# Geometrically Coupled Monte Carlo Sampling

**Mark Rowland**[*]
University of Cambridge
mr504@cam.ac.uk

**Krzysztof Choromanski**[*]
Google Brain Robotics
kchoro@google.com

**François Chalus**
University of Cambridge
chalusf3@gmail.com

**Aldo Pacchiano**
University of California, Berkeley
pacchiano@berkeley.edu

**Tamás Sarlós**
Google Research
stamas@google.com

**Richard E. Turner**
University of Cambridge
ret26@cam.ac.uk

**Adrian Weller**
University of Cambridge
Alan Turing Institute
aw665@cam.ac.uk

## Abstract

Monte Carlo sampling in high-dimensional, low-sample settings is important in many machine learning tasks. We improve current methods for sampling in Euclidean spaces by avoiding independence, and instead consider ways to couple samples. We show fundamental connections to optimal transport theory, leading to novel sampling algorithms, and providing new theoretical grounding for existing strategies. We compare our new strategies against prior methods for improving sample efficiency, including quasi-Monte Carlo, by studying discrepancy. We explore our findings empirically, and observe benefits of our sampling schemes for reinforcement learning and generative modelling.

## 1 Introduction and related work

Monte Carlo (MC) methods are popular in many areas of machine learning, including approximate Bayesian inference (Robert and Casella, 2005; Rezende et al., 2014; Kingma and Welling, 2014; Welling and Teh, 2011), reinforcement learning (RL) (Salimans et al., 2017; Choromanski et al., 2018c; Mania et al., 2018), and random feature approximations for kernel methods (Rahimi and Recht, 2007; Yu et al., 2016). Typically, Monte Carlo samples are drawn independently. In many applications, however, there may be an imbalance between the computational cost in drawing MC samples from the distribution of interest, and the subsequent cost incurred due to downstream computation with the samples. For example, when a sample represents the configuration of weights in a policy network for an RL problem, the cost of computing forward passes, backpropagating gradients through the network, and interacting with the environment, is much greater than drawing the sample itself. Since a high proportion of total time is spent *computing* with each sample relative to the cost of *generating* the sample, it may be possible to improve efficiency by replacing the default of independent, identically distributed samples by samples with some non-trivial *coupling*.

Such approaches have been studied in computational statistics for decades, often under the guise of variance reduction. Related methods such as control variates, quasi-Monte Carlo (QMC) (Halton, 1960; Aistleitner and Dick, 2015; Dick et al., 2015; Brauchart and Dick, 2012; Sloan and Wozniakowski, 1998; Avron et al., 2016)), herding (Chen et al., 2010; Huszar and Duvenaud, 2012) and

[*]Equal contribution

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antithetic sampling (Hammersley and Morton, 1956; Salimans et al., 2017) have also been explored. Methods used in recent machine learning applications include orthogonality constraints (Yu et al., 2016; Choromanski et al., 2018b,c, 2017, 2018a). In this paper, we investigate improvements to MC sampling through carefully designed joint distributions, with an emphasis on the low-sample, high-dimensional regime, which is often relevant for practical machine learning applications (Rezende et al., 2014; Kingma and Welling, 2014; Salimans et al., 2017). We call our approach *Geometrically Coupled Monte Carlo* (GCMC) since, as we will see, it is geometrically motivated. Importantly, we focus on Monte Carlo sampling, in contrast to (pseudo-)deterministic approaches such as QMC and herding, as unbiasedness of estimators is often an important property for stochastic approximation. Whilst approaches such as herding and QMC are known to have superior asymptotic performance to Monte Carlo methods in low dimensions, this may not hold in high-dimensional, low-sample regimes, where they do not provide any theoretical improvement guarantees.

We summarize our main contributions below. Throughout the paper, we save proofs of our results for the Appendix; where appropriate, we provide proof sketches to aid intuition.

- We frame the problem of finding an optimal coupling amongst a collection of samples as a multi-marginal transport (MMT) problem: this generalises the notion of optimal transport, which has seen many applications in machine learning (see for example Arjovsky et al., 2017). We show several settings where the MMT problem can be solved analytically. We recover some existing coupling strategies (based on orthogonal matrices), and derive novel strategies, involving coupling norms of pairs of samples.
- To connect to QMC, we show that sets of geometrically coupled Monte Carlo samples give rise to low discrepancy sequences. To our knowledge, we present the first explanation of the success of structured orthogonal matrices for scalable RBF kernel approximation via discrepancy theory.
- We provide exponentially small upper bounds on failure probabilities for estimators of gradients of Gaussian smoothings of blackbox functions based on the gradient sensing mechanism, both for unstructured and orthogonal settings (Choromanski et al., 2018c). These methods can be used to learn good quality policies for reinforcement learning tasks.
- We empirically measure the discrepancy of sequences produced by our method and show that they enable us to learn good quality policies for quadruped robot navigation in low-sample, high-dimensional regimes, where standard QMC approaches based on Halton sequences and related constructions fail.

## 2 Optimal couplings, herding, and optimal transport

Consider the problem of computing the expectation $I_f = \mathbb{E}_{X\sim\eta}[f(X)]$, where $\eta \in \mathscr{P}(\mathbb{R}^d)$ is a multivariate probability distribution and $f : \mathbb{R}^d \to \mathbb{R}$ is some measurable function in $L^1(\eta)$. A standard Monte Carlo approach is to approximate $I_f$ by $\widehat{I}_f^{\text{iid}} = \frac{1}{m}\sum_{i=1}^m f(X_i)$, where the samples $X_1, \ldots, X_m \sim \eta$ are taken independently. This estimator is clearly unbiased. The main question that we are interested in is what joint distributions (or couplings) over the ensemble of samples $(X_1, \ldots, X_m)$ lead to estimators of the expectation above which are still unbiased, but have lower *mean squared error* (MSE) than the i.i.d. estimator $\widehat{I}_f^{\text{iid}}$, defined for a general estimator $\widehat{I}_f$ by:

$$\text{MSE}(\widehat{I}_f) = \mathbb{E}\left[\left(\widehat{I}_f - I_f\right)^2\right]. \tag{1}$$

For sufficiently rich functions classes $\mathscr{F} \subseteq L^2(\eta)$, a coupling of the random variables $(X_1, \ldots, X_m)$ that achieves optimal MSE simultaneously for all functions $f \in \mathscr{F}$ need not exist. We illustrate this with examples in the Appendix Section 8.2. This motivates the approach below to define optimality of a coupling by taking into account average performance across a function class of interest.

### 2.1 *K*-optimal couplings

We begin by defining formally the notion of coupling.

**Definition 2.1.** Given a probability distribution $\eta \in \mathscr{P}(\mathbb{R}^d)$ and $m \in \mathbb{N}$, we denote by $\Lambda_m(\eta)$ the set of all joint distributions of $m$ random variables $(X_1, \ldots, X_m)$, where each random variable $X_i$

has the marginal distribution $\eta$. More formally,

$$\Lambda_m(\eta) = \{\mu \in \mathscr{P}(\mathbb{R}^{d\times m}) | (\pi_i)_{\#}\mu = \eta \text{ for } i = 1, \ldots, m\},$$

where $\pi_i : \mathbb{R}^{d\times m} \to \mathbb{R}^d$ denotes projection onto the $i^{\text{th}}$ set of $d$ coordinates, for $i = 1, \ldots, m$.

Note that if $X_{1:m} \sim \mu \in \Lambda_m(\eta)$, then because of the restriction on the marginals of $X_{1:m}$, the estimator $m^{-1}\sum_{i=1}^m f(X_i)$ is unbiased for $\mathbb{E}_{X\sim\eta}[f(X)]$, for any $f \in L^1(\eta)$.

We now define the following notion of optimality of a coupling. Similar notions have appeared in the literature when samples are taken to be non-random, or when selecting importance distributions, sometimes referred to as kernel quadrature (Rasmussen and Ghahramani, 2003; Briol et al., 2017).

**Definition 2.2** ($K$**-optimal coupling).** Given a kernel $K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$, a *$K$-optimal coupling* is a solution to the optimisation problem

$$\operatorname*{arg\,min}_{\mu\in\Lambda_m(\eta)} \mathbb{E}_{f\sim\mathrm{GP}(0,K)}\left[\mathbb{E}_{X_{1:m}\sim\mu}\left[\left(\frac{1}{m}\sum_{i=1}^m f(X_i) - I_f\right)^2\right]\right]. \tag{2}$$

That is, a $K$-optimal coupling is one that gives the best MSE on average when the function concerned is drawn from the Gaussian process $\mathrm{GP}(0, K)$. For background on Gaussian processes, see (Rasmussen and Williams, 2005).

**Remark 2.3.** There are measure-theoretic subtleties in making sure that the objective in Expression (2) is well-defined. For readability, we treat these issues in the Appendix (Section 7), but remark here that it is sufficient to restrict to kernels $K$ for which sample paths of the corresponding Gaussian process are continuous, which we do for the remainder of the paper.

Our ultimate aim is to characterise $K$-optimal couplings under a variety of conditions algorithmically to enable practical implementation. We discuss the identification of $K$-optimal couplings, along with precise statements of algorithms, in Section 2.3. First we develop the theoretical properties of $K$-optimal couplings, starting with the intimate connection between $K$-optimal couplings and multi-marginal transport theory (Pass, 2014). This theory is a generalisation of optimal transport theory to the case where there are more than two marginal distributions.

**Theorem 2.4.** The optimisation problem defining $K$-optimality in Equation (2) is equivalent to the following *multi-marginal transport problem*:

$$\operatorname*{arg\,min}_{\mu\in\Lambda_m(\eta)} \mathbb{E}_{X_{1:m}\sim\mu}\left[\sum_{i\neq j} K(X_i, X_j)\right].$$

**Remark 2.5.** The optimal transport problem of Theorem 2.4 has an interesting difference from most optimal transport problems arising in machine learning: in general, its cost function is *repulsive*, so it seeks a transport plan where transport paths are typically *long*, as opposed to the short transport paths sought when the cost is given by e.g. a metric. Intuitively, the optimal transport cost rewards *space-filling* couplings, for which it is uncommon to observe collections of samples close together.

### 2.2 Minimax couplings and herding

Definition 2.2 ($K$-optimality) considers best average-case behaviour. We could instead use a "minimax" definition of optimality, by examining best worst-case behaviour.

**Definition 2.6 (Minimax coupling).** Given a function class $\mathscr{F} \subseteq L^2(\eta)$, we say that $\mu \in \Lambda_m(\eta)$ is an *$\mathscr{F}$-minimax coupling* if it is a solution to the following optimisation problem:

$$\operatorname*{arg\,min}_{\mu\in\Lambda_m(\eta)} \sup_{f\in\mathscr{F}} \mathbb{E}_{X_{1:m}\sim\mu}\left[\left(\frac{1}{m}\sum_{i=1}^m f(X_i) - I_f\right)^2\right]. \tag{3}$$

In general, the minimax coupling objective appearing in Equation (3) is intractable. However, there is an elegant connection to concepts from the kernel herding literature that may be established by taking the function class $\mathscr{F}$ to be the unit ball in some reproducing kernel Hilbert space (RKHS).

**Proposition 2.7.** Suppose that the function class $\mathscr{F}$ is the unit ball in some RKHS given by a kernel $K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$. Then the component

$$\sup_{f \in \mathscr{F}} \mathbb{E}_{X_{1:m} \sim \mu} \left[ \left( \frac{1}{m} \sum_{i=1}^{m} f(X_i) - I_f \right)^2 \right]$$

of the minimax coupling objective in Equation (3) may be upper-bounded by the following objective:

$$\mathbb{E}_{X_{1:m} \sim \mu} \left[ \left\| \theta_K \left( \frac{1}{m} \sum_{i=1}^{m} \delta_{X_i} \right) - \theta_K (\eta) \right\|_{\mathcal{H}_K}^2 \right], \tag{4}$$

where $\theta_K : \mathscr{P}(\mathbb{R}^d) \to \mathcal{H}_K$ is the kernel mean embedding into the RKHS $\mathcal{H}_K$ associated with $K$.

We note the intimate connection of the objective in Equation (4) with maximum mean discrepancy (MMD) (Gretton et al., 2012) and herding (Chen et al., 2010; Huszar and Duvenaud, 2012). First, the integrand appearing in Equation (4) is exactly the MMD-squared between $m^{-1} \sum_{i=1}^{m} \delta_{X_i}$ and $\eta$ with respect to the kernel $K$. Second, if we instead take $m^{-1} \sum_{i=1}^{m} \delta_{X_i}$ to be a *non-random* measure of the form $m^{-1} \sum_{i=1}^{m} \delta_{x_i}$, viewing Expression (4) as a function of the delta locations $x_1, \ldots, x_k$ results in exactly the herding optimisation problem. A connection between variance-reduced sampling and herding has also been noted in the context of random permutations (Lomelí et al., 2018). As well as these similarities, there are important differences between herding and the notion described here. Because all samples are regarded as random variables which are constrained to be marginally distributed according to $\eta$, a coupling maintains the usual unbiasedness guarantees of finite-sample Monte Carlo estimators. In contrast, herding is theoretically supported by fast asymptotic rates of convergence for a wide variety of estimators, but because samples are chosen in a deterministic way, estimator properties based on finite numbers of herding samples are harder to describe statistically. Often there are good reasons to eschew unbiasedness of an estimator in favour of fast convergence rates; however, unbiasedness of gradient estimators is crucial in optimisation algorithms performing correctly, as is well-established in the stochastic approximation literature. Bellemare et al. (2017) provide a discussion of this phenomenon in the context of generative modelling.

Interestingly, the following result shows that solutions of Problem (4) coincide exactly with $K$-optimal couplings of Definition 2.2.

**Theorem 2.8.** Given a probability distribution $\eta \in \mathscr{P}(\mathbb{R}^d)$ and a kernel $K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$, a coupling $\mu \in \Lambda_m(\eta)$ is $K$-optimal iff it is solves the optimisation problem in Expression (4).

Connections similar to Theorem 2.8 have previously been established in the study of identifying *deterministic* quadrature points (Paskov, 1993) – we also highlight (Kanagawa et al., 2018) as a recent review of such connections. In contrast, here we take random quadrature points with fixed marginal distributions.

### 2.3 Solving for *K*-optimal couplings

In this section, we study the objective defining $K$-optimal couplings, as given in Definition 2.2. The problem is intractable to solve analytically in general, so we present several solutions in settings with additional restrictions, either on the number of samples $m$ in the problem, or on the types of couplings considered. The theoretical statements are given in Theorems 2.9 and 2.10, with the corresponding practical algorithms given as Algorithms 1 and 2. We emphasise that solving Problem (2) in general remains an interesting direction for future work.

**Theorem 2.9.** Let $\eta \in \mathscr{P}(\mathbb{R}^d)$ be isotropic, and let $K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ be a stationary isotropic kernel, such that $K(\mathbf{x}, \mathbf{y})$ is a strictly decreasing, strictly convex function of $\|\mathbf{x} - \mathbf{y}\|$. Then the $K$-optimal coupling of 2 samples $(X_1, X_2)$ from $\eta$ is given by first drawing $X_1 \sim \eta$, and then setting the direction of $X_2$ to be opposite to that of $X_1$, and setting the norm of $\|X_2\|$ so that

$$F_R(\|X_2\|) + F_R(\|X_1\|) = 1\,, \tag{5}$$

where $F_R$ is the CDF associated with the norm of a random vector distributed according to $\eta$.

The proof of this theorem can be found in the Appendix Section 9 and relies on first showing that any optimal coupling must be antithetic and second that an antithetic coupling must satisfy equation

**Algorithm 1** Antithetic inverse lengths coupling of Theorem 2.9

**for** $i = 1, \dots, m$ **do**
  Draw $X_i \sim \eta$.
  Set $X_{m+i} = -X_i \frac{F_R^{-1}(1-F_R(||X_i||))}{||X_i||}$.
**end for**
**Output:** $X_1, \dots, X_{2m}$ marginally $\eta$ distributed, with low MSE.

**Algorithm 2** Orthogonal coupling of Theorem 2.10

**for** $i = 1, \dots, m$ **do**
  Draw $X_i \sim \eta$ conditionally orthogonal to $X_1, \dots, X_{i-1}$.
  Set $X_{m+i} = -X_i$.
**end for**
**Output:** $X_1, \dots, X_{2m}$ marginally $\eta$ distributed, with low MSE.

(5) in order for the marginals to be equal to $\eta$. In the Appendix Section 8 we illustrate with a counterexample that the convexity assumption is required. Indeed if most of the mass of $\eta$ is near the origin and the RBF kernel is larger around 0 then the classical antithetic coupling $X_2 = -X_1$ performs better.

Further extending the above situation, we restrict our attention to antithetic couplings and establish that the optimal way to couple $m$ antithetic pairs $(X_i, X_{m+i}) = (X_i, -X_i)$ is to draw sequentially orthogonal samples if the dimension of the space allows it and the marginal $\eta$ is spherically symmetric. Introduce the following notation for the set of antithetic couplings with independent lengths:

$$\Lambda_{2m}^{\text{anti}}(\eta) = \{\text{Law}(X_1, \dots, X_{2m}) \in \Lambda_{2m}(\eta) |\ ||X_i||, 1 \leq i \leq m \text{ are independent}, X_i = -X_{m+i}\ \}\ .$$

**Theorem 2.10.** Let $\eta \in \mathscr{P}(\mathbb{R}^d)$ be isotropic and let $K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ be a stationary isotropic kernel, such that $K(\mathbf{x}, \mathbf{y}) = \Phi(||\mathbf{x} - \mathbf{y}||^2)$, where $\Phi$ is a decreasing, convex function. If $\text{Law}(X_1, \dots, X_{2m})$, with $m \leq d$, is a solution to the constrained optimal coupling problem

$$\underset{\mu \in \Lambda_{2m}^{\text{anti}}(\eta)}{\arg\min}\ \mathbb{E}_{X_{1:2m} \sim \mu} \left[ \sum_{i,j=1}^{2m} \Phi\left(||X_i - X_j||^2\right) \right],$$

then it satisfies $\langle X_i, X_j \rangle = 0$ a.s. for all $1 \leq i < j \leq m$.

The proof of this theorem can be found in the Appendix Section 9 and relies on reformulating the objective function and showing that the exact minimum is attained thanks to convexity. This result illustrates the advantage that orthogonal samples can have over i.i.d. samples, see (Yu et al., 2016) for earlier such settings. Details on how to efficiently sample orthogonal samples can be found in (Stewart, 1980); exact simulation of $d$ orthogonal samples is possible in $\mathcal{O}(d^3)$ time, whilst empirically good quality samples can be obtained from approximate algorithms in $\mathcal{O}(d^2 \log d)$ time. We emphasise that we focus on applications where these increases in sampling costs are insignificant relative to the downstream costs of computing with the samples (such as simulating rollouts in RL environments, as in Section 5.1). However, we note that an interesting direction for future work would be to incorporate a notion of computational complexity into the $K$-optimality objective, to trade off statistical efficiency against sampling costs.

## 3 Low discrepancy of geometrically coupled samples

Having described our notions of optimal couplings in the previous section and obtained several sampling schemes, we now provide an interesting connection between our geometrically coupled samples and low discrepancy sequences that are studied in the QMC literature. Our main interest is in the *local discrepancy function* $\text{disr}_S : \mathbb{R}^d \to \mathbb{R}$ parametrised by a given set of samples $S = \{X_1, ..., X_{|S|}\}$ and defined as follows:

$$\text{disr}_S(\mathbf{u}) = \text{Vol}(J_{\mathbf{u}}) - \frac{|\{i : X_i \in J_{\mathbf{u}}\}|}{|S|},$$

where: $J_{\mathbf{u}} = [0, u_1) \times ... \times [0, u_d)$ and $\text{Vol}(J_{\mathbf{u}}) = \prod_{j=1}^d u_j$. Now define the *star discrepancy function* $D^*(S)$ as: $D^*(S) = \sup_{\mathbf{u} \in [0,1]^d} |\text{disr}_S(\mathbf{u})|$. This function measures the discrepancy between the empirical sample $S$ from the uniform distribution on a hypercube $[0, 1]^d$.

Consider an expression $I_f = \mathbb{E}_{X\sim\lambda}[f(X)]$, where $\lambda \in \mathscr{P}(\mathbb{R}^1)$, and a set of samples $S = \{X_1, ..., X_{|S|}\}$ that is used in a given (Q)MC estimator to approximate $I_f$. The *star discrepancy function* $D^*_\lambda$ *with respect to a distribution* $\lambda$ is defined on $S$ as: $\mathrm{D}^*_\lambda(S) \stackrel{\mathrm{def}}{=} \mathrm{D}^*(F_\lambda(S)) = \sup_{u\in[0,1]} |\mathrm{disr}_{F_\lambda(S)}(u)|$, where $F_\lambda(S) = \{F_\lambda(X_i)\}_{i=1,...,|S|}$ and $F_\lambda$ stands for the cdf function for $\lambda$. In other words, to measure the discrepancy between arbitrary distribution $\lambda \in \mathscr{P}(\mathbb{R}^1)$ and a set of samples $S$, the set of samples is transformed to the interval $[0, 1]$ via the cdf $F_\lambda$ and the discrepancy between the uniform distribution on $[0, 1]$ and the transformed sequence $F_\lambda(S)$ is calculated.

We will focus here on distributions $\lambda \in \mathscr{P}(\mathbb{R}^1)$, which we call *regular distributions*, corresponding to random variables $X$ defined as $X = \mathbf{g}^\top \mathbf{z}$, where $\mathbf{z} \in \mathbb{R}^d$ is a deterministic vector and $\mathbf{g} \in \mathbb{R}^d$ is taken from some isotropic distribution $\tau$ (e.g. multivariate Gaussian distribution). Regular distributions play an important role in machine learning. It is easy to show that the random feature map approximation of radial basis function (RBF) kernels such as Gaussian kernels can be rewritten as $I_f = \mathbb{E}_{X\sim\lambda}[f(X)]$, where $f(x) \stackrel{\mathrm{def}}{=} \cos(x)$ and $\lambda$ is a regular distribution (Rahimi and Recht, 2007). To sample points from $\lambda$, we will use the standard set $S_{\mathrm{iid}}$ of independent samples as well as the set of orthogonal samples $S_{\mathrm{ort}}$, where marginal distributions of different $\mathbf{g}_i$ are $\lambda$ but different $\mathbf{g}_i$ are conditioned to be exactly orthogonal (see Choromanski et al., 2018b, for explicit constructions).Our main result of this section shows that local discrepancy $\mathrm{disr}_{F_\lambda(S)}(\mathbf{u})$ for a fixed $\mathbf{u} \in [0, 1]^d$ is better concentrated around 0 for regular distributions $\lambda$ if orthogonal sets of samples $S$ are used instead of independent samples. Indeed, in both cases one can obtain exponentially small upper bounds on failure probabilities but these are sharper when orthogonal samples are used.

**Theorem 3.1.** [Local discrepancy & regular distributions] Denote by $S_{\mathrm{iid}}$ a set of independent samples, each taken from a regular distribution $\lambda$ and by $S_{\mathrm{ort}}$ the set of orthogonal samples for that distribution. Let $s = |S_{\mathrm{iid}}| = |S_{\mathrm{ort}}|$. Then for any fixed $u \in [0, 1]$ and $a \in \mathbb{R}_+$ the following holds: $\mathbb{P}[|\mathrm{disr}_{F_\lambda(S_{\mathrm{iid}})}(u)| > a] \leq 2e^{-\frac{sa^2}{8}} \stackrel{\mathrm{def}}{=} p_{\mathrm{iid}}(a)$ and for some $p_{\mathrm{ort}}$ satisfying $p_{\mathrm{ort}} < p_{\mathrm{iid}}$ it holds pointwise: $\mathbb{P}[|\mathrm{disr}_{F_\lambda(S_{\mathrm{ort}})}(u)| > a] \leq p_{\mathrm{ort}}(a)$ . Also: $Var(\mathrm{disr}_{F_\lambda(S_{\mathrm{ort}})}(u)) < Var(\mathrm{disr}_{F_\lambda(S_{\mathrm{iid}})}(u))$.

Sharper concentration results regarding local discrepancies translate to sharper concentration results for the star discrepancy function $D^*_\lambda$ via the $\epsilon$-net argument and thus also ultimately to sharper results regarding approximation error of MC estimators using regular distributions via the celebrated Koksma-Hlawka Inequality ((Avron et al., 2016); see Theorem 10.4 in the Appendix).

We conclude that orthogonal samples (special instantiations of the GCMC mechanism) lead to strictly better guarantees regarding the approximation error of $I_f$ for functions $f$ with bounded variation and regular distributions $\lambda$ than standard MC mechanisms. This is the case in particular for random feature map based approximators of RBF kernels. The advantages of orthogonal samples in this setting were partially understood before for certain classes of RBF kernels (Choromanski et al., 2018b; Yu et al., 2016), but to the best of our knowledge, general non-asymptotic results and the connection with discrepancy theory were not known.

In Figure 1 we show a kernel density estimate of the distributions of the $D^*$ discrepancies of 50,000 sample sequences $\left(F^{-1}_{\mathcal{N}(0,1)}\left(\frac{\mathbf{g_i}^T\mathbf{z}}{||z||}\right)\right)_{i=1,...,40}$ for a range of coupling algorithms to generate Gaussian samples $\mathbf{g_i}$. We see that using antithetic samples with coupled lengths as in Algorithm 1 leads to a sequence with lower discrepancy on average. We also observe that coupling the samples to be orthogonal reduces the discrepancy. This

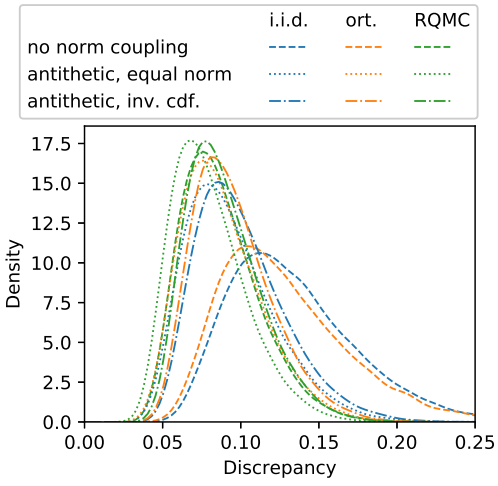



Figure 1: Histograms of the $D^*$ discrepancy for different sampling methods: samples $g_i$ have i.i.d., orthogonal or RQMC directions with uncoupled lengths or lengths coupled according to Algorithms 1 or 2

confirms the above results. Finally this figure shows that an algorithm designed to have a low discrepancy (RQMC) will still reach a lower discrepancy than a classical sampling method but this difference can be mitigated by using antithetic samples.

# 4 Geometric coupling for estimating gradients of function smoothings

Here we provide results on the concentration of zeroth order gradient estimators for reinforcement learning applications, helping to explain their efficacy. This area is one of the main applications of the GCMC methods introduced in Section 2, and we present experiments for these applications in Section 5.1. To our knowledge, we provide the first result showing exponential concentration for the Evolution Strategies (ES) gradient estimator (Salimans et al., 2017) in this setting. We also provide exponential concentration bounds for orthogonal gradient estimators.

Recall that given a function $F : \Theta \to \mathbb{R}$ to be minimised, the Vanilla ES gradient estimator is defined as:

$$\hat{\nabla}_N^V F_\sigma(\theta) = \frac{1}{N\sigma} \sum_{i=1}^{N} F(\theta + \sigma\epsilon_i)\epsilon_i, \quad \text{where } \epsilon_i \sim \mathcal{N}(0, I) \text{ are all i.i.d.}. \tag{6}$$

In what follows we assume that $F$ is uniformly bounded over its domain by $\mathcal{F}$. In the case that $F$ is a sum of discounted rewards, an upper bound of $\mathcal{R}$ for the reward function yields an upper bound of $\frac{1}{1-\gamma}\mathcal{R}$ for $F$, where $\gamma$ is the discount factor. Whenever $F$ is bounded in absolute value, the random vector $\hat{\nabla}_N^V F_\sigma(\theta)$ is sub-Gaussian.

**Theorem 4.1.** If $F$ is a bounded function such that $|F| \leq R_1$, then the vanilla ES estimator is a sub-Gaussian vector with parameter $\frac{\sqrt{2}R_1\sqrt{8c^2+1}}{\sqrt{N}\sigma}$; with $c = 24e$ and therefore for any $t \geq 0$:

$$\mathbb{P}\left( \max_{j=1,\ldots,d} \left| \left(\hat{\nabla}_N^V F_\sigma(\theta)\right)_j - \left(\mathbb{E}\left[\hat{\nabla}_N^V F_\sigma(\theta)\right]\right)_j \right| \geq t \right) \leq 2de^{\frac{-t^2 N\sigma^2}{2R_1^2(8c^2+1)}},$$

for a universal constant $c$.

For the case of pairs of antithetic coupled gradient estimators, one can obtain a similar bound with comparable performance using this technique.

## 4.1 Bounds for orthogonal estimators

We show that a general class of orthogonal gradient estimators present similar exponential concentration properties as the Vanilla ES estimator. Proving these bounds is substantially more challenging because of the correlation structure between samples. To our knowledge, these are the first results showing exponential concentration for structured gradient estimators, yielding insight as to why these perform well in practice. We provide concentration bounds for gradient estimators of the form:

$$\hat{\nabla}_d^{Ort} F(\theta) = \frac{1}{d\sigma} \sum_{i=1}^{d} \nu_i b_i F\left(\theta + \sigma\nu_i b_i\right),$$

where the random vectors $\nu_i \in \mathbb{R}^d$ are sampled uniformly from the unit sphere using a sequentially orthogonal process, and $b_i$ are zero mean signed lengths, sampled from sub-Gaussian distributions each with sub-Gaussian parameter $\beta_i$, independent from each other and from all other sources of randomness. Let $c := 2\sqrt{(24e)^2 + \frac{1}{2}}$. Whenever the function $F$ is bounded, the random variable vector $\hat{\nabla}_d^{Ort} F(\theta)$ is sub-Gaussian.

**Theorem 4.2.** Let $B = \max_i \mathbb{E}\left[|b_i|\right]$, and $\beta = \max_i \beta_i$, $|F| \leq R$, then the orthogonal gradient estimator $\hat{\nabla}_d^{Ort} F(\theta)$ is sub-Gaussian with parameter $\sqrt{\frac{\beta^2 c^2 R^2}{\sigma^2 d^2} + \frac{R^2 B^2}{4d\sigma^2}}$.

Assuming $N = Td$ and the availability of $T$ i.i.d. orthogonal estimators (indexed by $j$), define:

$$\hat{\nabla}_N^{Ort} F(\theta) = \frac{1}{T} \sum_{j=1}^{T} \hat{\nabla}_d^{Ort,j} F(\theta).$$

**Theorem 4.3.** The gradient estimator $\hat{\nabla}_N^{Ort} F(\theta)$ is sub-Gaussian with parameter $\frac{1}{\sqrt{T}}\sqrt{\frac{\beta^2 c^2 R^2}{\sigma^2 d^2} + \frac{R^2 B^2}{4\sigma^2 d}} = \frac{1}{\sqrt{N}}\sqrt{\frac{\beta^2 c^2 R^2}{d\sigma^2} + \frac{R^2 B^2}{4\sigma^2}}$; and therefore:

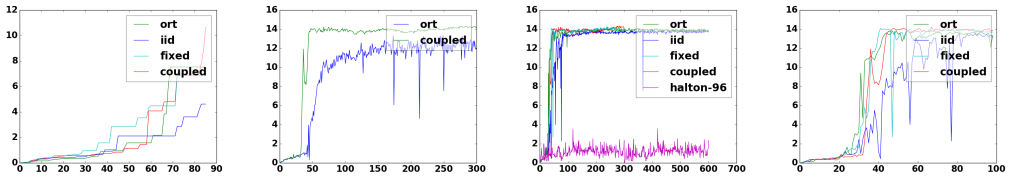
$$\mathbb{P}\left(\max_{j=1,\ldots,d}\left|\left(\hat{\nabla}_N^{Ort} F(\theta)\right)_j - \left(\mathbb{E}\left[\hat{\nabla}_N^{Ort} F(\theta)\right]\right)_j\right| \geq t\right) \leq 2de^{\frac{-t^2 N\sigma^2}{\frac{\beta^2 c^2 R^2 \sigma^2}{d} + \frac{R^2 B^2}{4}}}.$$

# 5 Experiments

## 5.1 Learning efficient navigation policies with ES strategies

We consider the task of closed-loop policy optimization to train stable walking behaviors for quadruped locomotion of the Minitaur platform on the Bullet simulator (Coumans and Bai, 2016–2018). We train neural network policies with $d \geq 96$ parameters and optimize the blackbox function $F$ that takes as input parameters of the neural network and outputs the total reward, by applying MC estimators of gradients of Gaussian smoothings of $F$, as described in Expression (6). The main aim of the experiments is to compare policies learnt by using i.i.d. samples, as in Expression (6), against estimators using GCMC methods. We test four different control variate terms that lead to four different variants of the MC algorithm: vanilla (no control variate), forward finite-difference (see Choromanski et al., 2018c, for details), antithetic and antithetic-coupled (see: below). For each of these four variants we use different sampling strategies of calculating the MC estimator: MCGaussian, Halton (baselines), MCGaussianOrthogonal, MCGaussianOrthogonalFixed, and MCRandomHadamard that correspond to: independent Gaussian samples (Salimans et al., 2017), samples constructed from randomized Halton sequences used on a regular basis in QMC methods, Gaussian orthogonal samples (introduced first in Choromanski et al. (2018c) but not tested for $m < d$ and in the locomotion task setting), Gaussian orthogonal samples with renormalized lengths (each length equals $\sqrt{d}$) and finally: rows of random Hadamard matrices (that approximate Gaussian orthogonal samples, but are easier to compute, (see Choromanski et al., 2018c)). For the antithetic variant using Gaussian orthogonal samples, we also test the variant which couples the lengths of antithetic pairs of samples as in Algorithm 1; we refer to this as antithetic $-$ coupled. We tested different number of samples $s$ with the emphasis on MC estimators satisfying: $m \ll d$. We chose: $m = 8, 16, 32, 48, 56, 64, 96$. Full details of the sampling mechanisms described above are given in the Appendix Section.

Figure 2 shows comparison of different MC methods using antithetic variant for $m = 8, 32, 48$ samples given to the MC estimator per iteration of the optimization routine (with an exception of the Halton approach, where we used $m = 96$ samples to demonstrate that even with the larger number of samples standard QMC methods fail). Walkable policies are characterized by total reward $R > 10.0$. We notice that structured approaches outperform the unstructured one and that QMC method based on Halton sequences did not lead to walkable policies. Since it will be also the case for other settings considered by us, we exclude it from the subsequent plots.




(a) $m = 8$ (b) $m = 32$ (c) $m = 48$, 600 iterations (d) $m = 48$, 100 iterations

Figure 2: Training curves for different MC methods. iid, ort, coupled, fixed, halton-96 correspond to: MCGaussian, MCGaussianOrthogonal, antithetic $-$ coupled, MCGaussianOrthogonalFixed and Halton-based QMC method. Subfigure (d) is a zoomed version of Subfigure (c) after just 100 iterations and with Halton approach excluded.

For $m = 32$ we excluded the comparison with MCGaussian since it performed substantially worse than other methods and with MCGaussianOrthogonalFixed since it was very similar to

$\mathrm{MCGaussianOrthogonal}$ (for clarity). Again, for clarity, for $m = 8$ we plot the max-reward-curves, where the maximal reward from already constructed policies instead of the current one is plotted (thus these curves are monotonic). In Subfigure (a) the curves stabilize after about $87$ iterations (for the $\mathrm{MCGaussianOrthogonal}$ strategy the curve ultimately exceeds reward 10.0 but after $> 500$ iterations).

We conclude that for $m = 8$ the coupling mechanism is the only one that leads to walkable policies and for $m = 32$ it leads to the best policy among all considered structured mechanisms. More experimental results are given in the Appendix. We also attach videos showing how policies learned by applying certain structured mechanisms work in practice (details in the Appendix). Testing all variants of the MC mechanism mentioned above, we managed to successfully train stable walking behaviours using only $m = 8$ samples per iteration only for $k = 5$ settings: $\mathrm{MCGaussianOrthogonal}$-$\mathrm{antithetic}$-$\mathrm{coupled}$, $\mathrm{MCGaussianOrthogonal}$-$\mathrm{antithetic}$, $\mathrm{MCGaussianOrthogonal}$-$\mathrm{forward}$-$\mathrm{fd}$, $\mathrm{MCRandomHadamard}$-$\mathrm{antithetic}$ and $\mathrm{MCRandomHadamard}$-$\mathrm{vanilla}$. Thus all $5$ policies correspond to some variants of our GCMC mechanism.

We did not conduct hyperparameters tuning to obtain the above curves. We used hyperparameters applied on a regular basis in other Monte Carlo algorithms for policy optimization, in particular chose $\sigma = 0.1$ and $\eta = 0.01$, where $\sigma$ stands for the standard deviation of the entries of Gaussian vectors used for MC and $\eta$ is the gradient step size. The experiments where conducted in a distributed environment on a cluster of machines, where each machine was responsible for evaluating exactly one sample.

### 5.2 Variance-reduced ELBO estimation for deep generative models

In this section, we test GCMC sampling strategies on a deep generative modelling application. We consider a variational autoencoder (VAE) (Rezende et al., 2014; Kingma and Welling, 2014) with latent variable $z$ with prior $p(z)$, observed variable $x$ with trainable generative model $p_\theta(x|z)$, and trainable recognition model $q_\phi(z|x)$. In the standard VAE training algorithm, the evidence lower-bound (ELBO) for a single training point $x$ is:

$$\mathbb{E}_{z\sim q_\phi(\cdot|x)}\left[\log p_\theta(x,z) - \log q_\phi(z|x)\right] .$$

This objective is then optimised by estimating gradients using a combination of $m \in \mathbb{N}$ i.i.d. Monte Carlo samples together with the reparametrisation trick. We adjust the training algorithm by using a variety of GCMC sampling algorithms, rather than i.i.d. sampling. We train on MNIST, and report the average train and test ELBO after 50 epochs for a variety of sampling algorithms and numbers of samples $K$, to understand the effect of these sampling methods on speeding up learning. The full results and experiment specifications are given in the Appendix Section 12. We observe that GCMC methods consistently lead to better log-likelihoods than i.i.d. sampling, in fact with GCMC methods with 2 samples performing better than i.i.d. methods using $8$ samples. We highlight concurrent work (Buchholz et al., 2018) that presents an in-depth study of quasi-Monte Carlo integration for variational inference.

## 6 Conclusion

We have introduced Monte Carlo coupling strategies in Euclidean spaces for improving algorithms that typically operate in a high-dimensional, low-sample regime, demonstrating fundamental connections to multi-marginal transport. In future work, it will be interesting to explore applications in other areas such as random feature kernel approximation. We also highlight more general solution of the $K$-optimality criterion, and incorporation of a sampling cost penalty into the corresponding objective as interesting problems left open by this paper.

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# APPENDIX: Geometrically Coupled Monte Carlo Sampling

## 7 Measure-theoretic considerations regarding *K*-optimality

In this section, we briefly address the measure-theoretic issues arising from the definition of $K$-optimality in Section 2.1, and establish several important integrability results that will be used in the proofs of the results appearing in Section 2. We re-emphasize here that, as stated in Section 2 of the main paper, we restrict to the case where the Gaussian process $\mathrm{GP}(0, K)$ has continuous sample paths in order to avoid unnecessary technical complications. More precisely, we restrict to Gaussian processes for which a continuous modification of the process exists, and assume in the following that it is always this modification that we are working with. The vast majority of commonly used GP kernels in machine learning lead to continuous GP sample paths, with the exception of special cases such as the white noise kernel. For further discussion of the properties of kernels that lead to continuous sample paths in GPs (see e.g. Marcus and Shepp, 1972; Talagrand, 1987; Gin and Nickl, 2015).

We begin by recalling the form of the objective for $K$-optimality, defined in the main paper in Expression (2):

$$\underset{\mu\in\Lambda_m(\eta)}{\arg\min}\ \mathbb{E}_{f\sim\mathrm{GP}(0,K)}\left[\mathbb{E}_{X_{1:m}\sim\mu}\left[\left(\frac{1}{m}\sum_{i=1}^{m}f(X_i)-I_f\right)^2\right]\right].$$

Firstly, we establish joint measurability of the random variable $(m^{-1}\sum_{i=1}^m f(X_i) - I_f)^2$. We consider the Gaussian process $f$ taking values in the measurable space $(C(\mathbb{R}^d;\mathbb{R}),\Sigma)$, where $C(\mathbb{R}^d,\mathbb{R})$ is the space of continuous functions from $\mathbb{R}^d$ to $\mathbb{R}$, and $\Sigma$ is the product sigma-algebra, and $(X_1,\ldots,X_m)$ taking values in the measurable space $((\mathbb{R}^d)^m,\mathcal{B}((\mathbb{R}^d)^m))$, where $\mathcal{B}((\mathbb{R}^d)^m)$ is the usual Borel sigma algebra on $(\mathbb{R}^d)^m$. We aim to establish that $(m^{-1}\sum_{i=1}^m f(X_i) - I_f)^2$ is measurable on $(C(\mathbb{R}^d;\mathbb{R})\times(\mathbb{R}^d)^m,\Sigma\otimes\mathcal{B}((\mathbb{R}^d)^m))$. Considering the types of terms that result from expanding $(m^{-1}\sum_{i=1}^m f(X_i) - I_f)^2$, we note that it is sufficient to prove joint measurability of terms of the form $f(X_i)$ and $f(X_i)f(X_j)$. We deal explicitly with the term $f(X_i)$ here; the treatment of the term $f(X_i)f(X_j)$ is analogous. To do this, we show that the evaluation function $\psi : (C(\mathbb{R}^d;\mathbb{R})\times(\mathbb{R}^d)^m,\Sigma\otimes\mathcal{B}((\mathbb{R}^d)^m))\to(\mathbb{R},\mathcal{B}(\mathbb{R}))$ defined by $\psi(g,x)=g(x)$, is measurable, and since $f(X_i)$ is given by the composition $\psi(f,X_i)$, we have that $f(X_i)$ is measurable, as required. To reach this conclusion, we will show that (i) for all $x\in\mathbb{R}^d$, the function $\psi(\cdot,x) : (C(\mathbb{R}^d;\mathbb{R}),\Sigma)\to\mathbb{R}$ is measurable, and (ii) for all $g\in C(\mathbb{R}^d;\mathbb{R})$, the function $\psi(g,\cdot):\mathbb{R}^d\to\mathbb{R}$ is continuous. $\psi$ is then said to be a Carathéodory function, and joint measurability follows (see Aliprantis and Border, 2006, Lemma 4.51). For (i), simply note that for all $A\in\mathcal{B}(\mathbb{R})$, $x\in\mathbb{R}^d$, the set $\{g\in C(\mathbb{R}^d;\mathbb{R})|g(x)\in A\}$ is a cylinder set, and hence in $\Sigma$. In addition, (ii) follows immediately by continuity of $g\in C(\mathbb{R}^d;\mathbb{R})$. Putting all this together, we have established joint measurability of the random variable $(m^{-1}\sum_{i=1}^m f(X_i) - I_f)^2$, which means that the $K$-optimality objective appearing in Definition 2.2 is well-defined.

Finally, we make several remarks on pathwise integrability of the Gaussian process $\mathrm{GP}(0,K)$. Firstly, we show that $f\in L^2(\eta)$ almost surely, via the following calculation:

$$\mathbb{E}_{X\sim\eta}\left[\mathbb{E}_{f\sim\mathrm{GP}(0,K)}\left[f(X)^2\right]\right]=\mathbb{E}_{X\sim\eta}\left[K(X,X)\right]<\infty,$$

with the bound following from stationarity of the kernel $K$. Thus, we may apply Fubini's theorem to obtain

$$\mathbb{E}_{f\sim\mathrm{GP}(0,K)}\left[\mathbb{E}_{X\sim\eta}\left[f(X)^2\right]\right]=\mathbb{E}_{X\sim\eta}\left[\mathbb{E}_{f\sim\mathrm{GP}(0,K)}\left[f(X)^2\right]\right].$$

It therefore follows that $f\in L^2(\eta)$ almost surely (under the law of the Gaussian process). The joint integrability with respect to $\eta$ and the law of the Gaussian process established above is important in justifying the use of Fubini's theorem in exchanging orders of expectation in the analysis presented in Section 9.

## 8 Examples and counterexamples relating to Section 2

In this section, we present several examples that serve to further illustrate results from the main text.

### 8.1 Convexity of the kernel is needed in Theorem 2.9

We present a counterexample illustrating that the convexity assumption on the kernel is required in theorem 2.9. Let $K(\mathbf{x}, \mathbf{y}) = e^{-||\mathbf{x}-\mathbf{y}||^2}$ be the Gaussian kernel and let $\eta \in \mathscr{P}(\mathbb{R}^d)$ be the spherically symmetric distribution such that if $X \sim \eta$ then $||X|| \sim \mathcal{U}([0, b])$ for some $b > 0$. Note that the kernel is not convex. Depending on the value of $b$, two different couplings of the norms will be optimal: either $||X_2|| = ||X_1||$ or $||X_2|| = F_R^{-1}(1 - F_R(||X_1||))$. Indeed it is easy to compute numerically the following expectations for this choice of $\eta$ and to note that

$$\mathbb{E}[K(X_1, -X_1)] < \mathbb{E}\left[K\left(X_1, \frac{X_1}{||X_1||} F_R^{-1}(1 - F_R(||X_1||)\right)\right] \iff b < \frac{3}{4}.$$

This illustrates that in the absence of convexity of the kernel the optimal choice of coupling for two samples also depends on $\eta$: if $\eta$ assigns a lot of mass to a small area around 0 ($b$ small) then the coupling of Theorem 2.9 suffers a lot in conjunction with the Gaussian kernel. On the other hand if $\eta$ spreads out mass more evenly further from 0 ($b$ large) then the antithetic coupling giving equal norms to both samples performs better.

### 8.2 Examples illustrating non-existence of uniformly optimal couplings

Below, we give two examples that expand on the remarks in Section 2 stating that in general, there does not exist a coupling of Monte Carlo samples $(X_1, \ldots, X_m)$ that achieves optimal MSE simultaneously for a range of functions $f$ for the objective appearing in Expression (1).

**Example 8.1.** Suppose we want to estimate the value of the following expectation:

$$\mathbb{E}_{X \sim N(0,I)}\left[f(X)\right],$$

where $f : \mathbb{R}^2 \to \mathbb{R}$ is specified in polar coordinates by

$$f(r, \theta) = \mathbb{1}_{\theta \in [0,\pi)}.$$

The exact value of this integral is $1/2$. An optimal coupling for two samples marginally distributed as $N(0, I)$ in this case can be shown to be any distribution for which $X_1$ and $X_2$ point in opposite directions almost surely (e.g. taking $X_2 = -X_1$). It is readily checked that the corresponding Monte Carlo estimator is in fact exact, having a mean squared error (MSE) of 0.

**Example 8.2.** Consider the same setup as Example 8.1, but now with the function

$$f(r, \theta) = \mathbb{1}_{\theta \in [0,\pi/2) \cup [\pi, 3\pi/2)}.$$

In this case, it is straightforward to show that the two coupled samples of Example 8.1 obtain the same MSE as a single Gaussian sample, whereas two i.i.d. Gaussian samples obtain half this MSE.

Examples 8.1 and 8.2 illustrate that it is not always possible for one coupling to outperform all others (in terms of MSE) across a given function class.

## 9 Proofs of results in Section 2

**Theorem 2.4.** The optimisation problem defining $K$-optimality in Equation (2) is equivalent to the following *multi-marginal transport problem*:

$$\underset{\mu \in \Lambda_m(\eta)}{\arg\min}\ \mathbb{E}_{X_{1:m} \sim \mu}\left[\sum_{i \neq j} K(X_i, X_j)\right].$$

*Proof.* We calculate as follows, beginning with the $K$-optimality objective:

$$\begin{aligned}
&\mathbb{E}_{f\sim\mathrm{GP}(0,K)}\left[\mathbb{E}_{X_{1:m}\sim\mu}\left[\left(\frac{1}{m}\sum_{i=1}^{m}f(X_i)-I_f\right)^2\right]\right]\\
=&\mathbb{E}_{f\sim\mathrm{GP}(0,K)}\left[\mathbb{E}_{X_{1:m}\sim\mu}\left[\left(\frac{1}{m}\sum_{i=1}^{m}f(X_i)-\mathbb{E}_{X\sim\eta}[f(X)]\right)^2\right]\right]\\
=&\mathbb{E}_{f\sim\mathrm{GP}(0,K)}\left[\mathbb{E}_{X_{1:m}\sim\mu}\left[\frac{1}{m^2}\sum_{i=1}^{m}f^2(X_i)+\frac{1}{m^2}\sum_{i\neq j}f(X_i)f(X_j)\right.\right.\\
&\left.\left.-\frac{2}{m}\mathbb{E}_{X\sim\eta}[f(X)]\sum_{i=1}^{m}f(X_i)+\mathbb{E}_{X\sim\eta}[f(X)]^2\right]\right].
\end{aligned}$$

Removing terms which depend only on the fixed marginal distribution $\eta$, and not the joint distribution $\mu$, the observe that up to a function of $\eta$ only, the objective above is equivalent to

$$\mathbb{E}_{f\sim\mathrm{GP}(0,K)}\left[\mathbb{E}_{X_{1:m}\sim\mu}\left[\sum_{i\neq j}f(X_i)f(X_j)\right]\right].$$

By Fubini's theorem, we obtain

$$\begin{aligned}
\mathbb{E}_{f\sim\mathrm{GP}(0,K)}\left[\mathbb{E}_{X_{1:m}\sim\mu}\left[\sum_{i\neq j}f(X_i)f(X_j)\right]\right]&=\mathbb{E}_{X_{1:m}\sim\mu}\left[\mathbb{E}_{f\sim\mathrm{GP}(0,K)}\left[\sum_{i\neq j}f(X_i)f(X_j)\right]\right]\\
&=\mathbb{E}_{X_{1:m}\sim\mu}\left[\sum_{i\neq j}K(X_i,X_j)\right],
\end{aligned}$$

as required. □

**Proposition 2.7.** Suppose that the function class $\mathscr{F}$ is the unit ball in some RKHS given by a kernel $K:\mathbb{R}^d\times\mathbb{R}^d\to\mathbb{R}$. Then the component

$$\sup_{f\in\mathscr{F}}\ \mathbb{E}_{X_{1:m}\sim\mu}\left[\left(\frac{1}{m}\sum_{i=1}^{m}f(X_i)-I_f\right)^2\right]$$

of the minimax coupling objective in Equation (3) may be upper-bounded by the following objective:

$$\mathbb{E}_{X_{1:m}\sim\mu}\left[\left\|\theta_K\left(\frac{1}{m}\sum_{i=1}^{m}\delta_{X_i}\right)-\theta_K\left(\eta\right)\right\|_{\mathcal{H}_K}^2\right], \tag{4}$$

where $\theta_K:\mathscr{P}(\mathbb{R}^d)\to\mathcal{H}_K$ is the kernel mean embedding into the RKHS $\mathcal{H}_K$ associated with $K$.

*Proof.* We begin by observing that for $f\in\mathcal{H}_K$,

$$\begin{aligned}
\mathbb{E}_{X_{1:m}\sim\mu}\left[\left(\frac{1}{m}\sum_{i=1}^{m}f(X_i)-I_f\right)^2\right]&=\mathbb{E}_{X_{1:m}}\left[\left(\int_{\mathbb{R}^d}f(x)\left(\frac{1}{m}\sum_{i=1}^{m}\delta_{X_i}-\eta\right)(\mathrm{d}x)\right)^2\right]\\
&=\mathbb{E}_{X_{1:m}}\left[\left\langle f,\theta_K\left(\frac{1}{m}\sum_{i=1}^{m}\delta_{X_i}\right)-\theta_K\left(\eta\right)\right\rangle_{\mathcal{H}_K}^2\right].
\end{aligned}$$

Using this observation, we next observe that

$$\sup_{f\in\mathscr{F}} \mathbb{E}_{X_{1:m}\sim\mu}\left[\left(\frac{1}{m}\sum_{i=1}^{m} f(X_i) - I_f\right)^2\right] = \sup_{f\in\mathscr{F}} \mathbb{E}_{X_{1:m}\sim\mu}\left[\left\langle f, \theta_K\left(\frac{1}{m}\sum_{i=1}^{m}\delta_{X_i}\right) - \theta_K(\eta)\right\rangle_{\mathcal{H}_K}^2\right]$$
$$\leq \mathbb{E}_{X_{1:m}\sim\mu}\left[\sup_{f\in\mathscr{F}}\left\langle f, \theta_K\left(\frac{1}{m}\sum_{i=1}^{m}\delta_{X_i}\right) - \theta_K(\eta)\right\rangle_{\mathcal{H}_K}^2\right].$$

We can now evaluate the supremum; it is realised when $f \in \mathcal{H}_K$ is the unit vector in the direction of $\theta_K\left(m^{-1}\sum_{i=1}^{m}\delta_{X_i}\right) - \theta_K(\eta)$, in which case the squared inner product evaluates to $\|\theta_K\left(m^{-1}\sum_{i=1}^{m}\delta_{X_i}\right) - \theta_K(\eta)\|_{\mathcal{H}_K}^2$. Substituting this in yields the result. □

**Theorem 2.8.** Given a probability distribution $\eta \in \mathscr{P}(\mathbb{R}^d)$ and a kernel $K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$, a coupling $\mu \in \Lambda_m(\eta)$ is $K$-optimal iff it is solves the optimisation problem in Expression (4).

*Proof.* The optimisation objective

$$\mathbb{E}_{X_{1:m}\sim\mu}\left[\left\|\theta_K\left(\frac{1}{m}\sum_{i=1}^{m}\delta_{X_i}\right) - \theta_K(\eta)\right\|_{\mathcal{H}_K}^2\right]$$

can be rewritten in the following form:

$$\mathbb{E}_{X_{1:m}\sim\mu}\left[\left\|\theta_K\left(\frac{1}{m}\sum_{i=1}^{m}\delta_{X_i}\right) - \theta_K(\eta)\right\|_{\mathcal{H}_K}^2\right]$$
$$=\mathbb{E}_{X_{1:m}\sim\mu}\left[\left\|\frac{1}{m}\sum_{i=1}^{m}K(X_i,\cdot) - \theta_K(\eta)\right\|_{\mathcal{H}_K}^2\right]$$
$$=\mathbb{E}_{X_{1:m}\sim\mu}\left[\left\|\frac{1}{m}\sum_{i=1}^{m}K(X_i,\cdot)\right\|_{\mathcal{H}_K}^2 - 2\left\langle\frac{1}{m}\sum_{i=1}^{m}K(X_i,\cdot), \theta_K(\eta)\right\rangle_{\mathcal{H}_K} + \|\theta_K(\eta)\|_{\mathcal{H}_K}^2\right].$$

Since the marginal distributions of $X_1, \ldots, X_m$ are fixed, the only term above that depends on the *coupling* between the random variables $X_1, \ldots, X_m$ is the first term. Thus, minimising the original objective is equivalent to minimising

$$\mathbb{E}_{X_{1:m}\sim\mu}\left[\left\|\frac{1}{m}\sum_{i=1}^{m}K(X_i,\cdot)\right\|_{\mathcal{H}_K}^2\right].$$

Expanding this term yields:

$$\mathbb{E}_{X_{1:m}\sim\mu}\left[\frac{1}{m^2}\sum_{i=1}^{m}K(X_i,X_i) + \frac{1}{m^2}\sum_{i\neq j}K(X_i,X_j)\right].$$

Again, the only term depending on the coupling is the final term, so minimising the original objective is equivalent to the following optimisation problem:

$$\min_{\mu\in\Lambda_m(\eta)} \mathbb{E}_{X_{1:m}\sim\mu}\left[\sum_{i\neq j}K(X_i,X_j)\right],$$

over all joint distribution of $X_{1:m}$ with marginals given by $\eta$. □

**Theorem 2.9.** Let $\eta \in \mathscr{P}(\mathbb{R}^d)$ be isotropic, and let $K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ be a stationary isotropic kernel, such that $K(\mathbf{x}, \mathbf{y})$ is a strictly decreasing, strictly convex function of $\|\mathbf{x} - \mathbf{y}\|$. Then the $K$-optimal coupling of 2 samples $(X_1, X_2)$ from $\eta$ is given by first drawing $X_1 \sim \eta$, and then setting the direction of $X_2$ to be opposite to that of $X_1$, and setting the norm of $\|X_2\|$ so that

$$F_R(\|X_2\|) + F_R(\|X_1\|) = 1\,, \tag{5}$$

where $F_R$ is the CDF associated with the norm of a random vector distributed according to $\eta$.

*Proof.* To demonstrate that the optimal coupling takes the form given in the statement of Theorem, we proceed in two steps: (i) we show that there exists an optimal coupling $\mu^*$ such that if $(X_1, X_2) \sim \mu^*$, then $X_1/\|X_1\| = -X_2/\|X_2\|$ almost surely, i.e. $X_1$ and $X_2$ point in opposite directions almost surely, and (ii) that the norms of $X_1$ and $X_2$ satisfy $\|X_2\| = F_R^{-1}(1 - F_R(\|X_1\|))$ almost surely. We begin with (i).

Let $\mu \in \Lambda_2(\eta)$ be optimal for the following optimisation problem:

$$\min_{\mu \in \Lambda_2(\eta)} \mathbb{E}_{(X_1,X_2)\sim\mu} \left[ K(X_1, X_2) \right] , \tag{7}$$

Then note that if we let $(X_1, X_2) \sim \mu$, then if $R$ is a random matrix draw independently from Haar measure on the orthogonal group $O_d$, then $\mu' = \mathrm{Law}((RX_1, -RX_1/\|X_1\| \times \|X_2\|))$ still lies in $\Lambda_2(\eta)$, and moreover yields an objective value for (7) at least as small as that achieved by $\mu$. The former claim comes from observing that since $\eta$ is radially symmetric, we have $\mathrm{Law}(RX_1) = \mathrm{Law}(X_1) = \eta$, and $\mathrm{Law}(-RX_1 \times \|X_2\|/\|X_1\|)$ is the law of a random vector with uniformly random direction (given by $-RX_1/\|X_1\|$), and independent norm given by $\|X_2\|$, and so is again distributed according to $\eta$. For the latter claim, note that we have

$$\|X_1 - X_2\| \leq \left\| X_1 - \left( -X_1 \frac{\|X_2\|}{\|X_1\|} \right) \right\| = \left\| RX_1 - \left( -RX_1 \frac{\|X_2\|}{\|X_1\|} \right) \right\| ,$$

and so by the assumption of the theorem that $K(\mathbf{x}, \mathbf{y})$ is a decreasing function of $\|\mathbf{x} - \mathbf{y}\|$, we have

$$K(X_1, X_2) \geq K \left( RX_1, -RX_1 \frac{\|X_2\|}{\|X_1\|} \right) ,$$

as required. We have therefore demonstrated that there exists an optimal coupling of $X_1, X_2 \sim \eta$ for (7) such that the vectors $X_1$ and $X_2$ point in opposite directions almost surely.

To establish claim (ii), we note that in order for the coupling to be optimal, under the condition of convexity of $K$, we must have $\|X_2\|$ decreasing monotonically as $\|X_1\|$ increases. It therefore follows that the optimal coupling must of the form stated in the theorem. □

**Theorem 2.10.** Let $\eta \in \mathscr{P}(\mathbb{R}^d)$ be isotropic and let $K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ be a stationary isotropic kernel, such that $K(\mathbf{x}, \mathbf{y}) = \Phi(||\mathbf{x} - \mathbf{y}||^2)$, where $\Phi$ is a decreasing, convex function. If $\mathrm{Law}(X_1, \ldots, X_{2m})$, with $m \leq d$, is a solution to the constrained optimal coupling problem

$$\operatorname*{arg\,min}_{\mu \in \Lambda_{2m}^{\mathrm{anti}}(\eta)} \mathbb{E}_{X_{1:2m}\sim\mu} \left[ \sum_{i,j=1}^{2m} \Phi \left( ||X_i - X_j||^2 \right) \right] ,$$

then it satisfies $\langle X_i, X_j \rangle = 0$ a.s. for all $1 \leq i < j \leq m$.

*Proof.* Because $X_i = -X_{i+m}$ a.s., the objective function can be rewritten as follows:

$$\begin{aligned}
&\sum_{i,j=1}^{2m} \Phi \left( ||X_i - X_j||^2 \right) = \sum_{i=1}^{2m} \Phi \left( ||X_i - X_i||^2 \right) + 2 \sum_{i=1}^{2m-1} \sum_{j=i+1}^{2m} \Phi \left( ||X_i - X_j||^2 \right) \\
&= 2m\Phi(0) + 2 \sum_{i=1}^{m-1} \sum_{j=i+1}^{m} \Phi \left( ||X_i - X_j||^2 \right) + 2 \sum_{i=m+1}^{2m-1} \sum_{j=i+1}^{2m} \Phi \left( ||X_i - X_j||^2 \right) \\
&+ 2 \sum_{i=1}^{m} \sum_{j=m+1}^{2m} \Phi \left( ||X_i - X_j||^2 \right) \\
&= 2m\Phi(0) + 4 \sum_{i=1}^{m-1} \sum_{j=i+1}^{m} \Phi \left( ||X_i - X_j||^2 \right) + 2 \sum_{i,j=1}^{m} \Phi \left( ||X_i + X_j||^2 \right) \\
&= 2m\Phi(0) + 2 \sum_{i=1}^{m} \Phi \left( ||2X_i||^2 \right) + 4 \sum_{1 \leq i < j \leq m} \Phi \left( ||X_i - X_j||^2 \right) + \Phi \left( ||X_i + X_j||^2 \right) .
\end{aligned}$$

Hence it becomes equivalent to minimise with $||X_i||$ fixed

$$E\left[\sum_{1\leq i<j\leq m}\Phi\left(||X_i-X_j||^2\right)+\Phi\left(||X_i+X_j||^2\right)\right]$$
$$=E\left[\sum_{1\leq i<j\leq m}\Phi\left(||X_i||^2+||X_j||^2-2\langle X_i,X_j\rangle\right)+\Phi\left(||X_i||^2+||X_j||^2+2\langle X_i,X_j\rangle\right)\right]. \quad (8)$$

Using convexity note that

$$2\Phi\left(||\mathbf{x}||^2+||\mathbf{y}||^2\right)=2\Phi\left(\frac{||\mathbf{x}||^2+||\mathbf{y}||^2-2\langle\mathbf{x},\mathbf{y}\rangle+||\mathbf{x}||^2+||\mathbf{y}||^2+2\langle\mathbf{x},\mathbf{y}\rangle}{2}\right)$$
$$\leq\Phi\left(||\mathbf{x}||^2+||\mathbf{y}||^2-2\langle\mathbf{x},\mathbf{y}\rangle\right)+\Phi\left(||\mathbf{x}||^2+||\mathbf{y}||^2+2\langle\mathbf{x},\mathbf{y}\rangle\right)$$

and equality is attained whenever $\langle\mathbf{x},\mathbf{y}\rangle=0$. Therefore, the expectation in equation (8) is minimized when $\langle X_i,X_j\rangle=0$ a.s. for $1\leq i<j\leq m$. This is a set of valid constraints as long as $d\geq m$. Also, if $X_1\sim\eta$ and the $X_j$'s are generated under $\eta$ conditioned on being orthogonal to $X_1,\ldots,X_{j-1}$ then $X_j$ also has marginal $\eta$ because drawing a uniform distribution conditional on being orthogonal to a uniform axis results in a uniform direction. Hence any optimal coupling must satisfy this condition. □

## 10 Proofs of results in Section 3

For the reader's convenience we restate our main result that we prove here.

**Theorem 3.1.** [Local discrepancy & regular distributions] Denote by $S_{\text{iid}}$ a set of independent samples, each taken from a regular distribution $\lambda$ and by $S_{\text{ort}}$ the set of orthogonal samples for that distribution. Let $s=|S_{\text{iid}}|=|S_{\text{ort}}|$. Then for any fixed $u\in[0,1]$ and $a\in\mathbb{R}_+$ the following holds: $\mathbb{P}[|\text{disr}_{F_\lambda(S_{\text{iid}})}(u)|>a]\leq 2e^{-\frac{sa^2}{8}}\stackrel{\text{def}}{=}p_{\text{iid}}(a)$ and for some $p_{\text{ort}}$ satisfying $p_{\text{ort}}<p_{\text{iid}}$ it holds pointwise: $\mathbb{P}[|\text{disr}_{F_\lambda(S_{\text{ort}})}(u)|>a]\leq p_{\text{ort}}(a)$ . Also: $Var(\text{disr}_{F_\lambda(S_{\text{ort}})}(u))<Var(\text{disr}_{F_\lambda(S_{\text{iid}})}(u))$.

*Proof.* Consider a set of samples $S=\{X_1,...,X_{|S|}\}$ with elements of marginal distributions $\text{Unif}[0,1]^d$. Denote $s=|S|$. Note that for any given $\mathbf{u}=(u_1,\ldots,u_d)\in[0,1]^d$ we have:

$$\mathbb{E}[\text{disr}_S(\mathbf{u})]=\prod_{j=1}^d u_j-\frac{\mathbb{E}[|\{i:X_i\in J_{\mathbf{u}}\}|]}{s}=\prod_{j=1}^d u_j-\frac{\sum_{i=1,\ldots,s}\mathbb{P}[X_i\in J_{\mathbf{u}}]}{s}$$
$$=\prod_{j=1}^d u_j-\frac{s\cdot\text{Vol}(J_{\mathbf{u}})}{s}=0$$

Thus we conclude that the expected value of $\text{disr}_S(\mathbf{u})$ is 0. Let $\eta\in\mathscr{P}(\mathbb{R}^d)$ be some isotropic distribution and denote by $\lambda$ the distribution corresponding to the random variable $X=\mathbf{z}^\top\mathbf{g}$, where $\mathbf{z}\in\mathbb{R}^d$ is some fixed deterministic vector and $\mathbf{g}$ is sampled from $\eta$.

Now consider a set of samples $S_{\text{iid}}$ of the form: $S_{\text{iid}}=\{\mathbf{z}^\top\mathbf{g}_1^{\text{iid}},...,\mathbf{z}^\top\mathbf{g}_s^{\text{iid}}\}$, where random vectors $\mathbf{g}_1^{\text{iid}},...,\mathbf{g}_s^{\text{iid}}$ are chosen independently from $\eta$. Similarly, consider a set of samples $S_{\text{ort}}$ of the form: $S_{\text{ort}}=\{\mathbf{z}^\top\mathbf{g}_1^{\text{ort}},...,\mathbf{z}^\top\mathbf{g}_s^{\text{ort}}\}$, where the marginal distributions of the random vectors $\mathbf{g}_1^{\text{ort}},...,\mathbf{g}_s^{\text{ort}}$ is $\eta$, but this time different $\mathbf{g}_i^{\text{ort}}$ are conditioned to be orthogonal.

For any given $u\in[0,1]$ we have the following:

$$\text{disr}_{\psi(S_{\text{iid}})}(u)=u-\frac{\sum_{i\in S}I[\psi(\mathbf{z}^\top\mathbf{g}_i^{\text{iid}})<u]}{s},$$

where $\psi\stackrel{\text{def}}{=}F_\lambda$ and $I$ is an indicator random variable.

Note that equivalently, we can rewrite $\mathrm{disr}_{\psi(S_{\mathrm{iid}})}(u)$ as:

$$\mathrm{disr}_{\psi(S_{\mathrm{iid}})}(u) = u - \frac{-\sum_{i\in S} I[\psi(\mathbf{z}^\top \mathbf{g}_i^{\mathrm{iid}}) \geq u] + s}{s} = u - 1 + \frac{-\sum_{i\in S} I[\psi(\mathbf{z}^\top \mathbf{g}_i^{\mathrm{iid}}) \geq u]}{s}.$$

From our previous analysis and standard properties of the cdf we conclude that $\frac{\sum_{i\in S} I[\psi(\mathbf{z}^\top \mathbf{g}_i^{\mathrm{iid}})\geq u]}{s}$ is an unbiased estimator of $u-1$.

Similarly, we obtain:

$$\mathrm{disr}_{\psi(S_{\mathrm{ort}})}(u) = u - 1 + \frac{-\sum_{i\in S} I[\psi(\mathbf{z}^\top \mathbf{g}_i^{\mathrm{ort}}) \geq u]}{s}.$$

Again, as before we note that $\frac{\sum_{i\in S} I[\psi(\mathbf{z}^\top \mathbf{g}_i^{\mathrm{ort}})\geq u]}{s}$ is an unbiased estimator of $u-1$ (since the marginal distributions of the $g_i^{\mathrm{ort}}$ are the same as those of the $g_i^{\mathrm{iid}}$). Denote $Y_i^{\mathrm{iid}} = I[\psi(\mathbf{z}^\top \mathbf{g}_i^{\mathrm{iid}}) \geq u]$ and $Y_i^{\mathrm{ort}} = I[\psi(\mathbf{z}^\top \mathbf{g}_i^{\mathrm{ort}}) \geq u]$. Note that $Y_i^{\mathrm{iid}}, Y_i^{\mathrm{ort}} \in \{0,1\}$ for $i = 1,\ldots,s$. Notice also that even though the random variables $(Y_i^{\mathrm{iid}})_{i=1}^s$ are independent, this is not true of $(Y_i^{\mathrm{ort}})_{i=1}^s$.

We will use the following Cramer's Theorem:

**Theorem 10.1.** Let $Y_1, ..., Y_s$ be random variables. Denote: $W_s = \frac{Y_1+...+Y_s}{s}$. Then $\mathbb{P}[W_s \geq a] \leq \min_{\theta>0} \frac{\mathbb{E}[e^{s\theta W_s}]}{e^{s\theta a}}$.

Denote: $Z_i^{\mathrm{iid}} = 1 - Y_i^{\mathrm{iid}}$ and similarly: $Z_i^{\mathrm{ort}} = 1 - Y_i^{\mathrm{ort}}$. Denote: $W_s^{\mathrm{iid}} = \frac{Y_1^{\mathrm{iid}}+...+Y_s^{\mathrm{iid}}}{s}$, $W_s^{\mathrm{iid},-} = \frac{Z_1^{\mathrm{iid}}+...+Z_s^{\mathrm{iid}}}{s}$ and similarly: $W_s^{\mathrm{ort}} = \frac{Y_1^{\mathrm{ort}}+...+Y_s^{\mathrm{ort}}}{s}$, $W_s^{\mathrm{ort},-} = \frac{Z_1^{\mathrm{ort}}+...+Z_s^{\mathrm{ort}}}{s}$. Note that for any $0 < c < 1$:

$$\mathbb{P}[|W_s^{\mathrm{iid}} - \mathbb{E}[W_s^{\mathrm{iid}}]| > c] = \mathbb{P}[W_s^{\mathrm{iid}} > \mathbb{E}[W_s^{\mathrm{iid}}] + c] + \mathbb{P}[W_s^{\mathrm{iid}} < \mathbb{E}[W_s^{\mathrm{iid}}] - c].$$

Denote: $\mu = \mathbb{E}[W_s^{\mathrm{iid}}]$. We get:

$$\mathbb{P}[|W_s^{\mathrm{iid}} - \mathbb{E}[W_s^{\mathrm{iid}}]| > c] = \mathbb{P}[W_s^{\mathrm{iid}} > \mu + c] + \mathbb{P}[W_s^{\mathrm{iid},-} > \mu_- + c],$$

where $\mu_- = 1 - \mu = \mathbb{E}[W_s^{\mathrm{iid},-}]$.

Therefore, using Cramer's Theorem, we get:

$$\mathbb{P}[|W_s^{\mathrm{iid}} - \mathbb{E}[W_s^{\mathrm{iid}}]| > c] \leq \min_{\theta>0} \frac{\mathbb{E}[e^{s\theta W_s^{\mathrm{iid}}}]}{e^{s\theta a_1}} + \min_{\theta>0} \frac{\mathbb{E}[e^{s\theta W_s^{\mathrm{iid},-}}]}{e^{s\theta a_2}},$$

where: $a_1 = \mu + c$ and $a_2 = \mu_- + c$. Thus, from independence and the fact that all $Y_j^{\mathrm{iid}}$ have the same distribution, we have:

$$\mathbb{P}[|W_s^{\mathrm{iid}} - \mathbb{E}[W_s^{\mathrm{iid}}]| > c] \leq \min_{\theta>0} \frac{(\mathbb{E}[e^{\theta Y_1^{\mathrm{iid}}}])^s}{e^{s\theta a_1}} + \min_{\theta>0} \frac{(\mathbb{E}[e^{\theta Z_1^{\mathrm{iid}}}])^s}{e^{s\theta a_2}}. \tag{9}$$

Notice that: $|\mathrm{disr}_{\psi(S_{\mathrm{iid}})}(u)| = |W_s^{\mathrm{iid}} - \mathbb{E}[W_s^{\mathrm{iid}}]|$. Straightforward calculation of the RHS of Equation (9) leads to the upper bound on $|\mathrm{disr}_{\psi(S_{\mathrm{iid}})}(u)|$ from Theorem 3.1.

Now notice, that by the same analysis as before, we get:

$$\mathbb{P}[|W_s^{\mathrm{ort}} - \mathbb{E}[W_s^{\mathrm{ort}}]| > c] \leq \min_{\theta>0} \frac{\mathbb{E}[e^{s\theta W_s^{\mathrm{ort}}}]}{e^{s\theta a_1}} + \min_{\theta>0} \frac{\mathbb{E}[e^{s\theta W_s^{\mathrm{ort},-}}]}{e^{s\theta a_2}}.$$

Thus to complete the proof of Theorem 3.1, it suffices to show that: $\mathbb{E}[e^{s\theta W_s^{\mathrm{ort}}}] < \mathbb{E}[e^{s\theta W_s^{\mathrm{iid}}}]$ and: $\mathbb{E}[e^{s\theta W_s^{\mathrm{ort},-}}] < \mathbb{E}[e^{s\theta W_s^{\mathrm{iid},-}}]$ for any $\theta > 0$. We will show the first inequality. The proof of the second inequality is completely analogous.

**Lemma 10.2.** The following holds for any fixed $\theta > 0$:

$$\mathbb{E}[e^{s\theta W_s^{\mathrm{ort}}}] < \mathbb{E}[e^{s\theta W_s^{\mathrm{iid}}}].$$

*Proof.* Notice first that:

$$\mathbb{E}[e^{s\theta W_s^{\mathrm{ort}}}] = \mathbb{E}[e^{\theta \sum_{i=1}^{s} Y_i^{\mathrm{ort}}}] = \sum_{j=0}^{\infty} \frac{\theta^j}{j!} \sum_{j_1+...+j_k=j} \sum_{i_1<...<i_k} \mathbb{E}[(Y_{i_1}^{\mathrm{ort}})^{j_1}...(Y_{i_k}^{\mathrm{ort}})^{j_k}]$$

$$= \sum_{j=0}^{\infty} \frac{\theta^j}{j!} \sum_{j_1+...+j_k=j} \sum_{i_1<...<i_k} \mathbb{E}[Y_{i_1}^{\mathrm{ort}}...Y_{i_k}^{\mathrm{ort}}],$$

where the sum over $j_1, ...j_k$ is the sum over all partitioning of $j$ into positive integers $j_1, ..., j_k$, the sum over $i_1 < ... < i_k$ is the sum over all increasing nonempty sequences $(i_1, ..., i_k)$ such that $i_1, ...i_k \in \{1, ..., s\}$ (thus $k \in \{1, ..., s\}$) and furthermore the last equality is true since each $Y_i^{\mathrm{ort}}$ is an indicator random variable (note that the infinite sum above is well-defined since random variables under consideration are indicators). Similarly,

$$\mathbb{E}[e^{s\theta W_s^{\mathrm{iid}}}] = \mathbb{E}[e^{\theta \sum_{j=1}^{s} Y_j^{\mathrm{iid}}}] = \sum_{j=0}^{\infty} \frac{\theta^j}{j!} \sum_{j_1+...+j_k=j} \sum_{i_1,...,i_k} \mathbb{E}[Y_{i_1}^{\mathrm{iid}}...Y_{i_k}^{\mathrm{iid}}],$$

Thus, since $\theta > 0$, it suffices to show that:

$$\mathbb{E}[Y_{i_1}^{\mathrm{ort}}...Y_{i_k}^{\mathrm{ort}}] < \mathbb{E}[Y_{i_1}^{\mathrm{iid}}...Y_{i_k}^{\mathrm{iid}}]$$

or equivalently:

$$\mathbb{P}[\mathcal{A}_{i_1}^{\mathrm{ort}} \wedge ... \wedge \mathcal{A}_{i_k}^{\mathrm{ort}}] < \mathbb{P}[\mathcal{A}_{i_1}^{\mathrm{iid}} \wedge ... \wedge \mathcal{A}_{i_k}^{\mathrm{iid}}],$$

where $\mathcal{A}_i^{\mathrm{iid}}$ and $\mathcal{A}_i^{\mathrm{ort}}$ stand for events corresponding to indicators $Y_i^{\mathrm{iid}}$ and $Y_i^{\mathrm{ort}}$ respectively. For clarity, we present the proof for the inequality above for $k = 2$, for $k > 2$ the analysis is analogous. Notice also that the inequality for $k = 2$ immediately leads to the inequality regarding the variance from the statement of the theorem.

Note that it suffices to show that for any $t$ and any $\mathbf{z} \in \mathbb{R}^d$ the following is true:

$$\mathbb{P}[\mathbf{z}^\top \mathbf{g}_i^{\mathrm{ort}} \geq t \wedge \mathbf{z}^\top \mathbf{g}_j^{\mathrm{ort}} \geq t] < \mathbb{P}[\mathbf{z}^\top \mathbf{g}_i^{\mathrm{iid}} \geq t \wedge \mathbf{z}^\top \mathbf{g}_j^{\mathrm{iid}} \geq t]$$

for $i \neq j$.

Since $t$ is arbitrary, we can assume without loss of generality that $\|\mathbf{z}\| = 1$. Note that then the following holds:

$$\mathbb{P}[\mathbf{z}^\top \mathbf{g}_i^{\mathrm{ort}} \geq t \wedge \mathbf{z}^\top \mathbf{g}_j^{\mathrm{ort}} \geq t] = \mathbb{P}\left[\frac{g_1}{\sqrt{g_1^2 + ... + g_d^2}} l_1 \geq t \wedge \frac{g_2}{\sqrt{g_1^2 + ... + g_d^2}} l_2 \geq t\right],$$

where $\mathbf{g} = (g_1, ..., g_n)^\top$ is a multivariate Gaussian vector taken from a distribution $\mathcal{N}(0, I_d)$ and $l_1, l_2$ are taken independently from the distribution of the length of $\mathbf{g}_i^{\mathrm{ort}}$ (or $\mathbf{g}_i^{\mathrm{iid}}$ since the marginal distributions of samples are the same). The last equality immediately follows from the fact that $\mathbf{g}_i^{\mathrm{ort}}$ are taken from the isotropic distribution.

We also have:

$$\mathbb{P}[\mathbf{z}^\top \mathbf{g}_i^{\mathrm{iid}} \geq t \wedge \mathbf{z}^\top \mathbf{g}_j^{\mathrm{iid}} \geq t] = \mathbb{P}[\mathbf{z}^\top \mathbf{g}_i^{\mathrm{iid}} \geq t]\mathbb{P}[\mathbf{z}^\top \mathbf{g}_j^{\mathrm{iid}} \geq t]$$

$$= \mathbb{P}\left[\frac{g_1}{\sqrt{g_1^2 + ... + g_d^2}} l_1 \geq t\right] \cdot \mathbb{P}\left[\frac{g_2}{\sqrt{g_1^2 + ... + g_d^2}} l_2 \geq t\right],$$

where we use the independence assumption. Thus it suffices to show that:

$$\mathbb{P}\left[g_1 \geq \frac{t}{l_1}\sqrt{g_1^2 + ... + g_d^2} \wedge g_2 \geq \frac{t}{l_2}\sqrt{g_1^2 + ... + g_d^2}\right]$$

$$< \mathbb{P}\left[g_1 \geq \frac{t}{l_1}\sqrt{g_1^2 + ... + g_d^2}\right] \cdot \mathbb{P}\left[g_2 \geq \frac{t}{l_2}\sqrt{g_1^2 + ... + g_d^2}\right].$$

Therefore we want to prove that:

$$\mathbb{P}\left[g_2 \geq \frac{t}{l_2}\sqrt{g_1^2+...+g_d^2}\middle| g_1 \geq \frac{t}{l_1}\sqrt{g_1^2+...+g_d^2}\right] < \mathbb{P}\left[g_2 \geq \frac{t}{l_2}\sqrt{g_1^2+...+g_d^2}\right].$$

Note that: $\frac{t}{l_1}$, $\frac{t}{l_2}$, $g_1$, $g_2$ and $g_3^2+...+g_d^2$ are independent random variables. Thus it suffices to show that for any $c>0$ and any $a,b$ the following is true:

$$\mathbb{P}\left[g_2 \geq b\sqrt{g_1^2+g_2^2+c}\middle| g_1 \geq a\sqrt{g_1^2+g_2^2+c}\right] < \mathbb{P}\left[g_2 > b\sqrt{g_1^2+g_2^2+c}\right].$$

Denote $g_i^+ = g_i|g_i>0$ and $g_i^- = g_i|g_i<0$. We will prove the inequality above by conditioning on four possible events" $\mathcal{E}_1 = \{g_1,g_2>0\}$, $\mathcal{E}_2 = \{g_1,g_2<0\}$, $\mathcal{E}_3 = \{g_1>0, g_2<0\}$, $\mathcal{E}_4 = \{g_1<0, g_2>0\}$. Consider all four cases, one can easily see that in order to prove the inequality it suffices to prove the following: for any $x,y$:

$$\mathbb{P}[(g_2^+)^2 > x|(g_2^+)^2 \leq y] < \mathbb{P}[(g_2^+)^2 > x],$$

and similarly:

$$\mathbb{P}[(g_2^+)^2 < x|(g_2^+)^2 \geq y] < \mathbb{P}[(g_2^+)^2 < x].$$

We will prove the first inequality. The proof for the second one is completely analogous.

Denote: $A_1 = \mathbb{P}[(g_2^+)^2 < x]$, $A_2 = \mathbb{P}[x < (g_2^+)^2 < y]$ and $A_3 = \mathbb{P}[(g_2^+)^2 > y]$. We want to prove that: $\frac{A_2}{A_1+A_2} < A_2 + A_3$, which is trivially true since $0 < A_1, A_2, A_3 < 1$ and $A_1+A_2+A_3 = 1$. That completes the proof of Lemma 10.2. □

As we have noticed, the proof of Lemma 10.2 completes the proof of Theorem 3.1. □

### 10.1 From low discrepancy to low approximation error

As mentioned in the main body of the paper, sharper concentration results regarding local discrepancies translate to sharper concentration results for the star discrepancy function $D_\eta^*$ and ultimately also to sharper results regarding approximation error of MC estimators. We show it in this section.

Define the error coming from the approximation $\hat{I}_f$ of $I_f$ that uses the set of samples $S$ as: $\epsilon_S(f) = |I_f - \hat{I}_f|$.

The following theorem establishes the connection between the discrepancy of a sequence $S$ used for estimation and the above approximation error $\epsilon_S(f)$.

**Theorem 10.3** (Koksma-Hlawka inequality)**.** For any function f with bounded variation and a sequence $S$, the approximation error $\epsilon_S(f)$ satisfies:

$$\epsilon_S(f) \leq D_\lambda^*(S) V_{\mathrm{HK}}(f) = \sup_{\mathbf{u}\in[0,1]^d} |\mathrm{disr}_{\psi(S)}(\mathbf{u})| V_{\mathrm{HK}}(f),$$

where $V_{\mathrm{HK}}$ stands for the Hardy-Krause variation of $f$ (Niederreiter, 1992) defined as follows:

$$V_{\mathrm{HK}}(f) = \sum_{I\subset[d], I\neq\emptyset} \int_{[0,1]^d} \left|\frac{\partial f}{\partial \mathbf{u}_I}|_{u_j=1, j\notin I}\right| d\mathbf{u}_I.$$

and $\psi = F_\lambda$.

Thus we can conclude that sequences $S$ of lower discrepancies lead to tighter upper bounds on the approximation error of $I_f$.

The following is our main result of this section:

**Theorem 10.4.** For any $N\in\mathbb{N}, a > \frac{1}{N}$, set of samples $S$, $\lambda \in \mathscr{P}([0,1])$ and a function $f$ of bounded variation the following holds for $\epsilon_S(f) = |\hat{I}_f - I_f|$, where $I_f = \mathbb{E}_{X\sim\eta}[f(X)]$:

$$\mathbb{P}[\epsilon_S(f) > a] \leq Np\left(a - \frac{1}{N}\right) V_{\mathrm{HK}}(f),$$

if $p$ is such that: $\mathbb{P}[|\mathrm{disr}_{\psi(S))}(x)| > a] \leq p(a)$ for any fixed $x \in [0,1]$. In particular, if $\lambda$ is a regular distribution and if we take: $a = \frac{\log(|S|)}{|S|}$ and $N = \frac{2\sqrt{|S|}}{\log(|S|)}$, then we obtain: $\mathbb{P}[\epsilon_{S_{\mathrm{iid}}}(f) > a] \leq \frac{4\sqrt{|S|}}{\log(|S|)} e^{-\frac{\log^2(|S|)}{32}} = \mathrm{neg}(|S|)$, and for $S_{\mathrm{iid}}$ replaced by $S_{\mathrm{ort}}$ the bounds are even tighter. In the above statement $\mathrm{neg}(|S|)$ is defined as $\mathrm{neg}(|S|) = \frac{1}{\mathrm{superpoly}(|S|)}$ and superpoly stands for some superpolynomial function.

*Proof.* Let $s = |S|$. Consider $D^*_\lambda(S) = \sup_{x\in[0,1]} |\mathrm{disr}_{\psi(S)}(x)|$ for some one-dimensional distribution $\lambda$. We partition interval $[0,1]$ into $N$ subintervals: $[x_j, x_{j+1}]$ of length $\frac{1}{N}$ each for $j = 0, ..., N-1$. Note that for a fixed $a > 0$:

$$\left\{ \sup_{x\in[0,1]} |\mathrm{disr}_{\psi(S)}(x)| > a \right\} = \left\{ \exists x^* \in [0,1] : |\mathrm{disr}_{\psi(S)}(x^*)| > a \right\}.$$

Denote: $X^x_j = I[s_j < x]$, where $s_j$ is the $j^{th}$ sample from $\psi(S)$. Assume that $x^*$ is in the subinterval with endpoints: $x_{j^*}$ and $x_{j^*+1}$. Note that we have:

$$\frac{X_1^{x_{j^*}} + ... + X_s^{x_{j^*}}}{s} \leq \frac{X_1^{x^*} + ... + X_s^{x^*}}{s} \leq \frac{X_1^{x_{j^*+1}} + ... + X_s^{x_{j^*+1}}}{s}$$

Thus we get:

$$\mathrm{disr}_{\psi(S)}(x^*) = \left| \frac{X_1^{x^*} + ... + X_s^{x^*}}{s} - x^* \right| \leq \max(A, B),$$

where $A = \left| \frac{X_1^{x_{j^*}} + ... + X_s^{x_{j^*}}}{s} - x^* \right|$ and $B = \left| \frac{X_1^{x_{j^*+1}} + ... + X_s^{x_{j^*+1}}}{s} - x^* \right|$.

Therefore, using triangle inequality, we obtain:

$$\{|\mathrm{disr}_{\psi(S)}(x^*)| > a\} \subseteq \{|\mathrm{disr}_{\psi(S)}(x_{j^*})| + |x^* - x_{j^*}| > a\} \cup \{|\mathrm{disr}_{\psi(S)}(x_{j^*+1})| + |x^* - x_{j^*+1}| > a\}.$$

Therefore we obtain:

$$\left\{ \sup_{x\in[0,1]} |\mathrm{disr}_{\psi(S)}(x)| > a \right\} \subseteq \left\{ \exists_j : |\mathrm{disr}_{\psi(S)}(x_j)| > a - \frac{1}{N} \right\}.$$

Thus, by the union bound, we conclude that:

$$\mathbb{P}\left[ \left\{ \sup_{x\in[0,1]} |\mathrm{disr}_{\psi(S)}(x)| > a \right\} \right] \leq \sum_{j=1}^{N} \mathbb{P}\left[ \left\{ |\mathrm{disr}_{\psi(S)}(x^j)| > a - \frac{1}{N} \right\} \right].$$

The statement of Theorem 10.4 follows now from Koksma-Hlawka inequality, and Theorem 3.1.

□

# 11 Proofs of results in Section 4

## 11.1 Exponential concentration

In this section we present the proofs of the results in 4. For completeness we start by reviewing the classical defnitions of sub-Gaussianity for random variables and random vectors.

**Definition 11.1** (Sub-Gaussian Random Variables)**.** A random variable $X$ with mean $\mu = \mathbb{E}[X]$ is sub-Gaussian if there is a positive number $\sigma$ such that:

$$\mathbb{E}[e^{\lambda(X-\mu)}] \leq e^{\sigma^2\lambda^2/2} \text{ for all } \lambda \in \mathbb{R}.$$

A standard Gaussian random variable is sub-Gaussian with parameter $\sigma$ equal to the said variable's standard deviation.

**Lemma 11.2** (Concentration for sub-Gaussian random variables)**.** Let $X$ be a sub-Gaussian random variable with parameter $\sigma$ and mean $\mu$. It satisfies the following concentration inequality:

$$\mathbb{P}[X - \mu \geq t] \leq e^{-\frac{t^2}{2\sigma^2}}.$$

Paying a factor of 2 we can get an equivalent two sided bound for $|X - \mu| \geq t$.

The following alternative characterization of sub-Gaussianity will prove useful:

**Lemma 11.3** (Alternative characterization of sub-Gaussianity )**.** A *centered* random variable $X$ is sub-Gaussian if there is a constant $c$ and a Gaussian random variable $Z \sim N(0, \tau^2)$ such that:

$$\mathbb{P}\left[|X| \geq s\right] \leq c\mathbb{P}\left[|Z| \geq s\right], \text{ for all } s \geq 0.$$

Additionally, we can switch from the definition in 11.1 to the characterization in Lemma 11.3 in the following way:

- If $X$ is zero mean sub-Gaussian with parameter $\sigma$, then taking $\tau^2 = 2\sigma^2$ and $c = \sqrt{8}e$ is enough for Lemma 11.3 to hold for $X$.
- If $X$ is zero mean sub-Gaussian with sub-Gaussian parameters $\tau^2$ and $c$ in Lemma 11.3, then $\sigma^2 = 2c^2\tau^2$ is a valid sub-Gaussian parameter for for $X$, as in Definition 11.1.

The concept of sub-Gaussianity extends to vector valued random variables:

**Definition 11.4** (Sub-Gaussian Vector)**.** A random vector $X$ is sub-Gaussian with parameter at most $\sigma$ if for every $v \in \mathbb{S}^{d-1}$ (where $\mathbb{S}^{d-1}$ is the unit $d-$dimensional sphere.)

$$\mathbb{E}\left[e^{\lambda\langle v, X\rangle}\right] \leq e^{\frac{\lambda^2\sigma^2}{2}} \text{ for all } \lambda \in \mathbb{R}.$$

We will be using these facts heavily in the following sections.

The following facts will prove useful. For a detailed survey of these results consult (Boucheron et al., 2013).

Fact 1 If $X$ is sub-Gaussian with parameter $\sigma$, $X + c$ is sub-Gaussian with parameter $\sigma$ for all $c \in \mathbb{R}$.

Fact 2 If $X_1$ and $X_2$ are independent with parameters $\sigma_1, \sigma_2$ respectively, then $X_1 + X_2$ is sub-Gaussian with parameter $\sqrt{\sigma_1^2 + \sigma_2^2}$.

Fact 3 Even without assuming independence, if $X_1$ and $X_2$ are sub-Gaussian with parameters $\sigma_1, \sigma_2$ respectively, then $X_1 + X_2$ is sub-Gaussian with parameter $\sqrt{2}\sqrt{\sigma_1^2 + \sigma_2^2}$.

Fact 4 If $X$ is sub-Gaussian with parameter $\sigma^2$, $cX$ is sub-Gaussian with parameter $c^2\sigma^2$.

We need the following result showing that the product of a sub-Gaussian random variable and a bounded random variable is again sub-Gaussian.

**Theorem 11.5** (Sub-Gaussian products)**.** Let $Y$ be a bounded random variable such that $Y \in [-R_1, R_2]$ for $R_1, R_2 \geq 0$ with $R_1 + R_2 = R$ for some constant $R$, and let $X$ be sub-Gaussian with parameter $\sigma$ and mean $\mu$. Then $XY$ is sub-Gaussian with parameter $\sqrt{2}\sqrt{2g(\sigma)^2R^2 + \mu^2R^2/2 + \sigma^2R_1^2}$ where $g(\sigma) = 24e\sigma$.

Theorem 11.5 allows us to prove fast concentration rates for the vanilla ES estimator. We believe this result is of independent interest, as it tackles a fundamental question regarding concentration of products of sub-Gaussian variables.

*Proof.* The proof has two steps, we first show it holds for non-negative and discrete $Y$. Then we generalize.

1 Case 1: $Y$ only attains discrete values $Y \in \{0, 1\}$ and $X$ is zero mean.

We will make use of lemma 11.3 to prove this result. Since $X$ is mean zero and sub-Gaussian there is $\tau^2$ and constant $c$ such that:

$$P(|X| \geq s) \leq cP(|Z| \geq s),$$

where $Z \sim N(0, \tau^2)$. In fact we can take $\tau^2 = 2\sigma^2$, and $c = \sqrt{8}e$.

Let $X'$ be an independent copy of $X$. By Fact 2, $X - X'$ is sub-Gaussian with parameter $\sqrt{2}\sigma$. Since $X - X'$ has mean zero by Lemma 11.3 we conclude there are constants $\tau_1$ such that $\tau_1^2 = 4\sigma^2$ and $c_1 = \sqrt{8}e$ such that $P(|X - X'| \geq s) \leq c_1 P(|Z'| \geq s)$, where $Z' \sim N(0, \tau_1^2)$.

Let $\mu_{XY}$ denote the mean of $XY$. Let $X'$ and $Y'$ be independent copies of $X$ and $Y'$ respectively. We proceed to invoke a symmetrization argument. We first show that in order to bound the MGF of $XY$ it is enough to bound the MGF of $XY - X'Y'$. For any $\lambda \in \mathbb{R}$:

$$\begin{aligned}\mathbb{E}\left[e^{\lambda(XY - \mu_{XY})}\right] &= \mathbb{E}\left[e^{\lambda(XY - \mathbb{E}[X'Y'])}\right] \\ &\leq \mathbb{E}\left[e^{\lambda(XY - X'Y')}\right].\end{aligned}$$

The inequality follows from Jensen's inequality. This means that sub-Gaussianity of $XY - X'Y'$ implies sub-Gaussianity of $XY - \mu_{XY}$.

We will show sub-Gaussianity of $XY - X'Y'$. Since $Y$ and $Y'$ only take values in $\{0, 1\}$ we can write:

$$|XY - X'Y'| = \begin{cases} |X - X'| & \text{if } Y = 1, Y' = 1, \\ |X| & \text{if } Y = 1, Y' = 0, \\ |X'| & \text{if } Y = 0, Y' = 1, \\ 0 & \text{o.w.} \end{cases}$$

Let $s > 0$. By the union bound:

$$\mathbb{P}(|XY - X'Y'| \geq s) \leq \mathbb{P}(|X - X'| \geq s) + \mathbb{P}(|X| \geq s) + \mathbb{P}(|X'| \geq s).$$

By sub-Gaussianity of $X$ and $X' - X$ and using their Gaussian tail bounds:

$$\mathbb{P}(|XY - X'Y'| \geq s) \leq c_1 \mathbb{P}(|Z'| \geq s) + 2c\mathbb{P}(|Z| \geq s),$$

where $Z \sim N(0, \tau^2)$ and $Z' \sim N(0, \tau_1^2)$.

Let $\tau_2 = \max(\tau, \tau_1)$ and $c_2 = 3\max(c, c_1, 1)$. Let $c_2 = 3\sqrt{8}e$ and $\tau_2^2 = 4\sigma^2$. We conclude that for all $s \geq 0$:

$$\mathbb{P}(|XY - X'Y'| \geq s) \leq c_2 \mathbb{P}(|Z''| \geq s),$$

where $Z'' \sim N(0, \tau_2^2)$. The inequality also holds for $s = 0$ since we have ensured $c_2 \geq 1$. By the series of observations right below Lemma 11.3, this implies that $XY$ is sub-Gaussian with parameter $\sqrt{2}c_3\tau_2 = \sqrt{2} * 3 * \sqrt{8} * e * 2 * \sigma = 24e\sigma \stackrel{\text{def}}{=} g(\sigma)$.

1 Case 2: $X$ centered, $Y \geq 0$ and supported on a finite set $a_1 < a_2 < \cdots < a_m$.

Denote by $\mu_{XY}$ the mean of $XY$. In order to show $XY$ is sub-Gaussian we have to bound its MGF $\mathbb{E}\left[e^{\lambda(XY - \mu_{XY})}\right]$. For $i \geq 1$ let $X_i = X1(Y \leq a_i)$. Define $a_0 = 0$ then $XY = \sum_{i=1}^n X_i(a_i - a_{i-1})$

and therefore $\mathbb{E}[XY] = \sum_{i=1}^{n}(a_i - a_{i-1})\mathbb{E}[X_i]$. Notice that $\sum_{i=1}^{n} a_i - a_{i-1} = a_n - a_0$. Let $p_i = \frac{a_n - a_0}{a_i - a_{i-1}}$. Let $\sigma$ be the sub-Gaussianity parameter of $X$.

$$\begin{aligned}
\mathbb{E}\left[e^{\lambda(XY-\mu_{XY})}\right] &= \mathbb{E}\left[e^{\sum_{i=1}^{n}\lambda(a_i-a_{i-1})(X_i-\mathbb{E}[X_i])}\right] \\
&\leq \prod_i \mathbb{E}\left[\left(e^{\lambda(a_i-a_{i-1})(X_i-\mathbb{E}[X_i])}\right)^{\frac{a_n-a_0}{a_i-a_{i-1}}}\right]^{\frac{a_i-a_{i-1}}{a_n-a_0}} \\
&= \prod_i \mathbb{E}\left[e^{\lambda(a_n-a_0)(X_i-\mathbb{E}[X_i])}\right]^{\frac{a_i-a_{i-1}}{a_n-a_0}} \\
&\leq \prod_i \left(e^{\frac{\lambda^2(a_n-a_0)^2 g(\sigma)^2}{2}}\right)^{\frac{a_i-a_{i-1}}{a_n-a_0}} \\
&= e^{\frac{\lambda^2 g(\sigma)^2(a_n-a_0)^2}{2}},
\end{aligned}$$

where $g(\sigma)$ is defined as in Case 1. The first inequality follows by Hölder's inequality with parameters $p_i$. The second inequality follows from the sub-Gaussianity bound from Case 1 since $X_i = X1(Y \leq a_i)$.

2 Case 2. $Y$ is non-negative but not necessarily discrete. $X$ has mean zero.

Assume $Y \in [0, R]$. If $Y \geq 0$ there is a sequence of simple random variables (all of which are discrete) $Y_n$ with $Y_n \to Y$ almost surely. Furthermore, all $Y_n \in [0, R]$, so that the maximal element in the domain of $Y_n$ is at most $R$.

For any $\lambda \in \mathbb{R}$ the previous observation implies $\lambda XY_n \to \lambda XY$ almost surely. Let $f_1(x, y) = |\lambda RX|$. Since $|X|$ is integrable, $\mathbb{E}[f_1(X)] < \infty$. Notice that pointwise $|\lambda XY_n| \leq f_1(X, Y)$. By the dominated convergence theorem (Halmos, 2013) we can conclude $\mathbb{E}[\lambda XY_n] \xrightarrow{n\to\infty} \mathbb{E}[\lambda XY]$. By continuity of the exponential function $h(x) = e^x$ this also implies $e^{\mathbb{E}[\lambda XY_n]} \xrightarrow{n\to\infty} e^{\mathbb{E}[\lambda XY]}$.

The random variables $e^{\lambda XY_n}$ converge to $e^{\lambda XY}$ almost surely. The function $f_2(x, y) = e^{f_1(x,y)}$ satisfies:

1. $|e^{\lambda XY_n}| = e^{\lambda XY_n} \leq f_2(X, Y)$ pointwise.
2. $\mathbb{E}[f_2(X, Y)] < \infty$. Indeed: $\mathbb{E}[f_2(X, Y)] \leq \mathbb{E}[e^{\lambda RX}] + \mathbb{E}\left[e^{-\lambda RX}\right] \leq 2e^{\lambda^2 R^2 \sigma^2/2} < \infty$. The first inequality holds by nonnegativity of the exponential function and because for any point $x$, one of $\lambda Rx$ or $-\lambda Rx$ equals $|\lambda Rx|$. The second inequality holds by sub-Gaussianity of $X$.

By the dominated convergence theorem again we conclude that $\mathbb{E}\left[e^{\lambda XY_n}\right] \to \mathbb{E}\left[e^{\lambda XY}\right]$. Since by Case 2, $\mathbb{E}\left[e^{\lambda XY_n}\right] \leq e^{\lambda^2 g(\sigma)^2 R^2/2}$ we conclude $\mathbb{E}\left[e^{\lambda XY_n}\right] \leq e^{\lambda^2 g(\sigma)^2 R^2/2}$.

Case 3 $X$ has mean $\mu$ and $Y \in [-R_1, R_2]$ can attain negative values.

Define $R := R_1 + R_2$ and let $-R_1$ be the smallest element in the support of $Y$. Let $Y_1 = Y + R_1$ and $X_1 = X - \mu$. Notice $Y_1 \in [0, R]$ and $X_1$ has mean zero and sub-Gaussianity parameter $\sigma$, like $X$. By Case 3 we conclude $X_1 Y_1$ is sub-Gaussian with parameter $g(\sigma)R$.

Since $Y$ is bounded, $Y$ is sub-Gaussian with parameter $R/2$, (see Boucheron et al., 2013). Therefore $\mu Y$ is sub-Gaussian with parameter $|\mu|R/2$.

Since $X$ is sub-Gaussian with parameter $\sigma$, $R_1 X$ is sub-Gaussian with parameter $\sigma R_1$.

Notice that $X_1 Y_1 = XY + R_1 X - \mu Y - R_1 \mu$. Therefore:

1. $X_1Y_1 + R_1\mu$ is sub-Gaussian with parameter $g(\sigma)R$ since it is the translate of a $g(\sigma)R$ sub-Gaussian random variable.
2. $X_1Y_1 + R_1\mu + \mu Y$ is sub-Gaussian with parameter $\sqrt{2}\sqrt{g(\sigma)^2R^2 + \mu^2R^2/4}$ by Fact 3.
3. $X_1Y_1 + R_1\mu + \mu Y - R_1X = XY$ is sub-Gaussian with parameter

$$\sqrt{2}\sqrt{2(g(\sigma)^2R^2 + \mu^2R^2/4) + \sigma^2R_1^2} = \sqrt{2}\sqrt{2g(\sigma)^2R^2 + \mu^2R^2/2 + \sigma^2R_1^2}.$$

This shows that $XY$ is sub-Gaussian with parameter $\sqrt{2}\sqrt{2g(\sigma)^2R^2 + \mu^2R^2/2 + \sigma^2R_1^2}$ which concludes the proof.

□

### 11.2 The vanilla ES estimator

In this section we focus on proving Theorem 4.1. Recall that given $F : \Theta \to \mathbb{R}$, the Vanilla ES estimator is defined as:

$$\hat{\nabla}_N^V F_\sigma(\theta) = \frac{1}{N\sigma}\sum_{i=1}^{N} F(\theta + \sigma\epsilon_i)\epsilon_i,$$

where $\epsilon_i \sim \mathcal{N}(0, I)$ are all i.i.d. and $\sigma$ is the variance of the length of the sensing direction.

In what follows we assume that $F$ is uniformly bounded over its domain by $\mathcal{F}$. If $F$ is a sum of discounted rewards, an upper bound of $\mathcal{R}$ for the reward function yields an upper bound of $\frac{1}{1-\gamma}\mathcal{R}$ for $F$, where $\gamma$ is the discount factor.

We show that whenever $F$ is bounded in absolute value the random vector $\hat{\nabla}_N^V F_\sigma(\theta)$ is sub-Gaussian.

**Theorem 11.6.** If $F$ is a bounded function such that $|F| \leq R_1$, the vanilla ES estimator is a sub-Gaussian vector with parameter $\frac{\sqrt{2}R_1\sqrt{8c^2+1}}{\sqrt{N}\sigma}$ for $c = 24e$.

*Proof.* Let $v \in \mathbb{S}^{d-1}$ be an arbitrary $d-$dimensional unit vector. We start by showing sub-Gaussianity of the vector $F(\theta + \sigma\epsilon)\epsilon$.

Notice that $\langle v, F(\theta + \sigma\epsilon)\epsilon\rangle = F(\theta + \sigma\epsilon)\langle\epsilon, v\rangle$. Since linear combinations of jointly Gaussian random variables are Gaussian, and $||v|| = 1$, the random variable $\langle\epsilon, v\rangle$ is a $\mathcal{N}(0, 1)$ Gaussian random variable and therefore $\langle\epsilon, v\rangle$ is 1-sub-Gaussian.

By Theorem 11.5, since $F$ is assumed to be in the range $[-R_1, R_1]$, it follows that $\langle v, F(\theta + \epsilon)\epsilon\rangle$ is $\sqrt{2}R_1\sqrt{8c^2 + 1}$ sub-Gaussian, where $c = g(1)$.

By noting that each $\epsilon_i$ is independent from all others, we can obtain that $\langle v, \hat{\nabla}_N^V F_\sigma(\theta)\rangle$ is $\frac{\sqrt{2}R_1\sqrt{8g(1)^2+1}}{\sqrt{N}\sigma}$ sub-Gaussian. Since $v$ was arbitrary this concludes the proof.

□

**Corollary 11.7** (Exponential Concentration for the Vanilla ES estimator)**.** If $F$ is a bounded function such that $|F| \leq R_1$:

$$\mathbb{P}\left(\max_{j=1,\cdots,d}\left|\left(\hat{\nabla}_N^V F_\sigma(\theta)\right)_j - \left(\mathbb{E}\left[\hat{\nabla}_N^V F_\sigma(\theta)\right]\right)_j\right| \geq t\right) \leq 2de^{\frac{-t^2N\sigma^2}{2R_1^2(8g(1)^2+1)}}$$

For any $t \geq 0$.

The combination of Theorem 11.6 and Corollary 11.7 conclude the proof of Theorem 4.1.

### 11.3 Orthogonal Bounds

In this section we prove Theorem 4.3. We prove concentration bounds for orthogonal gradient estimators of the form:

$$\hat{\nabla}_d^{Ort} F(\theta) = \frac{1}{d\sigma} \sum_{i=1}^{d} \nu_i b_i F\left(\theta + \sigma \nu_i b_i\right),$$

where the random vectors $\nu_i \in \mathbb{S}^{d-1}$ are in the unit sphere and are sampled uniformly from the unit sphere using a sequentially orthogonal process, the function $F$ is bounded $\sup_x |F(x)| \leq R < \infty$, and $b_i$ are zero mean signed lengths, sampled from sub-Gaussian distributions each with parameter $\beta_i$ and independent from each other and from all other sources of randomness.

**Theorem 11.8.** Let $B = \max_i \mathbb{E}\left[|b_i|\right]$, $\beta = \max_i \beta_i$, $|F| \leq R$, the orthogonal gradient estimator $\hat{\nabla}_d^{Ort} F(\theta)$ is sub-Gaussian with parameter $\sqrt{\frac{\beta^2 c^2 R^2}{\sigma^2 d^2} + \frac{R^2 B^2}{4\sigma^2 d}}$. Where $c = 2\sqrt{(24e)^2 + \frac{1}{2}}$, and $\ln(e) = 1$.

*Proof.* We start by lumping in $\frac{1}{\sigma}$ with $F$ so that $|F|/\sigma \leq R/\sigma$. We proceed with the proof, and at the end subsitute $R$ by $R/\sigma$.

In order to show the concentration of the random vector $\hat{\nabla}_d^{Ort} F(\theta)$, it is enough to show that for any fixed $u \in \mathbb{S}^{d-1}$, $\langle u, \hat{\nabla}_d^{Ort} F(\theta)\rangle$ is a sub-Gaussian random variable.

Given $u \in \mathbb{S}^{d-1}$, define $\alpha_i = \langle u, \nu_i \rangle$. Notice that $\sum_{i=1}^{d} \alpha_i^2 = 1$ and that:

$$\langle u, d\hat{\nabla}_d^{Ort} F(\theta)\rangle = \sum_{i=1}^{d} \alpha_i b_i F(\theta + \sigma^2 \nu_i b_i)$$

We wish to control:

$$\mathbb{E}\left[\exp\left(\lambda\left(\langle u, d\hat{\nabla}_d^{Ort} F(\theta)\rangle - \mathbb{E}\left[\langle u, d\hat{\nabla}_d^{Ort} F(\theta)\rangle\right]\right)\right)\right].$$

We start by decomposing the MGF above as follows:

$$\mathbb{E}\Bigg[\exp\Big(\lambda\Big(\langle u, d\hat{\nabla}_d^{Ort} F(\theta)\rangle - \mathbb{E}\left[\langle u, d\hat{\nabla}_d^{Ort} F(\theta)\rangle \Big| \nu_1, \cdots, \nu_d\right] + \\ \mathbb{E}\left[\langle u, d\hat{\nabla}_d^{Ort} F(\theta)\rangle \Big| \nu_1, \cdots, \nu_d\right] - \mathbb{E}\left[\langle u, d\hat{\nabla}_d^{Ort} F(\theta)\rangle\right]\Big)\Big)\Bigg].$$

And first bounding the conditional MGF:

$$\mathbb{E}\left[\exp\left(\lambda\left(\langle u, d\hat{\nabla}_d^{Ort} F(\theta)\rangle - \mathbb{E}\left[\langle u, d\hat{\nabla}_d^{Ort} F(\theta)\rangle \Big| \nu_1, \cdots, \nu_d\right]\right)\right) \Big| \nu_1, \cdots, \nu_d\right].$$

Notice that conditional on $\nu_1, \cdots, \nu_d$, the sum $\langle u, \hat{\nabla}_d^{Ort} F(\theta)\rangle = \sum_{i=1} \alpha_i b_i F(\theta + \sigma^2 \nu_i b_i)$ is made of $d$ (conditionally) independent random variables $\{\alpha_i b_i F(\theta + \sigma^2 \nu_i b_i)\}_{i=1}^{d}$, and therefore, by Theorem 11.5 and Fact 2, the conditional MGF is bounded by:

$$e^{\frac{\lambda^2}{2} \sum_{i=1}^{d} \alpha_i^2 \beta_i^2 c^2 R^2}.$$

For $c = \max_i \frac{\sqrt{2}\sqrt{2g(\beta_i)^2+\mathbb{E}[b_i]^2/2+\beta_i^2}}{\beta_i}$ derived from applying Theorem 11.5 to this case, where $\beta_i$ are the sub-Gaussian parameters of the random variables $b_i$. Since $\sum_{i=1}^d \alpha_i^2 = 1$ the bound reduces to:

$$\mathbb{E}\left[\exp\left(\lambda\left(\langle u, d\hat{\nabla}_d^{Ort}F(\theta)\rangle - \mathbb{E}\left[\langle u, d\hat{\nabla}_d^{Ort}F(\theta)\rangle\middle|\nu_1,\cdots,\nu_d\right]\right)\right)\middle|\nu_1,\cdots,\nu_d\right] \leq e^{\frac{\lambda^2}{2}\beta^2c^2R^2},$$

where $\beta$ is an uppper bound to $\beta_i$ for all $i$. Notice that this bound has no dependence on dimension.

To provide a bound for the MGF:

$$\mathbb{E}\left[\exp\left(\lambda\left(\mathbb{E}\left[\langle u, d\hat{\nabla}_d^{Ort}F(\theta)\rangle\middle|\nu_1,\cdots,\nu_d\right] - \mathbb{E}\left[\langle u, d\hat{\nabla}_d^{Ort}F(\theta)\rangle\right]\right)\right)\right].$$

The random variable:

$$\begin{aligned}\mathbb{E}\left[\langle u, d\hat{\nabla}_d^{Ort}F(\theta)\rangle\middle|\nu_1,\cdots,\nu_d\right] &= \sum_{i=1}^d \mathbb{E}\left[\alpha_i b_i f(\theta+\sigma\nu_i b_i)|\nu_1,\cdots,\nu_d\right] \\ &= \sum_{i=1}^d \alpha_i \mathbb{E}\left[b_i f(\theta+\sigma\nu_i b_i)|\nu_1,\cdots,\nu_d\right]\end{aligned}$$

is bounded. Indeed by Hölder:

$$\left|\sum_{i=1}^d \alpha_i \mathbb{E}\left[b_i f(\theta+\sigma\nu_i b_i)|\nu_1,\cdots,\nu_d\right]\right| \leq RB\|\alpha\|_1,$$

where $\mathbb{E}\left[|b_i|\right] \leq B, \forall i$ and $\alpha \in \mathbb{R}^d$ with $\alpha \in \mathbb{S}^{d-1}$. The later implies $\|\alpha\|_1 \leq \sqrt{d}$. And $R$ is a uniform upper bound for $f$.

The previous observations imply in turn that this random variable is bounded by $RB\sqrt{d}$, and therefore that it is sub-Gaussian because it is bounded (Boucheron et al., 2013). Therefore:

$$\mathbb{E}\left[\exp\left(\lambda\left(\mathbb{E}\left[\langle u, d\hat{\nabla}_d^{Ort}F(\theta)\rangle|\nu_1,\cdots,\nu_d\right] - \mathbb{E}\left[\langle u, d\hat{\nabla}_d^{Ort}F(\theta)\rangle\right]\right)\right)\right] \leq \exp\left(\frac{\lambda^2R^2B^2d}{8}\right).$$

Plugging these two bounds together:

$$\mathbb{E}\left[\exp\left(\lambda\left(\langle u, d\hat{\nabla}_d^{Ort}F(\theta)\rangle - \mathbb{E}\left[\langle u, d\hat{\nabla}_d^{Ort}F(\theta)\rangle\right]\right)\right)\right] \leq e^{\frac{4\lambda^2\beta^2c^2R^2+\lambda^2R^2B^2d}{8}}.$$

As a consequence:

$$\mathbb{E}\left[\exp\left(\lambda\left(\langle u, \hat{\nabla}_d^{Ort}F(\theta)\rangle - \mathbb{E}\left[\langle u, \hat{\nabla}_d^{Ort}F(\theta)\rangle\right]\right)\right)\right] \leq e^{\frac{\lambda^2\beta^2c^2R^2}{2d^2}+\frac{\lambda^2R^2B^2}{8d}}.$$

With $c = \max_i \sqrt{2}\sqrt{2 * g(\beta_i)^2 + \mathbb{E}[b_i]^2/2 + \beta_i^2}$ with $g$ the function defined in Theorem 11.5.

□

Assuming $N = Td$ and therefore availability of $T$ i.i.d. orthogonal estimators (indexed by $j$) define:

$$\hat{\nabla}_N^{Ort}F(\theta) = \frac{1}{T}\sum_{j=1}^T \hat{\nabla}_d^{Ort,j}F(\theta).$$

The following corollary is immediate:

**Corollary 11.9.** The gradient estimator $\hat{\nabla}_N^{Ort} F(\theta)$ is sub-Gaussian with parameter $\frac{1}{\sqrt{T}}\sqrt{\frac{\beta^2 c^2 R^2}{d^2\sigma^2} + \frac{R^2 B^2}{4\sigma^2 d}} = \frac{1}{\sqrt{N}}\sqrt{\frac{\beta^2 c^2 R^2}{d\sigma^2} + \frac{R^2 B^2}{4\sigma^2}}$ .

And therefore:

**Corollary 11.10.** The orthogonal gradient estimator $\hat{\nabla}_N^{Ort} F(\theta)$ satisfies the following concentration inequality:

$$\mathbb{P}\left(\max_{j=1,\cdots d}\left|\left(\hat{\nabla}_N^{Ort} F(\theta)\right)_j - \left(\mathbb{E}\left[\hat{\nabla}_N^{Ort} F(\theta)\right]\right)_j\right| \geq t\right) \leq 2de^{\frac{-t^2 N\sigma^2}{\frac{\beta^2 c^2 R^2}{d} + \frac{R^2 B^2}{4}}}.$$

This argument finalizes the proof of Theorem 4.3. Whenever the lengths of the scalings $B, \beta_i$ are of order $O(1)$, we recover a concentration rate of order $O(d\exp(-t^2 N))$, which is comparable to the rate for the vanilla estimator. The analysis of orthogonal estimators is substantially harder than in the vanilla case due to the non i.i.d nature of the sampling process. This is to our knowledge the first result of its type.

## 12 Experiments: further details for variational autoencoder implementation

In this section, we give further details on the setup of the variational autoencoder experiments on MNIST appearing in Section 5.2 of the main paper.

### 12.1 Architectures

We use a 64-dimensional $N(0, I)$ distribution for the prior over the latent state $z$. The generative model $p_\theta(x|z)$ is specified by a fully-connected neural network with $64$ input units and two hidden layers of $500$ units. The hidden unit activation functions are ReLUs, and the final layer activations are sigmoids. A Bernoulli likelihood is used to train the output of the network. Here, $\theta$ represents the trainable parameters of the network. The recognition model $q_\phi(z|x)$ is also given by a fully connected neural network with two hidden layers of $500$ units. The hidden layer activation functions are ReLUs, and the final layer is linear, outputting a mean vector $\mu_\phi(x)$ and a log-standard deviation vector $\log(\sigma_\phi(x))$, which parametrise an approximate factorised Gaussian posterior $N(\mu_\phi(x), \sigma_\phi^2(x))$ for the latent encoding given $x$. Here, $\phi$ are the trainable parameters of the network. We initialise all weights of the networks using the normalised initialisation of (Glorot and Bengio, 2010), and initialise biases to $0$.

### 12.2 Results

Table 1: Train and test ELBO achieved with various sampling algorithms. iid refers to independently sampled directions, in contrast to ort, which refers to orthogonally constrained directions as in Algorithm 2. anti-eq corresponds to antithetic pairs of samples with matching norms (as in Algorithm 2, and anti-inv corresponds to antithetic pairs with norm couplings as in Algorithm 1.

| | $m = 2$ | | | | | |
|---|---|---|---|---|---|---|
| | iid | iid-anti-eq | iid-anti-inv | ort | ort-anti-eq | ort-anti-inv |
| Train | -99.59 | -98.60 | -98.64 | -99.30 | -98.56 | **-98.47** |
| Test | -99.96 | -99.02 | -99.05 | -99.69 | -98.97 | **-98.94** |
| | $m = 8$ | | | | | |
| | iid | iid-anti-eq | iid-anti-inv | ort | ort-anti-eq | ort-anti-inv |
| Train | -98.88 | -98.48 | -98.55 | -98.79 | **-98.41** | -98.50 |
| Test | -99.26 | -98.92 | -98.98 | -99.24 | **-98.89** | -98.95 |

We train on minibatches of $50$ images, and use the Adam optimiser with a learning rate of $10^{-4}$, and all other parameters set to default settings; the learning rate was softly optimized for the performance of the i.i.d. method. It is thus possible that with further hyperparameter tuning for each individual sampling method, further improvements in performance may be observed for GCMC sampling schemes; intuitively, we might expect that the variance reduction in stochastic gradients that GCMC methods achieve would allow a larger learning rate to be used. We report average test and train log-likelihood after 50 epochs of training, to assess the impact of the considered sampling schemes on the speed of learning for the model. We summarize full results for a variety of sampling methods in Table 1. We note that GCMC methods always improve speed of training relative to i.i.d., and in general the most substantial improvement combines some variant of antithetic sampling with orthogonality constraints.

## 13 Experiments: Learning efficient navigation policies with ES strategies

In this section we give additional information on the ES gradient estimators described in Section 5.1,as well as a description of the video library that we attach to the paper, and additional experimental results.

### 13.1 Estimator specification

The vanilla ES gradient estimator is given by

$$\hat{\nabla}_N^V F_\sigma(\theta) = \frac{1}{N\sigma}\sum_{i=1}^{N} F(\theta+\sigma\epsilon_i)\epsilon_i, \text{ where } \epsilon_i \sim \mathcal{N}(0,I) \text{ are all i.i.d. .}$$

We consider three variants of control variates: $\mathrm{forward\ finite\text{-}difference}$, in which the estimator is given by

$$\frac{1}{N\sigma}\sum_{i=1}^{N}(F(\theta+\sigma\epsilon_i)-F(\theta))\epsilon_i\,,$$

$\mathrm{antithetic}$, in which the estimator is given by

$$\frac{1}{2N\sigma}\sum_{i=1}^{N}(F(\theta+\sigma\epsilon_i)-F(\theta-\sigma\epsilon_i))\epsilon_i\,,$$

and $\mathrm{antithetic\text{-}coupled}$, in which the estimator is given by

$$\frac{1}{2N\sigma}\sum_{i=1}^{N}(F(\theta+\sigma\epsilon_i)\epsilon_i + F(\theta+\sigma\epsilon_i')\epsilon_i' - F(\theta)(\epsilon_i+\epsilon_i'))\,,$$

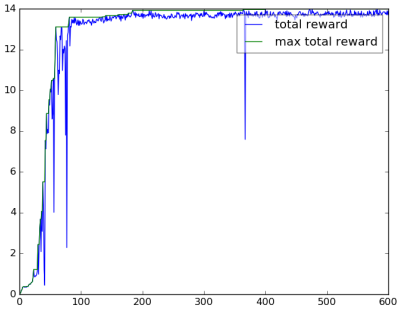
where $\varepsilon_i$ and $\varepsilon_i'$ are coupled as in Algorithm 1. Note the additional term dependent on $F(\theta)$ appearing in the $\mathrm{antithetic}-\mathrm{coupled}$ estimator, in order to cancel the zeroth order term in the Taylor expansion of the above objective.

### 13.2 Video library

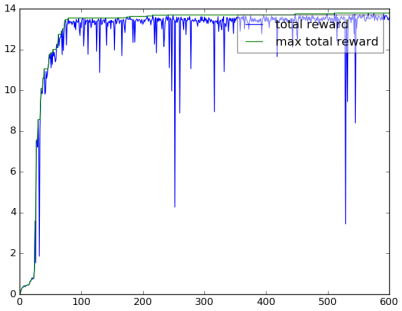
We attach to the paper a collection of videos showing how policies learned with different tested MC algorithms work in a simulator. Each file is in a $.\mathrm{webm}$ format and its name is using the following template: sensing_mechanism-control_variate-samples_number, where: sensing_mechanism stands for the sampling strategy and is chosen from the set: $\{\mathrm{MCGaussian}, \mathrm{MCGaussianOrthogonal}, \mathrm{MCRandomHadamard}\}$, control_variate-samples_number stands for the type of the control variate term used and is chosen from the set: $\{\mathrm{vanilla}, \mathrm{forward\ finite\text{-}difference}, \mathrm{antithetic}$ and $\mathrm{antithetic\text{-}coupled}\}$ and finally: samples_number stands for the number of samples used in the MC algorithm at each iteration of the optimization routine to approximate current gradient vector. These videos serve to illustrate the types of policies learnt under the variety of sampling mechanisms considered in Section 5.1.

### 13.3 RL experiments: additional results

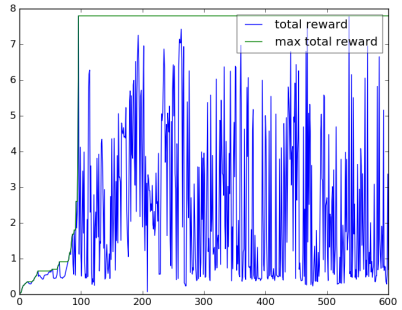
We present here the results of all experiments conducted to learn good quality navigation policies for the Minitaur platform for the following sampling strategies: MCGaussian, MCGaussianOrthogonal, MCRandomHadamard, the following control variate terms: vanilla, forward finite-difference, antithetic and the following number of samples: $m = 8, 48, 96$.



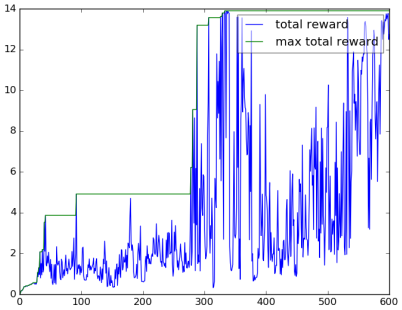

(a) MCGaussian-antithetic-48



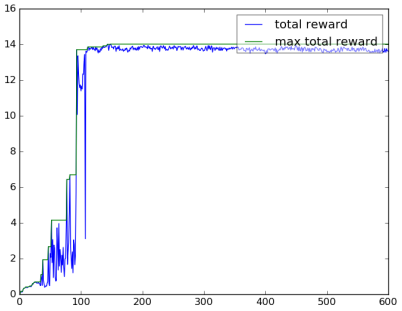

(b) MCGaussian-antithetic-96



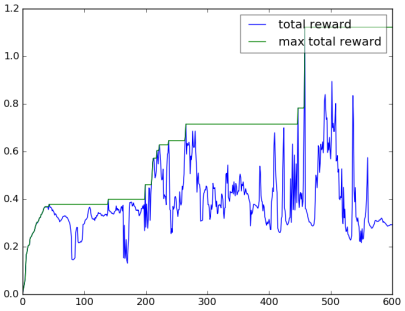

(c) MCGaussian-forward_fd-8




(d) MCGaussian-forward_fd-48

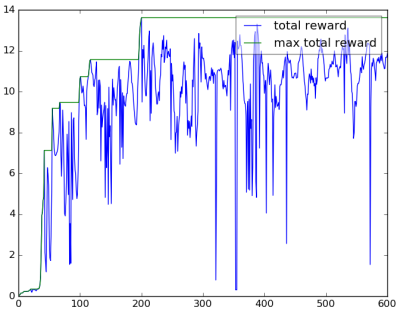



(e) MCGaussian-forward_fd-96

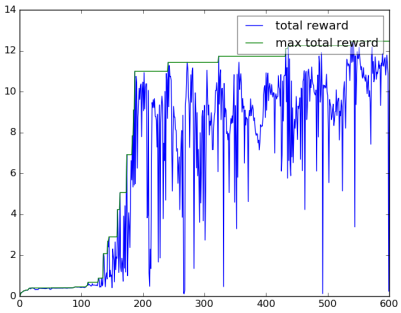



(f) MCGaussian-vanilla-8

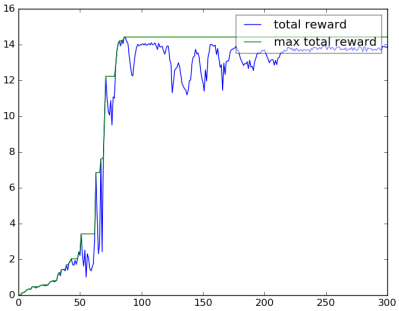
Figure 3: Additional experimental results showing training curves for different MC algorithms. Naming is borrowed from the video library section.



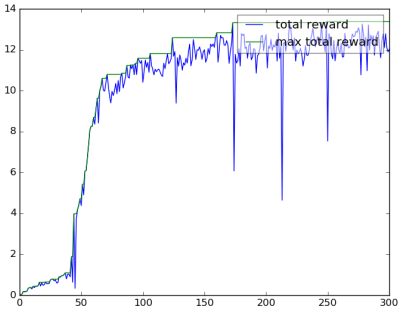

(a) MCGaussian-vanilla-48



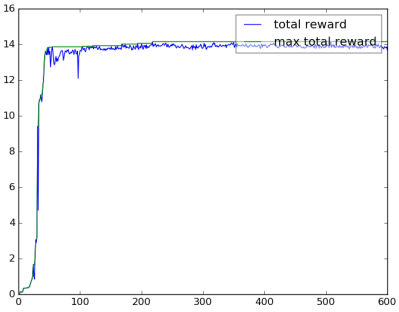

(b) MCGaussian-vanilla-96



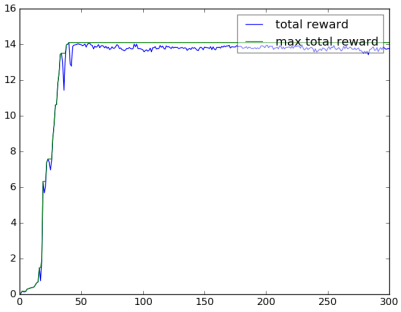

(c) MCGaussianOrthogonal-antithetic-16




(d) MCGaussianOrthogonal-antithetic-32

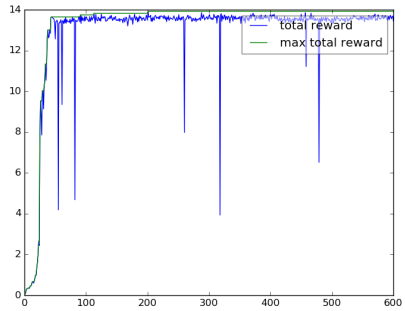



(e) MCGaussianOrthogonal-antithetic-48

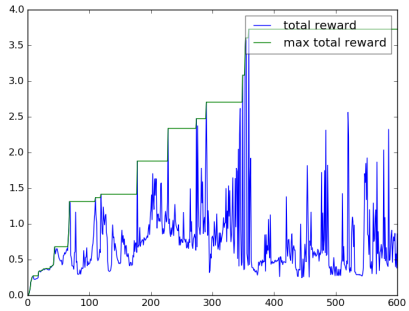



(f) MCGaussianOrthogonal-antithetic-64

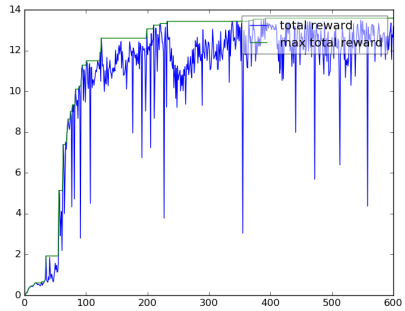
Figure 4: Additional experimental results showing training curves for different MC algorithms. Naming is borrowed from the video library section.



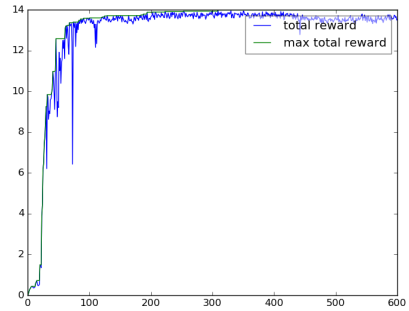

(a) MCGaussianOrthogonal-antithetic-96



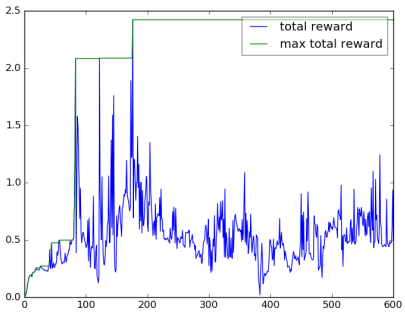

(b) MCGaussianOrthogonal-forward_fd-8



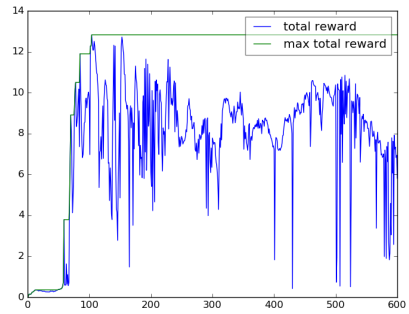

(c) MCGaussianOrthogonal-forward_fd-48




(d) MCGaussianOrthogonal-forward_fd-96

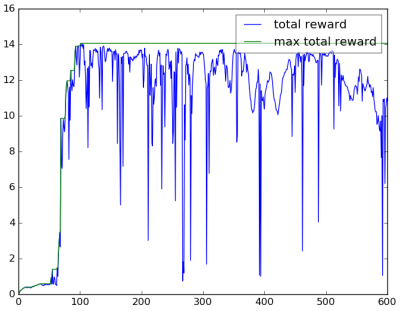



(e) MCGaussianOrthogonal-vanilla-8

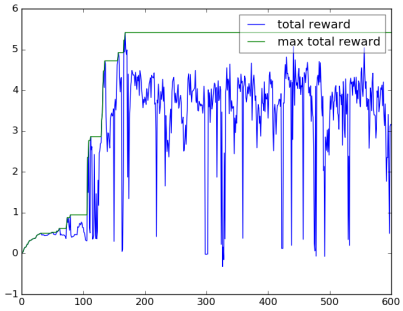



(f) MCGaussianOrthogonal-vanilla-48

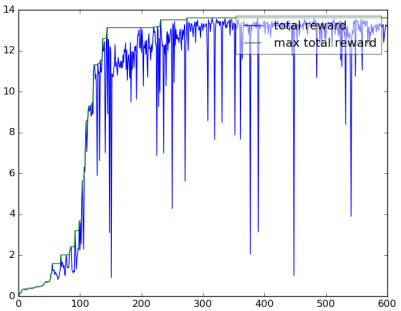
Figure 5: Additional experimental results showing training curves for different MC algorithms. Naming is borrowed from the video library section.



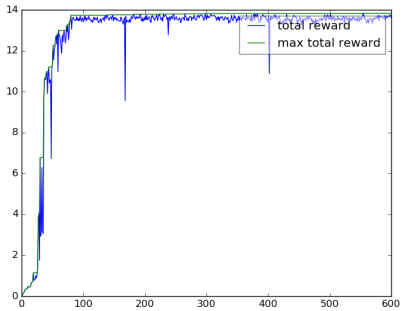

(a) MCGaussianOrthogonal-vanilla-96



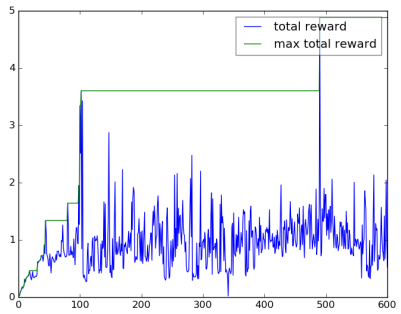

(b) MCRandomHadamard-vanilla-8



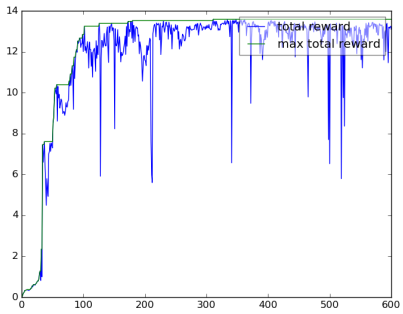

(c) MCRandomHadamard-vanilla-48




(d) MCRandomHadamard-vanilla-96

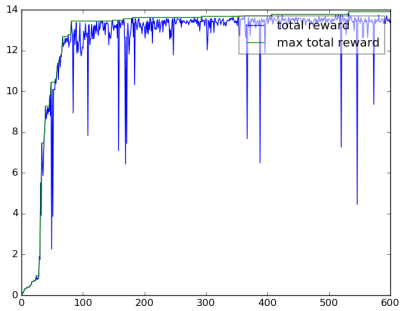



(e) MCRandomHadamard-forward_fd-8

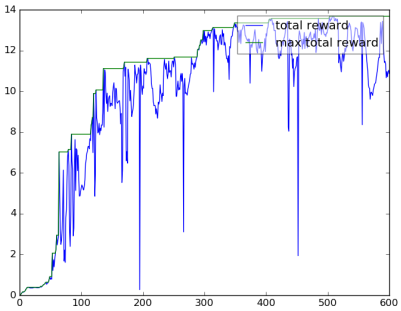



(f) MCRandomHadamard-forward_fd-48

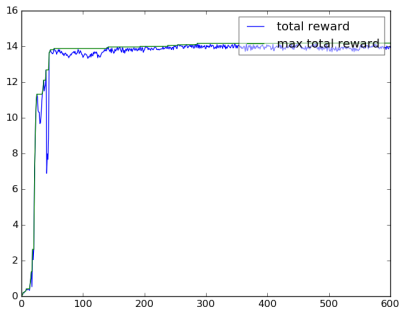
Figure 6: Additional experimental results showing training curves for different MC algorithms. Naming is borrowed from the video library section.



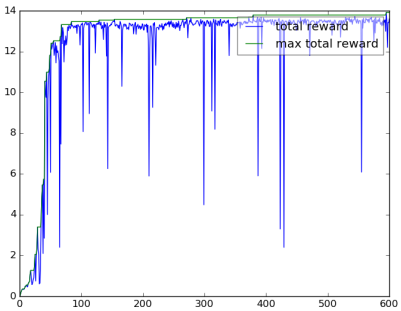

(a) MCRandomHadamard-forward_fd-96




(b) MCRandomHadamard-antithetic-8




(c) MCRandomHadamard-antithetic-48




(d) MCRandomHadamard-antithetic-96

Figure 7: Additional experimental results showing training curves for different MC algorithms. Naming is borrowed from the video library section.