATLAB).

We assume that the logarithm of the diffusivity field follows a zero mean Gaussian process with the Matérn covariance function

\[
C(s,t) = \frac{2^{1-\nu}}{\Gamma(\nu)} \left( \sqrt{2\nu} \frac{||s-t||_2}{\ell} \right)^\nu K_\nu \left( \sqrt{2\nu} \frac{||s-t||_2}{\ell} \right), \quad s, t \in D,
\]

where \( \nu \) is the smoothness parameter, and \( \ell \) is the correlation length. This definition includes the Gaussian covariance function as the limit \( \nu \to \infty \). Using the Karhunen-Loève (KL) expansion,
log \kappa(s, X) can be approximated by the finite representation
\[
\log \kappa(s, X) \approx \sum_{k=1}^{d} X_k \sqrt{\lambda_k} \psi_k(s),
\]
where \(\{\psi_k(s), \lambda_k\}\) is the \(k\)th eigenpair of the covariance operator in the descending order of eigenvalues and each random coefficient \(X_k\) follows a standard normal prior.

To setup the observation model, we measure the water table \(u(s, X)\) at \(m = 15 \times 15\) locations defined as the vertices of a uniform Cartesian grid on \(D = [0, 1]^2\) with grid size \(1/[(\sqrt{m} + 1)]\), as shown in Fig. 4. Measurements are corrupted by i.i.d. Gaussian noise. For a realization of \(X\), the observables are simulated numerically as the average of \(u_h(s, X)\) over subdomains \(D_i \subset D, i = 1, \ldots, m\), around the measurement locations. In our experiments, each \(D_i\) is a square with side length \(2/((\sqrt{m} + 1))\) centred at the \(i\)th location. This leads to the parameter-to-observable map
\[
y_i = Q_i(x) + \eta_i, \quad Q_i(x) = \frac{1}{|D_i|} \int_{D_i} u_h(s, x) ds, \quad \eta_i \sim \mathcal{N}(0, \sigma^2_n)
\]
for \(i = 1, \ldots, m\), where \(\sigma^2_n\) is the variance of the measurement noise.

**6.2. A posteriori risk versus a priori risk.** A common practice in the literature is to estimate the \(a priori\) risk by only considering the randomness induced by the prior of \(\kappa(s, X)\); see [47, 55] and references therein for examples. As shown in Fig. 4, depending on the structure of the true diffusivity field, the contaminant breakthrough time can change due to localized changes that are difficult to detect. Thus, it is critical to also assess the \(a posteriori\) risk, where the uncertainty due to the unobserved diffusivity field \(\kappa(s, X)\) can be better characterized by conditioning on observations of the water table.

![Empirical cumulative density function of the breakthrough time](image.png)

**Fig. 5:** Empirical cumulative density function of the breakthrough time, \(\log_{10} \tau\), computed using \(2^{17}\) samples from prior and posteriors conditional on two data sets shown in Figure 4. Left: zoom around the threshold \(\tau_a = 0.1\).

We first demonstrate the critical importance of computing the \(a posteriori\) risk rather than \(a priori\) risk in this example. We consider an experiment with the prior correlation length \(\ell = 1/\sqrt{50}\), prior smoothness \(\nu = \infty\), \(d = 20\) in the KL expansion, and a breakthrough time threshold \(\tau_a = 0.1\). Without any observed data, the \(a priori\) risk computes to \(6.3 \times 10^{-3} \pm 6.4 \times 10^{-4}\). Next, we generate the solution \(u\) from one of the “truth” coefficients depicted in Fig. 4 (left), and observe the solution at \(15 \times 15\) equispaced spatial points with a zero-mean normal noise with variance \(3 \times 10^{-2}\). Using the data generated from the diffusivity field with a low-diffusivity barrier in the top of Fig. 4, the \(a posteriori\) risk is \(9.4 \times 10^{-4} \pm 1.3 \times 10^{-4}\). In comparison, using the data generated from the diffusivity field with a high-diffusivity channel in the bottom of Fig. 4, the \(a posteriori\) risk is \(2.8 \times 10^{-2} \pm 0.2 \times 10^{-2}\), which is an order of magnitude higher. In addition, Fig. 5 shows cumulative density functions of the breakthrough time in the logarithmic scale. We observe that the law of breakthrough time significantly changes with observed data. In summary, the critical change of risk cannot be detected by computing the \(a\)
6.3. Additional experiments of \textit{A priori} rare events and comparison with cross entropy. Here, we provide additional experiments for changing the risk threshold $\tau_*$, the smoothing width $\gamma^*$, and the dimension of the truncated random field $d$. We also compare deep importance sampling with the cross entropy method. To enable computation using cross entropy and in a wide range of parameters, we change the smoothness parameter to $\nu = 2$, noise variance to $\sigma_n^2 = 10^{-2}$ and the correlation length to $\ell = 1$. With these parameters, the truncated representation of the dimension $d = 25$ can capture 99.99\% of the variance of the KL expansion. We also change the Dirichlet boundary conditions to $u|_{s_1=0} = 1$ and $u|_{s_1=1} = 0$.

To apply Alg. 3.1, we compute the approximation of the optimal importance density with TT rank $r = 9$, intermediate parameters $\beta_1 = 10^{-2}$, $\beta_{\ell+1} = \sqrt{10} \beta_\ell$, $\gamma_\ell = \beta_\ell \gamma^*$, and two options for the smoothing width $\gamma^* = 30/\tau_*$ and $\gamma^* = 100/\tau_*$. A total of $N_{\text{total}} = 159885$ density evaluations is required to construct the composite map. In the left plot of Fig. 6, we plot the Hellinger errors of the deep importance densities versus the risk thresholds $\tau_*$. We consider two Hellinger distances: the distance $D_H(\bar{p}, p^*)$ between the computed deep importance density $\bar{p}$ and the optimal importance density $p^*$, as well as the distance $D_H(\bar{p}, \phi^{(L)})$ between the deep importance density $\bar{p}$ and the final layer of smoothed importance densities $\phi^{(L)}$. As for \textit{a posteriori} risk estimation above, smaller $\tau_*$ values lead to smaller probabilities of a particle traversing the channel in a time below $\tau_*$, which increases the difficulty to approximate the importance densities and is reflected in higher Hellinger errors.

In Fig. 7, we compare deep importance sampling to the cross entropy method of [4], for the risk threshold fixed at $\tau_* = 0.03$. Here, the cross entropy method uses only one single Gaussian

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig6}
\caption{Hellinger errors in computed deep importance densities for \textit{a priori} risk estimation for different breakthrough time thresholds $\tau_*$ and smoothing widths $\gamma_*$ (left), as well as the associated values of the \textit{a priori} risk (right). Points denote average, and error bars denote one standard deviation over 10 runs.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig7}
\caption{Relative standard deviation of the \textit{a priori} risk, estimated using 10 runs, comparing deep importance sampling and the cross entropy method (left), as well as total number of density evaluations used in each case (right).}
\end{figure}
density, which is the best we were able to fit, while the smoothing width $\gamma^* = 100/\tau_*$ is used to build intermediate densities for deep importance sampling in Alg. 3.1. We run 10 replicas of each method to estimate relative standard deviations of the risk probabilities, which are shown in the left plot of Fig. 7. In the right plot of Fig. 7, we also show the total number of density evaluations used by each of the methods. In this example, the cross entropy method is able to compute qualitatively correct risk estimates in higher dimensions, albeit requiring a larger number of density evaluations (starting from $2 \times 10^5$ samples per iteration at $d = 5$, growing to $6 \times 10^5$ for $d = 18$). However, for $d \geq 20$, the cross entropy method is unable to converge, even using $N = 10^6$ samples per iteration. In comparison, the number of density evaluations in deep importance sampling demonstrates a linear scaling in the dimension and nearly constant errors that are about two orders of magnitude below those of the cross entropy method. Moreover, this is achieved using one order of magnitude fewer density evaluations compared to the cross entropy method.

### 6.4. Additional experiments of a posteriori rare events.

Here, we provide additional experiments for changing the risk threshold $\tau_*$, the smoothing width $\gamma^*$, and the dimension of the truncated random field $d$. In this set of experiments, we use the model setup in Section 6.3, a sample size of $N = 2^{15}$, a fixed TT rank 7, and intermediate parameters $\beta_t = 10^{-3}$, $\beta_{t+1} = \sqrt{10}\beta_t$, $\gamma_t = \beta_t \gamma^*$ and $\alpha_t = \beta_t$.

We first vary $\tau_*$ and calculate the a posteriori risks of breakthrough using a default smoothing width $\gamma^* = 100/\tau_*$. The results are shown in Fig. 8 together with Hellinger errors of the importance density functions used in the ratio estimator, as well as the total number of density evaluations needed in Alg. 3.1. As above, we consider three Hellinger errors: the distance $D_H(\bar{p}, p^*)$ between the computed deep importance density and the optimal importance density for the numerator of the ratio estimator, the distance $D_H(\bar{p}, \phi_n(L))$ between the deep importance density and the final layer of smoothed importance densities for the numerator of the ratio estimator, as well as the distance $D_H(\bar{q}, \pi^y)$ between the computed deep importance density and the optimal importance density for the denominator of the ratio estimator. Clearly smaller $\tau_*$ lead to smaller probabilities of a particle travelling through the channel in a time below $\tau_*$. Consequently, the optimal importance density of the numerator becomes harder to approximate when $\tau_*$ decreases. Correspondingly, we observe that the Hellinger errors $D_H(\bar{p}, p^*)$ and $D_H(\bar{p}, \phi_n(L))$ increase as $\tau_*$ decreases. Nevertheless, even extremely small probabilities (below $10^{-10}$) can be estimated accurately. For this set of experiments, the number of function evaluations stays constant, as the same parameters are used in Alg. 3.1.

Then, with a fixed risk threshold $\tau_* = 0.03$, we study the behaviour of Alg. 3.1 when the smoothing width $\gamma^*$ and the TT ranks are changed. The left plot of Fig. 9 shows the resulting Hellinger errors for approximating the optimal importance density of the numerator.
as a function of $\gamma^\ast$. The tensor-train approximation error increases with increasing $\gamma^\ast$ due to the loss of smoothness, while the bias error between the exact optimal importance density $p^\ast$ and the smoothed density $\phi(L)$ decreases. Thus, there is an optimal $\gamma^\ast$ to obtain the most accurate approximation of the optimal importance function $p^\ast(x)$, where the two error contributions balance. Regarding the dependency on the maximum rank $r$, for a fixed $\gamma^\ast = 100/\tau^\ast$ we observe that all Hellinger errors decay with $r$ until the discretisation error is reached, whereas the number of function evaluations in Alg. 3.1 appears to depend quadratically on $r$, as expected from the number of degrees of freedom in the tensor-train decomposition.

![Fig. 9: Hellinger errors for a posteriori risk estimation for different smoothing widths $\gamma^\ast$ (left) and TT ranks $r$ (middle) where $\tau^\ast = 0.03$. The right figure shows the total number of density evaluations in Alg. 3.1 as a function of the rank $r$ for $\gamma^\ast = 100/\tau^\ast$. Points denote averages, and error bars denote one standard deviation over 10 runs.](image)

Finally, we vary the dimension of the random field from $d = 5$ to 25 and take the threshold $\tau^\ast = 0.15$ to test the dimension scalability of deep importance sampling for estimating the a posteriori risk. The synthetic observations are generated using the diffusivity field with high diffusivity channel, depicted in the bottom of Fig. 4. The TT ranks are adaptively chosen using 5 iterations of the cross algorithm, starting from rank 1 and increasing the ranks by at most 2 in each iteration to obtain a relative Frobenius-norm error below $3 \times 10^{-2}$. We use piecewise linear basis functions on 17 grid points to discretize the density in each coordinate direction, truncating the unbounded domain to $[-5, 5]$. We choose a smoothing width of $\gamma^\ast = 100/\tau^\ast$.

The results are shown in Fig. 10. We observe that the computational complexity, measured in terms of density evaluations, depends no worse than linearly on the dimension, while the Hellinger error increases logarithmically with respect to the dimension.

7. Future work. We demonstrated that on problems constrained by differential equations, our proposed deep importance sampling is able to compute hitherto unattainable estimates of rare event probabilities for complex, high-dimensional posterior densities with $d > 20$. For problems with very high-dimensional parameters, e.g., $d > 10^3$, even though the computational complexity of TT may be independent of the apparent problem dimension if the underlying probability density lies in a Sobolev space with appropriately decaying dimension weights (see [33] and references therein), it can still be computationally demanding to build TT approximations if the decay in the weights is too slow. To alleviate this challenge, we can apply gradient-based dimension reduction methods [12, 16, 19, 55, 63] to identify subspaces that capture the most relevant variations of the optimal importance distribution with respect to the underlying weighted norm. The TT approximation in each layer of deep importance sampling can then be further improved using the variable reordering/reparametrization technique in [14] after the gradient-based dimension reduction.

Although deep importance sampling demonstrates good statistical efficiency in terms of the effective sample size per function evaluation in our numerical experiments, the failure function can be computationally costly to evaluate due to the use of numerical solvers for the differential equations. This may prevent a reliable estimation of the failure probability with a limited
Hellinger error

\[ D_{H}(\bar{q}, \pi^y) \]

\[ D_{H}(\bar{p}, \phi_u^L) \]

\[ D_{H}(\bar{p}, p^\star) \]

Fig. 10: Hellinger errors in the densities (left) and total number of function evaluations in Alg. 3.1 (right) for estimating the \textit{a posteriori} risk in Example 2 with \( \tau = 0.15 \) and varying the parameter dimension \( d \). Points denote averages, and error bars denote one standard deviation over 10 runs.

Computational budget. To address this bottleneck, one can use surrogate modeling techniques—for example, those based on polynomial chaos [1, 11, 60, 40, 52, 61], reduced order models [6, 8, 10, 17, 18, 30, 38, 58], and neural networks [37, 39, 54, 62, 64]—to replace the forward model, so that the training of the Rosenblatt transport can be accelerated. Furthermore, our method can also be combined with either the multilevel Monte Carlo estimator [28, 51, 56] or used in a multi-fidelity framework [47, 48] to achieve further variance reduction.

Appendix A. Proof of Lemma 3.4. Recall that the unnormalized optimal importance density \( \rho^\star \) is approximated by

\[ \rho = \tilde{g}^2 + \tau \lambda, \]

where \( \lambda \) is a normalized probability density, \( \tau > 0 \), and \( \tilde{g} \) satisfies \( \|\sqrt{\rho^\star} - \tilde{g}\|_2 \leq \epsilon \). Since \( \rho^\star \) and \( \lambda \) are non-negative functions and \( \tau > 0 \), we have the identity

\[
(\sqrt{\rho^\star} - \sqrt{\rho})^2 = (\sqrt{\rho^\star} - (\tilde{g}^2 + \tau \lambda)^{1/2})^2 \\
= \rho^\star + \tilde{g}^2 + \tau \lambda - 2\sqrt{\rho^\star}(\tilde{g}^2 + \tau \lambda)^{1/2} \\
\leq \rho^\star + \tilde{g}^2 + \tau \lambda - 2\sqrt{\rho^\star}\tilde{g} \\
= (\sqrt{\rho^\star} - \tilde{g})^2 + \tau \lambda,
\]

which leads to \( \|\sqrt{\rho^\star} - \sqrt{\rho}\|_2 \leq \|\sqrt{\rho^\star} - \tilde{g}\|_2 + \tau \leq \epsilon^2 + \tau \). Choosing \( \tau \leq \epsilon^2 \), we have

\[
\|\sqrt{\rho^\star} - \sqrt{\rho}\|_2 \leq \sqrt{2\epsilon}.
\]

Since the square roots of the normalising constants can be expressed as \( \sqrt{\zeta^\star} = \|\sqrt{\rho^\star}\|_2 \) and \( \sqrt{\zeta} = \|\sqrt{\rho}\|_2 \), we have

\[
|\sqrt{\zeta^\star} - \sqrt{\zeta}|(\sqrt{\zeta^\star} + \sqrt{\zeta}) = |\zeta^\star - \zeta| \\
= \int_{\chi} \rho^\star(x) - \rho(x)dx \\
= |(\sqrt{\rho^\star} - \sqrt{\rho}, \sqrt{\rho^\star} + \sqrt{\rho})| \\
\leq \|\sqrt{\rho^\star} - \sqrt{\rho}\|_2\|\sqrt{\rho^\star} + \sqrt{\rho}\|_2 \\
\leq \|\sqrt{\rho^\star} - \sqrt{\rho}\|_2(\|\sqrt{\rho^\star}\|_2 + \|\sqrt{\rho}\|_2) \\
= \|\sqrt{\rho^\star} - \sqrt{\rho}\|_2(\sqrt{\zeta^\star} + \sqrt{\zeta}).
\]

This leads to

\[
|\sqrt{\zeta^\star} - \sqrt{\zeta}| \leq \|\sqrt{\rho^\star} - \sqrt{\rho}\|_2.
\]

Thus, the result of the first property of Lemma 3.4 follows.
Recall that the Hellinger distance is proportional to the $L^2$ distance of the normalized densities, i.e.,

$$D_H(p^*, p) = \left[ \frac{1}{2} \int \{ \sqrt{p^*} - \sqrt{p} \}^2 \, dx \right]^{\frac{1}{2}} = \frac{1}{\sqrt{2}} \| \sqrt{p^*} - \sqrt{p} \|_2.$$  

The $L^2$ distance of the normalized densities follows the identity

$$\| \sqrt{p^*} - \sqrt{p} \|_2 = \left\| \sqrt{\rho^*} - \frac{\sqrt{\rho^* + \sqrt{\rho^* - \sqrt{\rho^*}}}}{\sqrt{\zeta^*}} \right\|_2$$

$$\leq \frac{1}{\sqrt{\zeta^*}} \| \sqrt{p^*} - \sqrt{\rho} \|_2 + \frac{1}{\sqrt{\zeta^*}} \left\| \sqrt{\rho} \left( 1 - \frac{\sqrt{\zeta^*}}{\sqrt{\zeta}} \right) \right\|_2$$

$$= \frac{1}{\sqrt{\zeta^*}} \| \sqrt{p^*} - \sqrt{\rho} \|_2 + \frac{\sqrt{\zeta}}{\sqrt{\zeta^*}} \left( 1 - \frac{\sqrt{\zeta^*}}{\sqrt{\zeta}} \right)$$

$$\leq \frac{2}{\sqrt{\zeta^*}} \| \sqrt{p^*} - \sqrt{\rho} \|_2,$$

where the last inequality follows from (A.2). Substituting (A.1) into the above inequality and the definition of the Hellinger distance, we obtain $D_H(p^*, p) \leq 2\epsilon/\sqrt{\zeta^*}$. This gives the second property.

**Appendix B. Sequential marginalisation.** Here we provide implementation details of the sequence of one-dimensional integrations for building the Rosenblatt transport in Section 3.2. To realize the map $Q$, our starting point is to construct a sequence of unnormalized marginal densities

$$g(x) = G_1(x_1) \cdots G_k(x_k) \cdots G_d(x_d),$$

where $G_k(x_k) = \prod_{j=1}^k \lambda_j(x_j)$, for all $1 \leq k < d$. Recalling the tensor-train decomposition

$$\tilde{g}(x) = G_1(x_1) \cdots G_k(x_k) \cdots G_d(x_d),$$

we can define

$$G_k(x_k) = G_1(x_1) \cdots G_k(x_k), \quad G_{k+1}(x_{k+1}) = G_{k+1}(x_{k+1}) G_{k+1}(x_{k+1}).$$

The integration of $\tilde{g}^2$ over $x_{>k}$ for any index $k$, and hence the unnormalized marginal densities, can be obtained dimension-by-dimension as follows.

1. For $k = d - 1$, we integrate $\tilde{g}^2$ over the last coordinate $x_d$ to obtain

$$\rho_{<d}(x_{<d}) = \int_{x_d} \left\{ \sum_{\alpha_{d-1}}^{r_d-1} G_{<d}(x_{<d}) G_{d}(x_d) \right\}^2 \, dx_d + \tau \lambda_{<d}(x_{<d})$$

$$= \sum_{\alpha_{d-1}=1}^{r_d-1} \sum_{\beta_d=1}^{r_d-1} G_{<d}(x_{<d}) G_{<d}(x_{<d}) M_{d}(x_{<d}) + \tau \lambda_{<d}(x_{<d}),$$

25
where $M_d \in \mathbb{R}^{r_d \times r_d}$ is a symmetric positive definite mass matrix such that

$$
M_d^{(\alpha_{d-1}, \beta_{d-1})} = \int_{X_d} G_d^{(\alpha_{d-1})}(x_d) G_d^{(\beta_{d-1})}(x_d) \, dx_d.
$$

Computing the Cholesky factorization $L_d L_d^T = M_d$, we have the simplification

$$
\rho_{<d}(x_{<d}) = \sum_{\alpha_{d-1}=1}^{r_{d-1}} \left\{ G_{<d}(x_{<d}) L_d^{(\alpha_{d-1})} \right\}^2 + \tau \lambda_{<d}(x_{<d}).
$$

2. For any index $1 < k < d$, suppose we have the symmetric positive definite mass matrix $M_{>k} \in \mathbb{R}^{r_k \times r_k}$ such that

$$
\bar{M}_{>k}^{(\alpha_k, \beta_k)} = \int_{X_{>k}} G_k^{(\alpha_k)}(x_d) \bar{G}_{>k}^{(\beta_k)}(x_{>k}) \, dx_k
$$

and its Cholesky factorization $\bar{L}_{>k} \bar{L}_{>k}^T = \bar{M}_{>k}$. Then, similar to the above case, we have the unnormalized marginal density

$$
\rho_{<k}(x_{<k}) = \sum_{\alpha_k=1}^{r_k} \left\{ G_{<k}(x_{<k}) \bar{G}_{>k}^{(\alpha_k)} \right\}^2 + \tau \lambda_{<k}(x_{<k}).
$$

This way, the next unnormalized marginal density $\rho_{<k}(x_{<k})$ can be constructed by a one-dimensional integration over $x_k$, which takes the form

$$
\rho_{<k}(x_{<k}) = \sum_{\alpha_k=1}^{r_k} \int_{X_k} \left\{ \sum_{\alpha_{k-1}=1}^{r_{k-1}} G_{<k}^{(\alpha_{k-1})}(x_{<k}) G_k^{(\alpha_{k-1}, \cdot)}(x_k) \bar{L}_{>k}^{(\cdot, \alpha_k)} \right\} \, dx_k + \tau \lambda_{<k}(x_{<k})
$$

and

$$
= \sum_{\alpha_{k-1}=1}^{r_{k-1}} \sum_{\beta_{k-1}=1}^{r_{k-1}} G_{<k}^{(\alpha_{k-1})}(x_{<k}) G_{>k}^{(\beta_{k-1}, \cdot)}(x_{<k}) \bar{M}_{>k}^{(\alpha_{k-1}, \beta_{k-1})} + \tau \lambda_{<k}(x_{<k}),
$$

where $\bar{M}_{>k} \in \mathbb{R}^{r_{k-1} \times r_{k-1}}$ is the next mass matrix such that

$$
\bar{M}_{>k}^{(\alpha_{k-1}, \beta_{k-1})} = \sum_{\alpha_k=1}^{r_k} \int_{X_k} \left\{ G_k^{(\alpha_{k-1}, \cdot)}(x_k) \bar{L}_{>k}^{(\cdot, \alpha_k)} \right\} \left\{ G_k^{(\beta_{k-1}, \cdot)}(x_k) \bar{L}_{>k}^{(\cdot, \alpha_k)} \right\} \, dx_k.
$$

Again, by computing the Cholesky factorization $\bar{L}_{>k} \bar{L}_{>k}^T = \bar{M}_{>k}$, we have the simplified marginal density

$$
\rho_{<k}(x_{<k}) = \sum_{\alpha_k=1}^{r_k} \left\{ G_{<k}(x_{<k}) \bar{L}_{>k}^{(\cdot, \alpha_k)} \right\}^2 + \tau \lambda_{<k}(x_{<k}).
$$

Following the above procedure, initializing $\bar{M}_{>k}$ with $\bar{M}_{>d} = M_d$ for $k = d - 1$, we can recursively construct all unnormalized marginal densities. In each iteration, we only need to solve a one-dimensional integration problem in (B.4). Given $n_k$ number of discretization basis functions in $x_k$, the total computational complexity of solving the integration in (B.4) and computing the Cholesky factorization $L_{>k}$ is $O(n_k r_k^2) + r_k^3$.

3. For $k = 1$, we have the unnormalized marginal density

$$
\rho_{<1}(x_1) = \sum_{\alpha_1=1}^{r_1} \left\{ G_1(x_1) \bar{L}_{>1}^{(\cdot, \alpha_1)} \right\}^2 + \tau \lambda_{<1}(x_1).
$$

Carrying out one extra integration defined in (B.4), we obtain $\bar{M}_{>1} \in \mathbb{R}$ as $r_0 = 1$. This gives the normalising constant $\zeta = \bar{M}_{>1} + \tau$.
Appendix C. Pushforward density of the composite map. Here we provide a
detailed derivation of the normalized density \( \hat{p} = \{ T^{(L)} \}_{T} \) \( \lambda \) in (3.9), which is the pushforward density of the reference \( \lambda \) under the composition of maps \( T^{(L)} = Q^{(1)} \circ Q^{(2)} \circ \cdots \circ Q^{(L)} \). As a
starting point, we derive the Jacobian of the incremental map \( u' = Q^{(i)}(u) \), which has the form

\[
Q^{(i)} = F^{-1} \circ R,
\]

with \( F_\sharp p^{(i)} = \mu \) and \( R_\sharp \lambda = \mu \), where \( \mu \) is the uniform density on \([0,1]^d\) and

(C.1) \[
p^{(i)}(u') = \frac{1}{\zeta^{(i)}} \left\{ \hat{g}^{(i)}(u')^2 + \tau^{(i)} \lambda(u') \right\}
\]
is the \( \ell \)-th approximate density. Thus, we have the identity

(C.2) \[
p^{(i)}(u') = \{ Q^{(i)} \}_{\sharp} \lambda(u') = \lambda \left[ \{ Q^{(i)} \}^{-1}(u') \right] |\nabla \{ Q^{(i)} \}^{-1}(u')|,
\]
which gives the Jacobian

\[
|\nabla \{ Q^{(i)} \}^{-1}(u')| = \frac{p^{(i)}(u')}{\lambda \left[ \{ Q^{(i)} \}^{-1}(u') \right]}.
\]

Given a composite map \( T^{(i)} = T^{(\ell-1)} \circ Q^{(i)} \), to avoid confusion, we define the associated change of variables as

\[
x = T^{(i)}(u) \iff u' = Q^{(i)}(u), \quad x = T^{(\ell-1)}(u'),
\]
and the reverse transform as

\[
u = \{ T^{(i)} \}^{-1}(x) \iff u' = \{ T^{(\ell-1)} \}^{-1}(x), \quad u = \{ Q^{(i)} \}^{-1}(u').
\]

This way, the Jacobian of the inverse map satisfies

\[
|\nabla \{ T^{(i)} \}^{-1}(x)| = |\nabla \{ Q^{(i)} \}^{-1}(u')| |\nabla \{ T^{(\ell-1)} \}^{-1}(x)|,
\]
by the chain rule. Substituting (C.2) and \( u' = \{ T^{(\ell-1)} \}^{-1}(x) \) into the above identity, the Jacobian of the composite map satisfies the recurrence relationship

(C.3) \[
\begin{align*}
|\nabla \{ T^{(i)} \}^{-1}(x)| &= \frac{|\nabla \{ T^{(\ell-1)} \}^{-1}(x)|}{\lambda \left[ \{ Q^{(i)} \}^{-1}(x) \right]} \\
&= \frac{|\nabla \{ T^{(\ell-1)} \}^{-1}(x)| p^{(i)}(\mu \left[ \{ T^{(\ell-1)} \}^{-1}(x) \right])}{\lambda \left[ \{ T^{(i)} \}^{-1}(x) \right]}
\end{align*}
\]

Thus, by induction, the Jacobian of the composite of \( L \) layers of maps, \( T^{(L)} \), satisfies

(C.4) \[
|\nabla \{ T^{(L)} \}^{-1}(x)| = \frac{p^{(1)}(x)}{\lambda \left[ \{ T^{(L)} \}^{-1}(x) \right]} \prod_{i=2}^{L} \frac{p^{(i)}(\mu \left[ \{ T^{(\ell-1)} \}^{-1}(x) \right])}{\lambda \left[ \{ T^{(L)} \}^{-1}(x) \right]}
\]

Substituting (C.4) into the identity

\[
\{ T^{(L)} \}_{\sharp} \lambda(x) = \lambda \left[ \{ T^{(L)} \}^{-1}(x) \right] |\nabla \{ T^{(L)} \}^{-1}(x)|
\]
Fig. 11: Samples drawn from the approximate importance densities, colored by their density
values, for $R_0^2 = 10^{-2}$, $R_i^2 = R_0^2 - 10^{-4}$ (left) and for $R_0^2 = 10^{-3}$, $R_i^2 = 0$ (right).

and applying (C.1), the pushforward density of $\lambda$ under $T^{(L)}$ has the density

$$
(C.5) \quad \{ T^{(L)} \}_{T^{(L)}} \lambda(x) = p^{(1)}(x) \prod_{\ell=2}^{L} p^{(\ell)} \left[ \{ T^{(\ell-1)} \}^{-1}(x) \right] \lambda \left[ \{ T^{(\ell-1)} \}^{-1}(x) \right]^{-1} \left[ \prod_{\ell=1}^{\ell} \zeta^{(\ell)} \right]^{-1} \left\{ \tilde{g}^{(1)}(x)^2 + \tau^{(1)} \lambda(x) \right\} \prod_{\ell=2}^{L} \left( \frac{\tilde{g}^{(\ell)} \{ T^{(\ell-1)} \}^{-1}(x)^2 + \tau^{(\ell)} \lambda(x) \} \right).
$$

This concludes the derivation. \qed

Appendix D. Areas of annulus and disk. We consider a 2-dimensional toy example for estimating a priori failure probabilities, where the prior distribution that is uniform on the unit square, i.e., $\pi_0(x) = 1$ with $x \in [0, 1]^2$ and the failure function

$$
(D.1) \quad f(x) = 1_{\{R_i \leq \|x-x_0\| \leq R_0 \}}(x),
$$

for given radii $0 \leq R_i < R_0$ and center $x_0 = [0.4, 0.4]$. Thus, the event probability is the area of the annulus, $\zeta^* := \text{pr}_{\pi_0}(X \in A) = \pi_i (R_0^2 - R_i^2)$, where $\pi_i$ is Archimedes’ constant.

The smoothed indicator function for Alg. 3.1 is defined as a product of two sigmoids,

$$
\tilde{f}_\gamma(x) = \left[ 1 + \exp \left( \gamma (\|x - x_0\|^2 - R_i^2) \right) \right]^{-1} \left[ 1 + \exp \left( \gamma (R_0^2 - \|x - x_0\|^2)^2 \right) \right]^{-1}.
$$

To approximate the smoothed optimal importance density with Alg. 3.1, we tune various control variables in the deep importance sampling procedure such that the Hellinger distance between the approximate density and the optimal importance density $p^*(x)$ is about 0.3 for all choices of $R_i$ and $R_0$. This involves varying the final smoothing variable $\gamma_L = \gamma^*$, the univariate grid size $n$, the tensor rank $r$, and the initial smoothing variable $\gamma_1$. The intermediate densities are defined throughout by $\gamma_{\ell+1} = \sqrt{10} \gamma_\ell$. Once the approximation of the optimal importance density is computed, we use $N = 2^{16}$ samples to compute the deep importance sampling estimator $\hat{c}_{p, N}$ in (3.10).

In the first experiment, we fix the outer radius $R_0 = 0.1$, and vary the inner radius $R_i$, as shown in Fig. 11 (left), such that it approaches $R_0$. The results are shown in Table 2. This setup requires finer discretizations, that is, larger values of $n$, as the width of the annulus decreases. As a result, the number of function evaluations to approximate the optimal importance density, $N_{TTT}$, grows rapidly.

In contrast, if the inner radius is fixed to $R_i = 0$ and the outer radius $R_0$ is varied, the optimal importance density function $p^*(x) \propto f(x)\pi_0(x)$ is unimodal, representing just the indicator function of the disk with radius $R_0$. As we can see in Table 3, in that case the approximation complexity, in terms of function evaluations, depends only logarithmically on the value of $\zeta^*$. 28
Table 2: Annulus test with $R_0 = 0.1$ fixed. $N_{TT}$ is the total number of function evaluations used in Alg. 3.1 to approximate the smoothed optimal importance density. The last column gives the relative bias of the estimator in each case.

| $R^2_2 - R^2_1$ | $\gamma$ | $n$ | $\bar{r}$ | $\bar{\gamma}_i$ | $N_{TT}$ | $D_H(p^*, \bar{p})$ | $|\zeta_{p,N} - \zeta^*|/\zeta^*$ |
|------------------|---------|-----|----------|------------------|--------|----------------|------------------|
| $10^{-3}$        | $10^2$  | 35  | 3        | $10^{-3}$        | 3550   | 0.3292±0.0033  | 0.000152±0.000158 |
| $10^{-4}$        | $10^2$  | 257 | 5        | $10^{-4}$        | 23130  | 0.3292±0.0159  | 0.00293±0.00570  |
| $10^{-6}$        | $10^2$  | 513 | 10       | $10^{-6}$        | 112860 | 0.304±0.0111   | 0.00232±0.00180  |
| $10^{-7}$        | $10^2$  | 1025| 20       | $10^{-7}$        | 533000 | 0.379±0.0230   | 0.00616±0.00445  |

Table 3: Disk test with $R_i = 0$ fixed. $N_{TT}$ is the total number of function evaluations used in Alg. 3.1 for approximating the smoothed optimal importance densities. The last column gives the relative bias of the estimator in each case.

| $R^2_2$ | $\gamma$ | $n$ | $\bar{r}$ | $\bar{\gamma}_i$ | $N_{TT}$ | $D_H(p^*, \bar{p})$ | $|\zeta_{p,N} - \zeta^*|/\zeta^*$ |
|---------|---------|-----|----------|------------------|--------|----------------|------------------|
| $10^{-3}$ | $10^2$  | 17  | 2        | $10^{-2}$        | 340    | 0.224±0.0015  | 0.00136±0.00094  |
| $10^{-4}$ | $10^2$  | 17  | 2        | $10^{-2}$        | 340    | 0.221±0.0036  | 0.000111±0.00078 |
| $10^{-5}$ | $10^2$  | 17  | 2        | $10^{-3}$        | 476    | 0.218±0.0017  | 0.000105±0.00090 |
| $10^{-6}$ | $10^2$  | 17  | 2        | $10^{-4}$        | 612    | 0.218±0.0015  | 0.000144±0.00095 |
| $10^{-7}$ | $10^2$  | 17  | 2        | $10^{-5}$        | 748    | 0.218±0.0015  | 0.000193±0.00100 |

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