Unbalanced Kantorovich-Rubinstein distance and barycenter for finitely supported measures: A statistical perspective

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Abstract

We propose and investigate several statistical models and corresponding sampling schemes for data analysis based on unbalanced optimal transport (UOT) between finitely supported measures. Specifically, we analyse Kantorovich-Rubinstein (KR) distances with penalty parameter $C > 0$. The main result provides non-asymptotic bounds on the expected error for the empirical KR distance as well as for its barycenters. The impact of the penalty parameter $C$ is studied in detail. Our approach justifies randomised computational schemes for UOT which can be used for fast approximate computations in combination with any exact solver. Using synthetic and real datasets, we empirically analyse the behaviour of the expected errors in simulation studies and illustrate the validity of our theoretical bounds.

1 Introduction

Optimal transport (OT) [for a detailed mathematical discussion see e.g. Villani, 2008, Santambrogio, 2015] has been a focus of attention in various research fields for a long time. More recently, its powerful geometric features promoted by improved computational tools [see e.g. Chizat et al., 2018a, Peyré and Cuturi, 2019, Guo et al., 2020, Lin et al., 2020] have turned OT into a promising new tool for modern data analysis with applications in machine learning [Frogner et al., 2015, Arjovsky et al., 2017, Schmitz et al., 2018, Yang et al., 2018, Vacher et al., 2021], computer vision [Baumgartner et al., 2018, Kolkkin et al., 2019], genetics [Evans and Matsen, 2012, Schiebinger et al., 2019], cell biology [Gellert et al., 2019, Klatt et al., 2020, Tameling et al., 2021], image processing [Pitié et al., 2007, Rabin and Papadakis, 2015, Bonneel et al., 2016, Tartavel et al., 2016] and statistical inference [Sommerfeld and Munk, 2018, Lee and Raginsky, 2018, Mena and Niles-Weed, 2019, Panaretos and Zemel, 2019], among others.

However, the wide range of such applications also surfaced some limitations of classical OT. In particular, the assumption of equal total mass intensity of the measures is often inappropriate. A straightforward strategy to overcome this issue is to normalise the measures’ total intensities. However, this preprocessing step has an immediate impact on data analysis, in particular on the underlying transport plan. For example, when matching point clouds of different sizes the resulting plan distributes mass among several points, whereas often it is desired to match points one-to-one which is favourable in many applications (see Figure 1). Attempts to circumvent this issue have led to a range of unbalanced optimal transport (UOT) proposals [see e.g. Figalli, 2010, Liero et al., 2018, Chizat et al.,...
Figure 1: Transport between two measures (blue and brown) with their support points located in $[0, 1]^2$. The respective transport plans between them are displayed by red lines where the thickness of a line is proportional to the transported mass. (a) The measures have been normalised to probability measures (the blue points have mass 1/6 and the brown points with mass 1/13). (b) The UOT plan for the $(2, 2)$-KRD between the two unnormalised measures (all points have mass 1).

2018b, Balaji et al., 2020, Mukherjee et al., 2021, Heinemann et al., 2022a]. These formulations extend optimal transport concepts to general positive measures by either fixing the total amount of mass to be transported in advance or by penalising the hard marginal constraints inherent in OT. All these approaches also give rise to associated barycenters, generalising the popular notion of OT barycenters [Agueh and Carlier, 2011] to measures of unequal total intensity [Chizat et al., 2018a, Friesecke et al., 2021, Heinemann et al., 2022a].

The UOT formulation considered here is the $(p, C)$-Kantorovich-Rubinstein distance (KRD) (see Section 1.1) whose structural properties and related $(p, C)$-barycenter have recently been studied in detail [Heinemann et al., 2022a]. The $(1, 1)$-KRD essentially corresponds to the notion of extended Kantorovich norms [Kantorovich and Rubinstein, 1958, Hanin, 1992] considered in the context of Lipschitz spaces and signed measures. In this context, Guittet [2002] first introduced a discrete formulation of the problem, where he established a Linear Program (LP) formulation which carries over to the general $(p, C)$-KRD. For illustration, a comparison between the $(p, C)$-barycenter and the $p$-Wasserstein barycenter in a simple example is displayed in Figure 2. From a data analysis point of view we find it particularly appealing that for the $(p, C)$-KRD there is a clear geometrical connection between its penalty $C$ and the structural properties of the corresponding UOT plans and $(p, C)$-barycenter. More precisely, it is shown in Heinemann et al. [2022a] that $C$ controls the largest scale at which mass transport is possible in an optimal plan. This interpretation of the $(p, C)$-KRD allows to easily design it to respect different structural properties of the data and thus makes it a prime candidate for statistical tasks in data analysis. Furthermore, each support point of any $(p, C)$-barycenter is contained in a finite set characterised by the value of $C$. This allows to adapt OT solvers for the unbalanced problems.

Though, due to the unbalanced nature of the problem, the task of sampling from the underlying measures requires alternative sampling schemes and different statistical modelling. While for OT between probability measures there is a canonical sampling model by i.i.d. replications from the measures, this fails for UOT, since the considered mea-
sures are not necessarily probability measures. In this work, we address this issue and suggest a framework underpinning UOT based statistical data analysis. To this end, we analyse the \((p,C)\)-KRD and its barycenter in three specific statistical models motivated by applications in randomised algorithms and microscopy tasks. Notably, these models also provide a framework which potentially allows to treat the alternative UOT models mentioned above.

1.1 Kantorovich-Rubinstein Distance

Let \((X,d)\) be a finite metric space with finite cardinality \(M\) and denote by
\[
\mathcal{M}_+(X) := \left\{ \mu \in \mathbb{R}^{|X|} \mid \mu(x) \geq 0 \ \forall x \in X \right\}
\]
the set of non-negative measures\(^1\) on \(X\). For a measure \(\mu \in \mathcal{M}_+(X)\) its total mass is defined as
\[
\mathbb{M}(\mu) := \sum_{x \in X} \mu(x)
\]
and the subset \(\mathcal{P}(X) \subset \mathcal{M}_+(X)\) of measures with total mass one is the set of probability measures. If \(\pi \in \mathcal{M}_+(X \times X)\) is a measure on the product space \(X \times X\) its marginals are defined as
\[
\pi(x,X) := \sum_{x' \in X} \pi(x,x') \quad \text{and} \quad \pi(X,x') := \sum_{x \in X} \pi(x,x'),
\]
respectively. For two measures \(\mu, \nu \in \mathcal{M}_+(X)\) define the set of non-negative sub-couplings as
\[
\Pi_{\leq}(\mu, \nu) := \{ \pi \in \mathcal{M}_+(X \times X) \mid \pi(x,X) \leq \mu(x), \pi(X,x') \leq \nu(x') \ \forall x, x' \in X \}. \tag{1}
\]
Following Heinemann et al. [2022a], for \(p \geq 1\) and a parameter \(C > 0\), the \((p,C)\)-Kantorovich-Rubinstein distance (KRD) between two measures \(\mu, \nu \in \mathcal{M}_+(X)\) is defined as
\[
\text{KR}_{p,C}(\mu, \nu) := \left( \min_{\pi \in \Pi_{\leq}(\mu, \nu)} \sum_{x,x' \in X} d^p(x,x') \pi(x,x') + C^p \left( \frac{\mathbb{M}(\mu) + \mathbb{M}(\nu)}{2} - \mathbb{M}(\pi) \right) \right)^{\frac{1}{p}}. \tag{2}
\]
For any \(p \geq 1\), it defines a distance on the space of non-negative measures \(\mathcal{M}_+(X)\) and it naturally extends the well-known \(p\)-th order OT distance defined for measures of equal total mass [Heinemann et al., 2022a].

1.2 Kantorovich-Rubinstein Barycenters

The \((p,C)\)-KRD also allows to define a notion of a barycenter for a collection of measures with (potentially) different total masses. Assume \((X,d)\) to be embedded in some connected ambient space\(^2\) \((Y,d)\), e.g., a Euclidean space. Define the (unbalanced) \((p,C)\)-Fréchet functional
\[
F_{p,C}(\mu) = \frac{1}{J} \sum_{i=1}^{J} \text{KR}_{p,C}^\mu(\mu_i, \mu).
\]
Any minimiser of this functional in \(\mathcal{M}_+(Y)\) is said to be a \((p,C)\)-Kantorovich-Rubinstein barycenter of \(\mu_1, \ldots, \mu_J\) or \((p,C)\)-barycenter for short\(^3\). The objective functional \(F_{p,C}\)

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\(^1\)A non-negative measure on a finite space \(X\) is uniquely characterized by the values it assigns to each singleton \(\{x\}\). To ease notation we write \(\mu(x)\) instead of \(\mu(\{x\})\). The corresponding \(\sigma\)-field is always to be understood as the powerset of \(X\).

\(^2\)We assume the metric on \(X \subset \mathcal{Y}\) to be the metric of \(\mathcal{Y}\) restricted to \(X\).

\(^3\)For the sake of readability, the weights in this definition are fixed to \(1/J\). Adaptation of all results to arbitrary positive weights \(\lambda_1, \ldots, \lambda_J\) summing to one is straightforward.
Figure 2: (a) $J = 10$ measures with mass 1 at each support point and different total mass intensities (each colour corresponds to a different measure) superimposed on top of each other. (b) The OT barycenter (for squared Euclidean cost) of the normalised measures. (c) The $(2, 0.3)$-barycenter of the unnormalised measures (see (3) for a rigorous definition).

is referred as (unbalanced) $(p, C)$-Fréchet functional and the so called Borel barycenter application is defined as

$$T^{L,p}(x_1, \ldots, x_L) \in \arg\min_{y \in \mathcal{Y}} \sum_{i=1}^{L} d^p(x_i, y).$$

Define the full centroid set\footnote{There are scenarios where multiple sets fulfil the definition of the centroid set, since there might be multiple points that minimise the barycentric application. In this case, a fixed representative is chosen and there still exists a choice of centroid set which contains the support of the $(p, C)$-barycenter.} of the measures

$$\mathcal{C}_{KR}(J, p) = \left\{ y \in \mathcal{Y} \mid \exists L \geq \lceil J/2 \rceil, \ \exists (i_1, \ldots, i_L) \subset \{1, \ldots, J\}, \right.$$ \[ x_1, \ldots, x_L : x_l \in \text{supp}(\mu_l) \]
$$\forall l = 1, \ldots, L : y = T^{L,p}(x_1, \ldots, x_L) \right\},$$

and based on it the restricted centroid set

$$\mathcal{C}_{KR}(J, p, C) = \left\{ y = T^{L,p}(x_1, \ldots, x_L) \in \mathcal{C}_{KR}(J, p) \mid \forall 1 \leq l \leq L : \right.$$ \[ d^p(x_1, y) \leq C^p; \ \sum_{i=1}^{L} d^p(x_i, y) \leq \frac{C^p(2L - J)}{2} \right\}. \tag{5}$$

According to Heinemann et al. [2022a], any $(p, C)$-barycenter is finitely supported and its support is included in the restricted centroid set $\mathcal{C}_{KR}(J, p, C)$. This is critical, as it allows to restrict theoretical analysis as well as computational methods to the scenario all measures involved have finite support.

1.3 Statistical Models and Contributions

In practice, one often does not have access to the population measures $\mu, \nu, \mu^1, \ldots, \mu^J$, respectively. Instead, these measures have to be estimated from data. For probability measures the most common statistical model assumes access to (i.i.d.) data $X_1, \ldots, X_N \sim \mu$ (and similar for $\nu, \mu^1, \ldots, \mu^J$). A commonly used estimator is the empirical measure
\[ \hat{\mu}_N = \frac{1}{N} \sum_{k=1}^{N} \delta_{X_k}, \] where \( \delta_X \) denotes the (random) point measure at location \( X \). This can be used to estimate OT and its plan. In general, this yields a statistically efficient estimator [Dudley, 1969, Ajtai et al., 1984, Sommerfeld et al., 2019, Weed and Bach, 2019, Hütter and Rigollet, 2021, Manole et al., 2021, Hundrieser et al., 2022] see, however, Niles-Weed and Berthet [2022] for certain improvements. For OT barycenters based on empirical measures significantly less is known, though recently some progress has been made in the context of finitely supported measures [Heinemann et al., 2022b]. Extending such results to general measures is not obvious and requires the need for alternative statistical modelling which is the topic of this paper. Exemplary, we propose three approaches motivated by different applications.

**Multinomial Model**

For the *multinomial model* the measures are normalised to define probability measures such that sampling as described above is possible. The resulting empirical estimators are rescaled to the original total intensities. More precisely, consider i.i.d. random variables \( X_1, \ldots, X_N \)

\[ i.i.d. \sim \frac{\mu}{M(\mu)}, \]

where the total intensity \( M(\mu) \) is assumed to be known. The corresponding unbiased empirical estimator is then defined as

\[ \hat{\mu}_N := \frac{M(\mu)}{N} \sum_{x \in \mathcal{X}} \prod_{k \in \{1, \ldots, N\}} |\{ k \in \{1, \ldots, N\} \mid X_k = x \}| \delta_x. \]  

This approach can be understood as extension of the classical sampling approach for probability measures to measures of arbitrary total intensities. A key motivation for this model is resampling for randomised computations of UOT. In real world data analysis it is common to encounter data (e.g. high-resolution images) which are out of reach for current state of the art solvers for OT. One idea in this scenario is to replace each measure by its empirical version and then use these measures as surrogates. This idea has been considered in detail for the \( p \)-Wasserstein distance [Sommerfeld et al., 2019] and the \( p \)-Wasserstein barycenter [Heinemann et al., 2022b]. Statistical deviation bounds allow to balance computational complexity and accuracy of approximation in terms of the sample size \( N \). In the context of this model we extend these results to the \( (p,C) \)-KRD for measures of unequal total intensities.

**Bernoulli Model**

For the *Bernoulli model* we consider measures \( \mu \) with \( \mu(x) = 1 \) for all \( x \in \text{supp}(\mu) \). Thus, the measure \( \mu \) represents a point cloud in the ambient space \( \mathcal{Y} \) with the total mass being the cardinality of the point cloud. We restrict the model to this setting, but we stress that generalisations to arbitrary masses at the individual locations are straightforward. We then assume to observe independent Bernoulli random variables \( B_x \sim \text{Ber}(s_x) \) with a fixed success probability \( s_x \in [0, 1] \) for each location \( x \in \mathcal{X} \). We denote \( s_X := (s_{x_1}, \ldots, s_{x_M}) \) and refer to \( s_X \) as success vector. A suitable unbiased estimator for \( \mu \) is defined by

\[ \hat{\mu}_{s_X} := \sum_{x \in \mathcal{X}} \frac{B_x}{s_x} \delta_x. \]  

The corresponding Bernoulli field \((B_x)_{x \in \mathcal{X}}\) is a prototypical model for incomplete data, where data is missing at random and the Bernoulli variables serve as labels for this. It further arises, e.g. in the context of generalised linear models where the regressor \( X \) is linked to \( B_x \) by a link function in a non-parametric fashion. The Bernoulli model also underlies the sampling scheme for the subsequent Poisson intensity model, which occurs e.g. in various imaging devices, such as fluorescence cell microscopy. There, fluorescent
markers are, e.g. chemically attached to each protein within a complex protein ensemble and then are excited with a laser beam. The resulting, emitted photons indicate the spatial position of the objects of interest in the proper experimental setup [Kulaitis et al., 2021]. However, the marker has a limited labelling efficiency \( s_x \in (0,1] \) at each location \( x \in X \) and we only observe a location which has been labelled by the marker and finally emits photons.

**Poisson Intensity Model**

For the *Poisson intensity model* we fix a parameter \( t > 0 \) and a success probability \( s \in [0,1] \). Consider a collection of \( |X| \) independent Poisson random variables \( P_x \sim \text{Poi}(t \mu(x)) \) with intensity \( t \mu(x) \) at each location \( x \in X \) and independently from that Bernoulli random variables \( B_x \sim \text{Ber}(s) \) for each \( x \in X \). A suitable unbiased estimator for \( \mu \) is defined by

\[
\hat{\mu}_{t,s} := \frac{1}{st} \sum_{x \in X} B_x P_x \delta_x. \tag{8}
\]

In contrast to the Bernoulli model, in this model the success probability is assumed to be homogeneous (as opposed to the inhomogeneous probabilities in the Bernoulli model, though such generalisations are straightforward) and the values of the population measures at each support point are not necessarily equal to one. Hence, we have two independent layers of randomness in the construction of this empirical measure. First, we draw a location \( x \) with a certain probability \( s \), then we observe random photon counts driven by a Poisson distribution based on the mass of \( \mu \) and the value of \( t \). This model is motivated by various tasks in photonic imaging, for example, fluorescence microscopy, X-ray imaging and positron emission tomography (PET), see Munk et al. [2020] for a survey. The finite space \( X \) represents the center of bins of a detection interface used to measure the emitted photons. The value \( \mu(x) \) corresponds to the integrated underlying photon intensity over its respective bin. This intensity is proportional to an external source, such as a laser duration in fluorescence microscopy and modelled by the parameter \( t > 0 \). The Bernoulli random variable \( B_x \) models the possibility that in the bin of \( x \) a photon can not be recorded. This might be due to various effects that cause thinning, such as limited labelling efficiency, dead time of cameras or a loss of photons due to sparse detector tubes. The value of \( P_x \) corresponds to the number of photons which have been measured at the bin of \( x \). Note, that besides \( B_x \), there might be also additional effects present which do not disable the whole bin, but just prevent a single photon from being measured. All this causes a thinning of the process and is incorporated in the probability \( s' \in (0,1] \) that a single photon at any bin and any point in time can not be measured. In this case, the model can be shown to be equivalent to a Poisson model with parameter \( ts' > 0 \) instead of \( t \) [Aspelmeier et al., 2015]. Hence, this kind of thinning corresponds to a reparametrisation of the original model and is thus a special case of this general Poisson intensity model.

1.3.1 Sampling Bounds

Let \( \mu, \nu \in \mathcal{M}_+(X) \) and let \( \hat{\mu}, \hat{\nu} \) be empirical versions of these measures generated with one of the aforementioned sampling mechanisms (recall (6),(7) and (8)). We are interested in tight upper bounds for the quantities

\[
(i) \ E\left[KR_{p,C}(\hat{\mu}, \mu)\right], \quad (ii) \ E\left[\|KR_{p,C}(\hat{\mu}, \hat{\nu}) - KR_{p,C}(\mu, \nu)\|\right].
\]
In particular, we show that there exist constants $E^{\text{Mult}}_{p,\mathcal{X},\mu}(C)$, $E^{\text{Pois}}_{p,\mathcal{X},\mu}(C)$, $E^{\text{Ber}}_{p,\mathcal{X},\mu}(C)$ such that for any $p \geq 1$ and for any measure $\mu$ and its estimator $\hat{\mu}$ in each of the three statistical models it holds

$$\mathbb{E}[\text{KR}_{p,C}(\hat{\mu},\mu)] \leq \begin{cases} E^{\text{Mult}}_{p,\mathcal{X},\mu}(C)^{\frac{1}{p}} N - \frac{1}{2p}, & \text{if } \hat{\mu} = \hat{\mu}_N, \\ E^{\text{Pois}}_{p,\mathcal{X},\mu}(C)^{\frac{1}{p}} \phi(t,s)^{\frac{1}{p}}, & \text{if } \hat{\mu} = \hat{\mu}_{t,s}, \\ E^{\text{Ber}}_{p,\mathcal{X},\mu}(C)^{\frac{1}{p}} \psi(s_{\mathcal{X}})^{\frac{1}{p}}, & \text{if } \hat{\mu} = \hat{\mu}_{s_{\mathcal{X}}}, \end{cases}$$

where

$$\phi(t,s) = \begin{cases} \left(2(1-s)M(\mu) + \frac{s}{\sqrt{t}} \sum_{x \in \mathcal{X}} \sqrt{\mu(x)} \right), & C \leq \min_{x \neq x'} d(x,x') \\ \left(\frac{1}{\sqrt{t}} M(\mu) + \frac{1-s}{t} \sum_{x \in \mathcal{X}} \mu(x)^2 \right)^{\frac{1}{2}}, & \text{else}, \end{cases}$$

and

$$\psi(s_{\mathcal{X}}) = \begin{cases} \left(2 \sum_{x \in \mathcal{X}} (1 - s_x) \right), & C \leq \min_{x \neq x'} d(x,x') \\ \left(\sum_{x \in \mathcal{X}} \frac{1-s_x}{1-s_x} \right)^{\frac{1}{2}}, & \text{else}. \end{cases}$$

Notably, in the multinomial model for $N \to \infty$, in the Poisson model for $t \to \infty$, $s \to 1$ and in the Bernoulli model for $s_{\mathcal{X}} \to 1_M$, these upper bounds tend to zero. The proof of these bounds (see Section 2) is inspired by partitioning strategies used to control the empirical deviation of the OT distance between probability measures [Dereich et al., 2013, Fournier and Guillin, 2015, Weed and Bach, 2019] and based on a tree approximation empirically observed on ultra-metric trees by Heinemann et al. [2022a].

The constants in these bounds depend on the structural properties of the measures and space, such as covering numbers and total mass intensity. For a detailed discussion of the constants see Section 2. Exemplary, for measures supported in $([0,1]^D, d_2)$, $p = 2$ and $d_{\text{min}}^\infty := \min_{x \neq x'} d_{\infty}(x,x')$, it holds for $D < 4$ (see for details Section 2.4)

$$E^{\text{Poi}}_{2,\mathcal{X},\mu}(C) \leq D \begin{cases} \frac{C^2}{2^{D/2 + 3}} - \frac{2D/2+3}{1-2^{D/2-2}}, & \text{if } C \geq 2 \\ \frac{2^{5+(D/2-2)}}{1-2^{D/2-2}}, & \text{if } 2^{1-l} \leq C < 2^{2-l}, \\ \frac{C^2}{2}, & \text{if } C \leq d_{\text{min}}^\infty. \end{cases}$$

For $D = 4$ it holds

$$E^{\text{Poi}}_{2,\mathcal{X},\mu}(C) \leq D \begin{cases} \frac{C^2}{4} - 2 \left(2 - \left|\mathcal{X}\right|^{-\frac{1}{2}} \right)^2 + (2 + 8 \log_2 (\left|\mathcal{X}\right|)), & \text{if } C \geq 2, \\ (2 + 8 \log_2 (\left|\mathcal{X}\right|) - l), & \text{if } 2^{1-l} \leq C < 2^{2-l}, \\ \frac{C^2}{2}, & \text{if } C \leq d_{\text{min}}^\infty, \end{cases}$$

and for $D > 4$, it holds

$$E^{\text{Poi}}_{p,\mathcal{X},\mu}(C) \leq D \begin{cases} \frac{C^2}{2^{D/2}} - 2 \left(2 - \left|\mathcal{X}\right|^{-\frac{1}{2}} \right)^2 + 2\left|\mathcal{X}\right|^{\frac{1}{2}} - \frac{2}{p} \left(1 + \frac{2^{2+D/2}}{2^{D/2-2}-1} \right), & \text{if } C \geq 2, \\ \left|\mathcal{X}\right|^{\frac{1}{2}} - \frac{2}{p} + \frac{2^{2+D/2}}{2^{D/2-2}-1} \left|\mathcal{X}\right|^{\frac{1}{2}} - \frac{2}{p} \left(2^{(D/2-2)(l-1)} \right), & \text{if } 2^{1-l} \leq C < 2^{2-l}, \\ \frac{C^2}{2}, & \text{if } C \leq d_{\text{min}}^\infty. \end{cases}$$
In particular, for $D < 4$ the constants are independent of the cardinality of the space $|\mathcal{X}|$, for $D = 4$ the dependence is logarithmic and for $D > 4$ of order $1/2 - 2/D$. However, it should be stressed that the upper bound in general depends on the measure’s intrinsic dimension, e.g. if a measure is supported on a $D' < D$ dimensional subspace of $[0,1]^D$, then these upper bounds could be stated in terms of $D'$.

The constants in the Bernoulli model coincide with those for the Poisson model. For the multinomial model it holds for $C \leq d^\infty_{\min}$ and any $D \geq 1$ that

$$E_{\text{Mult},\mathcal{X},\mu}(C) \leq 2^{-1}D\sqrt{\mathcal{M}}(\mu)\sum_{x \in \mathcal{X}}\sqrt{\mu(x)}.$$  

For $C > 2$, it holds

$$E_{\text{Mult},\mathcal{X},\mu}(C) \leq \begin{cases} \frac{2^{D+3}}{1-2^{D/2}} & \text{if } D < 4, \\ (2 + 8\log_2(|\mathcal{X}|)) & \text{if } D = 4, \\ 2|\mathcal{X}|^{1-\frac{3}{D}} \left(1 + \frac{2^{2+D/2}}{2D/2-2-1}\right), & \text{if } D > 4. \end{cases}$$

Otherwise, the constants also coincide with those in the Poisson model. Hence, the main difference between the multinomial and the Poisson model is the fact that for large $C$ the latter contains an additional term which originates from having to estimate the population level total mass intensity, while in the multinomial model, this is assumed to be known.

To further extend these bounds to the context of the $(p,C)$-Fréchet functionals and $(p,C)$-barycenters (3), we utilise certain structural properties of the $(p,C)$-barycenter. Let $\mu^*$ be any $(p,C)$-barycenter of the population measures $\mu_1,\ldots,\mu_J$ and let $\hat{\mu}^*$ be any barycenter of the empirical measures $\hat{\mu}_1,\ldots,\hat{\mu}_J$. From (i), we can derive a bound on the error in the Fréchet functional and in conjunction with theory from linear programming, we then extend this control to a more refined statement on the $(p,C)$-barycenters (see Theorem 3.2). The caveat is the fact that neither $\mu^*$ nor $\hat{\mu}^*$ is necessarily unique. Thus, we need to control the error in terms of the respective optimal set $B^*$ and its empirical counterpart $\hat{B}^*$. For this, we consider the quantities

$$(iii) \quad E\left[F_{p,C}(\hat{\mu}^*) - F_{p,C}(\mu^*)\right], \quad (iv) \quad E\left[\sup_{\hat{\mu}^* \in \hat{B}^*} \inf_{\mu^* \in B^*} KR_{p,C}(\mu^*,\hat{\mu}^*)\right].$$

The term (iv) is the expected deviation of the empirical barycenter which has the largest $(p,C)$-KRD to the set of barycenters of the population measures. The bounds on (iii) and (iv) generalise recent bounds in the context of OT barycenters established in Heinemann et al. [2022b].

As a major application, we stress that these bounds enable randomised computations of UOT with statistical guarantees. If the size of the population measures is computationally infeasible, then empirical versions of these measures can be used as a proxy for the population level distances and barycenter. The bounds (i) – (iv) allow to tune the problem size against the quality of the approximation. While theoretically all three models allow this approximation approach, the most suitable candidate is clearly the multinomial model. In this resampling scenario, the assumption of known total intensities is natural, as the population measures are known, but solving UOT between them is computationally infeasible. Here, the sample size $N$ provides a strict upper bound on the computational complexity of a given approximation. This is not the case though, for the other two models, where the sampling schemes do not allow to bound the required computational complexity beforehand.

One alternative approach, closely related to the multinomial model, is to make use of
a subsampling\(^5\) method instead of a resampling one, i.e. to replace the i.i.d. samples
\(X_1, \ldots, X_N\) from \(\mu\) by ones drawn without replacement. A natural choice of estimator in
this scenario is
\[
\hat{\mu}_N = \frac{1}{\sum_{i=1}^N \mu(X_i)} \sum_{i=1}^N \mu(X_i) \delta_{X_i},
\]
where the mass at each drawn location \(x \in \mathcal{X}\) is proportional to the mass of the population
measure at \(x\) and the total mass intensity is rescaled to the known, true total intensity.
This estimator is, due to the sampling without replacement, guaranteed to have \(N\) support
points, which yields close control on the required runtime for a given approximation.
This approach has become popular within the machine learning community where it is referred
to as mini-batch OT [Fatras et al., 2021, Nguyen et al., 2021]. An illustration of the potential
runtime advantages using the suggested randomised methods is displayed in Figure 3.
For this example, the resampling approach provides an expected relative KRD error of
about 5\% while achieving a speedup of about a factor of 1000 compared to the original
runtime, while the subsampling approach requires nearly 10\% of the original runtime to
achieve the same accuracy. A more detailed comparison of the empirical performance of
the re- and subsampling model is found in Section 4.4. Though, we note that, in the
considered data examples, the resampling approach consistently performed better than
the subsampling one. We also study the convergence properties of (i) – (iv) for all three
described models in extended simulation studies on a wide range of synthetic datasets.

In summary, we provide non-asymptotic deviation bounds for UOT distances and corre-
sponding barycenters. A major finding in this regard is that UOT can be analysed in a
variety of statistical models. This extends results for classical OT which has been tradi-
tionally only considered in the context of comparing probability distributions. Our results
are explicit in their dependency on the cardinality of the measures’ support sizes and their
total mass intensities. Most importantly, the upper bounds reveal an interesting interac-
tion between the structural properties of the measures and the regularisation parameter
\(C\). Our results can be used for statistically sound UOT based analysis of data generators
with different intensities, as well as for randomised computational schemes with statistical
error control.

2 Sampling Bounds for Kantorovich-Rubinstein Distances

In this section we investigate the Poisson model and its estimator in (8) in detail. We
provide theoretical guarantees for the accuracy of the approximation in terms of their
expected Kantorovich-Rubinstein deviation. Results for the multinomial and Bernoulli
model follow along the same reasoning. Corresponding deviation bounds and the proofs
are provided in Appendix A and Appendix B.
The proof of the main result and the explicit construction of its constant relies on a tree
approximation of the space \(\mathcal{X}\). This approximation requires some depth level \(L \in \mathbb{N}\) and
resolution \(q > 1\), based on which we construct minimal \(q^{-d} \text{diam}(\mathcal{X})\)-coverings\(^6\) on \(\mathcal{X}\) to
obtain our bounds. An illustration of this approximation is given in Figure 4.

2.1 Tree Approximation for the Kantorovich-Rubinstein Distance

Let \(\mathcal{T} = (V, E)\) be a rooted, ultrametric tree with height function \(h : V \rightarrow \mathbb{R}_+\) and root
\(r\). For two nodes \(u, v \in V\), denote the unique path between \(u\) and \(v\) in \(\mathcal{T}\) by \(P(u, v)\). For
\(^5\)Here, subsampling refers to sampling without replacement, while resampling refers to sampling with
replacement.
\(^6\)For a metric space \((\mathcal{X}, d)\) an \(\epsilon\)-cover is a set of points \(\{x_1, \ldots, x_m\} \subset \mathcal{X}\) such that for each \(x \in \mathcal{X}\),
there exists some \(1 \leq i \leq m\) such that \(d(x, x_i) \leq \epsilon\). The smallest such set is denoted as \(\mathcal{N}(\mathcal{X}, d, \epsilon)\).
a node \( v \in V \) its children are the elements of the set \( C(v) = \{ w \in V \mid v \in P(w, r) \} \). The parent \( \text{par}(v) \) of a node \( v \) is the unique node with \( (\text{par}(v), v) \in E \) and \( h(v) < h(\text{par}(v)) \).

For any \( C > 0 \), define the set

\[
\mathcal{R}(C) := \{ v \in V \mid h(v) \leq C/2 < h(\text{par}(v)) \}
\]

with the convention that \( \mathcal{R}(C) = \{ r \} \) if \( C/2 \geq h(r) \). The goal is to control the \((p, C)\)-KRD on the finite metric space \((X, d)\) by bounding it from above by a dominating distance \( d_T \) induced from a tree \( T \) with the elements of \( X \) as vertices and a height function \( h \) such that \( d(x, x') \leq d_T(x, x') \). In this case and by the definition of the Kantorovich-Rubinstein distance it holds for all measures \( \mu, \nu \in M_+(X) \) that

\[
\text{KR}_{p,C}(\mu, \nu) \leq \text{KR}_{d_T, C}(\mu, \nu),
\]

where \( \text{KR}_{d_T, C}(\mu, \nu) \) denotes the \((p, C)\)-KRD w.r.t. the ground space \((X, d_T)\). Moreover, if \( T \) is an ultrametric tree with leaf nodes \( L \) and height function \( h: V \to \mathbb{R}_+ \) inducing the tree metric \( d_T \) and the two measures \( \mu^L, \nu^L \in M_+(L) \) supported on the leaf nodes of \( T \), then it holds [Heinemann et al., 2022a] that

\[
\text{KR}_{d_T, C}^{p}(\mu^L, \nu^L) =
\sum_{v \in \mathcal{R}(C)} \left( 2^{p-1} \sum_{w \in C(v) \setminus \{v\}} \left( (h(\text{par}(w)) - h(w))^p \right) |\mu^L(C(w)) - \nu^L(C(w))| \right) \right.
\]

\[
+ \left( \frac{C^p}{2} - 2^{p-1}h(v)^p \right) |\mu^L(C(v)) - \nu^L(C(v))|. \]

The construction of \( T \), such that (11) holds, is as follows. Fix some depth level \( L \in \mathbb{N} \). For

---

7For two vertices of the tree \( T \), we define their distance \( d_T \) as the sum of the weights of the edges included in the unique path between the two vertices. Here, the weight of an edge joining two vertices \( v \) and \( \text{par}(v) \) is given by \( h(\text{par}(v)) - h(v) \).
Figure 4: **Ground metric approximation by an ultrametric tree distance:** (a) A finite metric space \((X, d)\) and its covering sets \(Q_0\) (black), \(Q_1\) (red) and \(Q_2\) (green) for \(L = 2\). (b) Based on the covering sets from (a) an ultrametric tree is constructed. The metric space \(X\) is embedded in level \(L + 1 = 3\) and equal to all leaf nodes of that tree.
some \( q > 1 \) and level \( j = 0, \ldots, L \) define the covering set \( Q_j := N(\mathcal{X}, q^{-j} \text{diam}(\mathcal{X})) \subseteq \mathcal{X} \) and let \( Q_{L+1} := \mathcal{X} \). Any point \( x \in Q_j \) is considered as a node at level \( j \) of a tree \( T \) and denoted as \((x, j)\) to emphasise its level position. For level \( j = 0 \) this yields a single element in \( Q_0 \) which serves as the root of the tree. For \( j = 0, \ldots, L \) a node \((x, j)\) at level \( j \) is connected to one node \((x', j+1)\) at level \( j + 1 \) if their distance satisfies \( d(x, x') \leq q^{-j} \text{diam}(\mathcal{X}) \) (ties are broken arbitrarily). The edge weight of the corresponding edge is set equal to \( q^{-j} \text{diam}(\mathcal{X}) \). Consequently, the height of each node only depends on its assigned level \( 0 \leq l \leq L + 1 \) and is defined as \( h_{q,L} : \{0, \ldots, L + 1\} \to \mathbb{R} \) by

\[
    h_{q,L}(l) = \sum_{j=l}^{L} q^{-j} \text{diam}(\mathcal{X}) = \frac{q^{1-l} - q^{-L}}{q-1} \text{diam}(\mathcal{X}). \tag{13}
\]

By definition the space \( \mathcal{X} \) is embedded in level \( L + 1 \) as the leaf nodes of \( T \) with height \( h_{q,L}(L + 1) = 0 \). By a straightforward computation it holds for two points \( x, x' \in \mathcal{X} \) considered as embedded in \( T \) as \((x, L + 1)\) and \((x', L + 1)\) that

\[
    d^{p}(x, x') \leq d_{T}^{p}((x, L + 1), (x', L + 1)). \tag{14}
\]

The measures \( \mu, \nu \) are embedded into \( T \) as measures \( \mu^{L}, \nu^{L} \) supported only on leaf nodes of \( T \) and thus it follows from (14) that

\[
    \text{KR}_{p,C}(\mu, \nu) \leq \text{KR}_{p,C}(\mu^{L}, \nu^{L}).
\]

In combination with the closed formula from (12) this yields an upper bound on the \((p, C)\)-KRD. Whenever clear from the context the notation is alleviated by writing \( \nu \in Q_l \) instead of \((\nu, l) \in Q_l \).

**Lemma 2.1.** Let \((\mathcal{X}, d)\) be a finite metric space and let \( \mu, \nu \in \mathcal{M}_{+}(\mathcal{X}) \) with total mass \( \mathbb{M}(\mu) \) and \( \mathbb{M}(\nu) \), respectively. Let \( p \geq 1 \) and \( C > 0 \). Then for any resolution \( q > 1 \), depth \( L \in \mathbb{N} \) and height function (13) with

\[
    h_{q,L}(k) = \frac{q^{1-k} - q^{-L}}{q-1} \text{diam}(\mathcal{X})
\]

it holds that

\[
    \text{KR}_{p,C}^{0}(\mu, \nu) \leq \left\{ \begin{array}{ll}
    \left( \frac{C_{p}}{2} - 2^{p-1} h_{q,L}(0)^{p} \right) |\mathbb{M}(\mu) - \mathbb{M}(\nu)| \\
    + B_{q,p,L,\mathcal{X}}(1), & \text{if } C \geq 2h_{q,L}(0), \\
    B_{q,p,L,\mathcal{X}}(l), & \text{if } 2h_{q,L}(l) \leq C < 2h_{q,L}(l - 1), \\
    \frac{C_{p}}{2} \text{TV}(\mu, \nu), & \text{if } C \leq \left( 2h_{q,L}(L) \lor \min_{x \# x'} d(x, x') \right),
    \end{array} \right.
\]

where \( \text{TV}(\mu, \nu) = \sum_{x \in \mathcal{X}} |\mu(x) - \nu(x)| \) is the total variation distance and

\[
    B_{q,p,L,\mathcal{X}}(l) = 2^{p-1} \sum_{j=l}^{L+1} \sum_{x \in Q_j} (h_{q,L}(j-1)^{p} - h_{q,L}(j)^{p}) \left| \mu^{L}(\mathcal{C}(x)) - \nu^{L}(\mathcal{C}(x)) \right|.
\]

The proof is given in Appendix D.
2.2 \((p, C)\)-Kantorovich-Rubinstein Deviation Bound

Given Lemma 2.1 based on the tree-approximation, we are able to state our main result explicitly.

**Theorem 2.2.** Let \((\mathcal{X}, d)\) be a finite metric space and \(\mu \in \mathcal{M}_+(\mathcal{X})\). Let \(\hat{\mu}_{t,s}\) be the estimator from (8). Then, for any \(p \geq 1\), resolution \(q > 1\) and depth \(L \in \mathbb{N}\) it holds that

\[
\mathbb{E}[KR_{p,C}(\hat{\mu}_{t,s}, \mu)] \leq \mathcal{E}_{p,\mathcal{X},\mu}^{\text{PoI}}(C, q, L)^{1/p} \begin{cases} \left( \frac{2(1-s)}{s} M(\mu) + \frac{s}{\sqrt{q}} \sum_{x \in \mathcal{X}} \sqrt{\mu(x)} \right)^{1/p}, & \text{if } C \leq (2h_{q,L}(L) \lor \min_{x \neq x'} d(x, x')) \\ \left( \frac{1}{s} M(\mu) + \frac{1-s}{s} \sum_{x \in \mathcal{X}} \mu(x)^2 \right)^{\frac{1}{p}}, & \text{else.} \end{cases}
\]

For

\[
A_{q,p,L,\mathcal{X}}(l) := \text{diam}(\mathcal{X})^p 2^{p-1} \left( q^{-Lp} |\mathcal{X}| \right)^{1/2} + \left( \frac{q}{q-1} \right)^p \sum_{j=1}^{L} q^{p-jL} |Q_j|^{1/2},
\]

the constant is equal to

\[
\mathcal{E}_{p,\mathcal{X},\mu}^{\text{PoI}}(C, q, L) = \begin{cases} \left( \frac{C^p}{2} - 2^{p-1} \left( \frac{q^{-L}}{q-1} \text{diam}(\mathcal{X}) \right)^p \right) + A_{q,p,L,\mathcal{X}}(1), & \text{if } C \geq 2h_{q,L}(0), \\
A_{q,p,L,\mathcal{X}}(l), & \text{if } 2h_{q,L}(l) \leq C < 2h_{q,L}(l-1), \\
\frac{C^p}{2}, & \text{if } C \leq (2h_{q,L}(L) \lor \min_{x \neq x'} d(x, x')) \end{cases}
\]

Furthermore, for \(p = 1\) the factor \(\frac{q}{(q-1)}\) in \(A_{q,1,L,\mathcal{X}}(l)\) can be removed for all \(l = 1, \ldots, L\).

The constant \(\mathcal{E}_{p,\mathcal{X},\mu}^{\text{PoI}}(C, q, L)\) is reminiscent of the constants for similar deviation bounds for optimal transport between finitely supported measures [Boissard and Le Gouic, 2014, Sommerfeld et al., 2019]. However, in the case of UOT one finds an interesting case distinction into roughly three cases depending on the relation between the penalty parameter \(C\) of the \((p, C)\)-KRD and the resolution \(q\) and depth \(L\) of the tree approximation. The different constants arise from the fact that \(C\) controls the maximal range at which transport occurs in an UOT plan. In particular, if \(d(x, x') > C^p\), then for any UOT plan \(\pi\) it holds \(\pi(x, x') = 0\). If \(C\) is sufficiently large, i.e. larger than the diameter of \(\mathcal{X}\), then \(\mathcal{E}_{p,\mathcal{X},\mu}^{\text{PoI}}(C, q, L)\) coincides with the deviation bounds for usual optimal transport, however, there is an additional summand arising from the necessary estimation of the true total mass \(M(\mu)\). For sufficiently small \(C\), e.g. \(C < \min_{x \neq x'} d(x, x')\), the \((p, C)\)-KRD is proportional to the TV distance, hence we obtain a constant which is oblivious to the geometry of the ground space (see Lemma 2.5). For an intermediate value of \(C\), the UOT problem on the ultra-metric tree \(T\) decomposes into smaller problems on subtrees of \(T\) (for details see the proof of (12) in Heinemann et al. [2022a]) depending on \(C\). The expected \((p, C)\)-KRD error then depends on the size of these subtrees and the mass estimation error inherent to the total mass on these subtrees.
Hence, it suffices to show that
\[ \text{observe that each location.} \]
and then the strong law of large numbers guarantees the convergence of the weights at
\[ \text{However, for } s < 1, \text{ the error vanishes for } t \to \infty, \text{ as we observe all support points of } \mu \text{ and then the strong law of large numbers guarantees the convergence of the weights at each location.} \]
It remains to verify whether the rate in \( t > 1 \) and depth \( L \in \mathbb{N} \) is optimal. For this, fix \( s = 1 \) and observe that
\[ \min\{C, \min_{x \neq x'} d(x, x')\} PTV(\mu, \nu) \leq \text{KR}_p^C(\mu, \nu) \leq \min\{C, \text{diam}(\mathcal{X})\} PTV(\mu, \nu). \]

Hence, it suffices to show that \( t^{-1/2} \) is the optimal rate for the convergence in total variation distance. It holds
\[ \mathbb{E}[TV(\mu, \hat{\mu}_{t,1})] = \sum_{x \in \mathcal{X}} \mathbb{E}[|\mu(x) - \hat{\mu}_{t,1}(x)|] = \sum_{x \in \mathcal{X}} t^{-1} \mathbb{E}[|P_x - P_{x^t}|], \]
where \( P_x \sim \text{Poi}(\mu(x)t) \). Using the closed form solution of the mean absolute deviation of a Poisson random variable [Ramasubban, 1958] and Stirling’s formula, we obtain the asymptotic equivalence (in the sense that their ratio converges to one as \( t \to \infty \))
\[ \mathbb{E}[TV(\mu, \hat{\mu}_{t,1})] \approx \sum_{x \in \mathcal{X}} (t\mu(x))^{\mu(x)}(\mu(x)t)^{-1/2} \sqrt{\mu(x)} \sqrt{2/\pi}. \]
For \( t > \inf_{x \in \text{supp}(\mu)} \mu(x) \), this is bounded from below by
\[ \left( \sqrt{2/\pi} \sum_{x \in \mathcal{X}} \sqrt{\mu(x)} \right) t^{-1/2}. \]
All combined, the expectation \( \mathbb{E}[\text{KR}_p^C(\mu, \hat{\mu}_{t,1})] \) has a lower bound which is asymptotically equivalent to \( t^{-1/2} \) and hence the rate in \( t \) of Theorem 2.2 is sharp.

Remark 2.3. Since the deviation bound holds for any resolution \( q > 1 \) and depth \( L \in \mathbb{N} \) one can optimise and equivalently state upper bounds in terms of the infimum over those parameters. When the dependence on \( q \) or \( L \) is omitted, it is assumed that the infimum over those parameters has been taken, i.e.
\[ \mathcal{E}_{p,\mathcal{X},\mu}^{\text{Poi}}(C) = \inf_{L \in \mathbb{N}, q \geq 1} \mathcal{E}_{p,\mathcal{X},\mu}^{\text{Poi}}(C, q, L). \]
From the reverse triangle inequality we immediately obtain the following corollary from Theorem 2.2.

Corollary 2.4. Let \((\mathcal{X}, d)\) be a finite metric space and \( \mu, \nu \in \mathcal{M}_+(\mathcal{X}) \). Let \( \hat{\mu}_{t,1}, \hat{\nu}_{t,1} \) be the estimator from (8) for each of these measures, respectively. Then, for any \( p \geq 1 \), resolution \( q > 1 \) and depth \( L \in \mathbb{N} \) it holds that
\[ 2^{p-1} \mathcal{E}_{p,\mathcal{X},\mu}^{\text{Poi}}(C, q, L)^{1/p} \left\{ \begin{array}{ll}
2(1-s)M(\mu) + \frac{s}{diam(\mathcal{X})} \sum_{x \in \mathcal{X}} \sqrt{\mu(x)} \frac{1}{2p}, & \text{if } C < \min_{x,x' \in \mathcal{X}} d(x, x'), \\
(1-s)M(\mu) + \frac{1-s}{4} \sum_{x \in \mathcal{X}} \mu(x)^2 \frac{1}{2p}, & \text{else},
\end{array} \right. \]
where \( \mathcal{E}_{p,\mathcal{X},\mu}^{\text{Poi}}(C, q, L) \) is defined as in Theorem 2.2.
2.4 Explicit Bounds for Euclidean Spaces

While the constants in the previous theorem are valid on arbitrary metric spaces, more explicit bounds can be derived for many practical applications. Thus, assume that \( \mathcal{X} \subset \mathbb{R}^D \) and that \( d_{\infty}(x, x') = \max_{d=1, \ldots, D} |x_d - x'_d| \) be the uniform distance and \( \text{diam}_\infty(\mathcal{X}) \) be the diameter of \( \mathcal{X} \). Using the fact that

\[
d_2(x, x') \leq \sqrt{D}d_{\infty}(x, x'),
\]

we bound the \((p, C)\)-KRD with respect to the Euclidean distance by the \((p, C)\)-KRD with respect to the uniform distance at a price of a factor of \( \sqrt{D} \). In particular, we also apply this to the definition of the height function (13) given for \( q = 2 \) and any \( l \in \{0, \ldots, L\} \) by

\[
h_L(l) = \left(2^{1-l} - 2^{-L}\right)\text{diam}_\infty(\mathcal{X}).
\]

Within this framework, we can compute explicit upper bounds on the constants in Theorem 2.2. For \( D < 2p \) and \( L \to \infty \), it holds

\[
\mathcal{E}_{p, \mathcal{X}, \mu}^{\text{Poi}}(C) \leq D^{p/2} \begin{cases} 
\frac{C_p}{2\sqrt{D}} - 2^{2p-1}\text{diam}_\infty^p(\mathcal{X}) + \text{diam}_\infty^p(\mathcal{X})2^{3p-1}\frac{2^{D/2-p}}{1-2^{D/2-p}}, & \text{if } C \geq 2h_L(0), \\
\text{diam}_\infty^p(\mathcal{X})2^{3p-1}\frac{2^{(D/2-p)}}{1-2^{D/2-p}}, & \text{if } 2h_L(l) \leq C < 2h_L(l - 1), \\
\frac{C_p}{T}, & \text{if } C \leq \left(2h_L(L) \wedge \min_{x \neq x'} d_{\infty}(x, x')\right).
\end{cases}
\]

For \( D = 2p \) and \( L = \lceil \frac{1}{D} \log_2(|\mathcal{X}|) \rceil \), it holds

\[
\mathcal{E}_{p, \mathcal{X}, \mu}^{\text{Poi}}(C) \leq D^{p/2} \begin{cases} 
\frac{C_p}{2\sqrt{D}} - 2^{2p-1}\left(2 - |\mathcal{X}|^{-\frac{1}{p}}\right)^p\text{diam}_\infty^p(\mathcal{X}) + \text{diam}_\infty^p(\mathcal{X})2^{3p-1}(2^{-2p} + D^{-1}\log_2(|\mathcal{X}|)), & \text{if } C \geq 2h_L(0), \\
\text{diam}_\infty^p(\mathcal{X})2^{3p-1}(2^{-2p} + D^{-1}\log_2(|\mathcal{X}|) - l), & \text{if } 2h_L(l) \leq C < 2h_L(l - 1), \\
\frac{C_p}{T}, & \text{if } C \leq \left(2h_L(L) \wedge \min_{x \neq x'} d_{\infty}(x, x')\right).
\end{cases}
\]
For $D > 2p$ and $L = \lceil \frac{1}{2} \log_2 (|\mathcal{X}|) \rceil$, it holds

$$
E_{\text{Poi}, X, \mu} (C) \leq \frac{C p}{2} - 2^{p-1} \left( 2 - \left\lceil \frac{1}{2} \frac{1}{L} \right\rceil \right)^p \text{diam}_{\infty}^p (\mathcal{X})
$$

$$
+ \text{diam}_{\infty}^p (\mathcal{X}) 2^{p-1} |\mathcal{X}|^{\frac{1}{2} - \frac{1}{p}} \left( 1 + \frac{2^{p} + D/2}{2^{D/2 - p} - 1} \right),
$$

if $C \geq 2h_L(0)$,

$$
\text{diam}_{\infty}^p (\mathcal{X}) \left( \left| \mathcal{X} \right|^{\frac{1}{2} - \frac{1}{p}} \right)
$$

$$
+ \frac{2^{p} + D/2}{2^{D/2 - p} - 1} \left( \left| \mathcal{X} \right|^{\frac{1}{2} - \frac{1}{p}} - 2^{(D/2 - p)}(l-1) \right),
$$

if $2h_L(l) \leq C < 2h_L(l - 1)$,

$$
\frac{C p}{2},
$$

if $C \leq (2h_L(L) \wedge \min_{x \neq x'} d_{\infty}(x, x'))$.

These bounds distinguish cases, based on the value of the penalty $C$, as well as the dimension $D$. The most critical part of these bounds is the impact of the cardinality of $\mathcal{X}$. If $D < 2p$, then there is no dependence on $|\mathcal{X}|$ and the convergence of approximation error of the empirical measure is independent of its support size. If $D = 2p$, then $|\mathcal{X}|$ enters through a logarithmic term. If $D > 2p$, then the dependence becomes polynomial in $|\mathcal{X}|$. These phase transitions for the dependence on the support size match those for empirical optimal transport [Sommerfeld et al., 2019]. A novelty for the UOT setting is the additional dependency on the different scales of $C$. This is explained by the previously discussed control of $C$ on the maximal distance at which transport occurs in an optimal plan. The height function is again used to specify the scale induced by a particular choice of the parameter $C$. Notably, the dependence on $|\mathcal{X}|$ does not change on most scales of $C$. There is an exception, however, for sufficiently small values of $C$, where the $(p, C)$-KRD is equal to a scaled total variation distance. Thus, these bounds are completely oblivious to the geometry of $\mathcal{X}$ in $\mathcal{Y}$, though they scale as $\left| \mathcal{X} \right|^{\frac{1}{2} - \frac{1}{p}}$ which is the same rate we obtain for the TV bound (recall lemma 2.5). As a final observation, we note that for $C > 2h_L(0)$, these bounds essentially recover analogue bounds for empirical optimal transport [Sommerfeld et al., 2019]. However, for the $(p, C)$-KRD the bounds include an additional summand based on the estimation error for the measure’s total mass intensity.

### 2.5 Proofs

As a preparatory step to prove Theorem 2.2, we treat the significantly simpler case of an empirical deviation bound with respect to the total variation distance.

**Lemma 2.5** (Total Variation Bound). Let $(\mathcal{X}, d)$ be a finite metric space and $\mu \in \mathcal{M}_+(\mathcal{X})$ with total mass $M(\mu)$. Let $\hat{\mu}_{t,s}$ be the estimator from (8). Then, for any $p \geq 1$ it holds that

$$
E \left[ K^{p}_{p,C} (\hat{\mu}_{t,s}, \mu) \right] \leq \frac{C p}{2} \left( 2(1 - s)M(\mu) + \frac{s}{\sqrt{t}} \sum_{x \in \mathcal{X}} \sqrt{\mu(x)} \right).
$$

**Proof.** Let $\mu, \nu \in \mathcal{M}_+(\mathcal{X})$. By retaining all common mass between $\mu$ and $\nu$ at place and delete (resp. create) excess mass (resp. deficient mass) we obtain a feasible solution for (2) with objective value in terms of a total variation distance between $\mu$ and $\nu$. Thus, it
holds

\[ \text{KR}_{p,C}^p(\mu, \nu) \leq \frac{C^p}{2} \text{TV}(\mu, \nu). \]

In particular, this holds for \( \nu = \hat{\mu}_{t,s} \). Taking expectations yields

\[
\mathbb{E}[\text{TV}(\hat{\mu}_{t,s}, \mu)] = \frac{1}{st} \sum_{x \in \mathcal{X}} \mathbb{E}[|P_x B_x - st \mu(x)|]
\]

\[
= \frac{1}{st} \sum_{x \in \mathcal{X}} s \mathbb{E}[|P_x - st \mu(x)|] + (1 - s) st \mu(x)
\]

\[
\leq \frac{1}{st} \sum_{x \in \mathcal{X}} s(1 - s) \mathbb{E}[P_x] + s^2 \mathbb{E}[|P_x - t \mu(x)|] + (1 - s) st \mu(x)
\]

\[
\leq \frac{1}{st} \sum_{x \in \mathcal{X}} 2s(1 - s) t \mu_x + s^2 \sqrt{t} \sqrt{\mu(x)}
\]

\[
= 2(1 - s) \mathbb{M}(\mu) + \frac{s}{\sqrt{t}} \sum_{x \in \mathcal{X}} \sqrt{\mu(x)}.
\]

With Lemma 2.1 and Lemma 2.5 at our disposal we are able to prove Theorem 2.2.

**Proof of Theorem 2.2.** Let \( \hat{\mu}_{t,s} \) be the estimator from (8). We fix \( p = 1 \) and detail the case \( p > 1 \) at the end of the proof. Suppose first that \( C \leq \min_{x \neq x'} d(x, x') \). According to [Heinemann et al., 2022a, Theorem 2.2 (ii)] it holds that

\[
\mathbb{E}[\text{KR}_{1,C}(\hat{\mu}_{t,s}, \mu)] = C^2 \mathbb{E} \left[ \sum_{x \in \mathcal{X}} |\hat{\mu}_{t,s} - \mu(x)| \right] = \frac{C}{2} \mathbb{E}[\text{TV}(\hat{\mu}_{t,s}, \mu)].
\]

This yields the total variation bounds (see Lemma 2.5). Next, consider the tree approximation as outlined in Section 2.1 and construct an ultrametric tree \( T \) such that \( \text{KR}_{1,C}(\hat{\mu}_{t,s}, \mu) \leq \text{KR}_{d_T,C}(\hat{\mu}_{L,s}, \mu^L) \). Applying Lemma 2.1 for \( p = 1 \) where by definition the difference of height function is equal to

\[
h_{q,L}(j - 1) - h_{q,L}(j) = \frac{\text{diam}(\mathcal{X})}{q - 1} (q^2 - q^{2j}) = \text{diam}(\mathcal{X})q^{1-j}
\]

and yields the upper bound

\[
\mathbb{E}[\text{KR}_{1,C}(\hat{\mu}_{t,s}, \mu)] \leq \mathbb{E}[\text{KR}_{d_T,C}(\hat{\mu}_{L,s}, \mu^L)]
\]

\[
= \begin{cases}
\left( \frac{C}{2} - h_{q,L}(0) \right) \mathbb{E} \left[ |\mathbb{M}(\hat{\mu}_{t,s}) - \mathbb{M}(\mu)| \right] \\
+ \text{diam}(\mathcal{X}) \sum_{j=1}^{L+1} q^{-j} \sum_{x \in \mathcal{X}_j} \mathbb{E} \left[ |\hat{\mu}_{t,s}(C(x)) - \mu^L(C(x))| \right], & C \geq 2h_{q,L}(0) \\
\text{diam}(\mathcal{X}) \sum_{j=1}^{L+1} q^{-j} \sum_{x \in \mathcal{X}_j} \mathbb{E} \left[ |\hat{\mu}_{L,s}(C(x')) - \mu^L(C(x'))| \right], & 2h_{q,L}(l) \leq C < 2h_{q,L}(l - 1), \\
\frac{C^p}{2} \mathbb{E}[\text{TV}(\hat{\mu}_{t,s}, \mu)], & C \leq (2h_{q,L}(L) \vee \min_{x \neq x'} d(x, x')).
\end{cases}
\]
For the estimator from (8) with \( B_x \sim \text{Ber}(s) \) and \( P_x \sim \text{Poi}(t\mu(x)) \) for all \( x \in \mathcal{X} \), it holds
\[
\sum_{x \in Q_t} \mathbb{E} \left[ |\hat{\mu}_{t,s}(C(x)) - \mu^L(C(x))| \right] = \sum_{x \in Q_t} \frac{1}{st} \mathbb{E} \left[ \left| \sum_{y \in C(x)} P_y B_y - st \sum_{y \in C(x)} \mu(y) \right| \right] \leq \sum_{x \in Q_t} \frac{1}{st} \sqrt{\text{Var} \left( \sum_{y \in C(x)} P_y B_y \right)}
\]
\[
= \sum_{x \in Q_t} \frac{1}{st} \sqrt{\sum_{y \in C(x)} \text{Var}(P_y B_y)}
\]
\[
= \sum_{x \in Q_t} \frac{1}{st} \sqrt{\sum_{y \in C(x)} s(1-s)t\mu(y) + s(1-s)\mu(y)^2 + t\mu(y)s^2}
\]
\[
= \sum_{x \in Q_t} \frac{1}{st} \sqrt{\sum_{y \in C(x)} \mu(y) + \frac{1-s}{s} \sum_{y \in C(x)} \mu(y) + \frac{1}{t} \sum_{y \in C(x)} \mu(y)}
\]
\[
= \sum_{x \in Q_t} \frac{1}{st} \sqrt{\mu(C(x)) + \frac{1-s}{s} \sum_{y \in C(x)} \mu(y)^2}
\]
\[
\leq \sqrt{|Q_t|} \frac{1}{st} \sum_{x \in Q_t} \mu(C(x)) + \frac{1-s}{s} \sum_{x \in Q_t} \sum_{y \in C(x)} \mu(y)^2
\]
\[
= \sqrt{|Q_t|} \frac{1}{st} \mathbb{M}(\mu) + \frac{1-s}{s} \sum_{x \in \mathcal{X}} \mu(x)^2
\]

Following an analogous computation one bounds the estimation error for the total mass intensity as
\[
\mathbb{E} \left[ |\mathbb{M}(\hat{\mu}_{t,s}) - \mathbb{M}(\mu)| \right] \leq \sqrt{\text{Var}(\mathbb{M}(\hat{\mu}_{t,s}))} \leq \sqrt{\mathbb{E} \left[ \frac{1}{st} \mathbb{M}(\mu) + \frac{1-s}{s} \sum_{x \in \mathcal{X}} \mu(x)^2 \right]}.
\]

Applying both of these bounds to the previous upper bound on the \((p,C)\)-KRD in Lemma 2.1 yields the claim.

For \( p > 1 \), we first observe again that if \( C \leq \min_{x \neq x'} d(x, x') \) then according to Heinemann et al. [2022a] it holds that
\[
\mathbb{E} \left[ \text{KR}_{p,C}^p(\hat{\mu}_{t,s}, \mu) \right] = \frac{C^p}{2} \mathbb{E} \left[ \text{TV}(\hat{\mu}_{t,s}, \mu) \right]
\]
which yields the total variation bounds. For more general \( C \), we simply repeat the previous calculations with the upper bounds on the difference of height function \( h_{q,L}(j - 1)^p - h_{q,L}(j)^p \leq \text{diam}(\mathcal{X})^p \left( \frac{q}{q-1} \right)^p q^{p-jp} \). Since \( h_{q,L}(L+1) = 0 \) we also have \( h_{q,L}(L)^p - h_{q,L}(L+1)^p = \text{diam}(\mathcal{X})^p q^{-Lp} \). The expectations are bounded identically as before. Finally, using Jensen’s inequality to bound
\[
\mathbb{E} \left[ \text{KR}_{p,C}(\mu, \hat{\mu}_{t,s}) \right] \leq \left( \mathbb{E} \left[ \text{KR}_{p,C}^p(\mu, \hat{\mu}_{t,s}) \right] \right)^{\frac{1}{p}}
\]
finishes the proof. \( \square \)
Then, for Theorem 3.1. Let $p, C$ the mean absolute deviation of $(p, C)$ between a measure and its empirical version is used to achieve control on $\infty_{J, \mu, q, L}$ in the appendix. The previous upper bound on the Kantorovich-Rubinstein distance in (8). We again focus on the Poisson model and treat the remaining two models as defined in (8). We denote $\hat{\mu}^t \in \arg\min_{\mu \in \mathcal{M}_+(\mathcal{X})} \frac{1}{J} \sum_{i=1}^J \text{KR}_{p, C}^p(\mu^i, \mu)$ and measure the accuracy of approximation of $\mu^*$ by $\hat{\mu}^*$ in terms of their mean absolute $p$-Fréchet deviation.

**Theorem 3.1.** Let $\mu^1, \ldots, \mu^J \in \mathcal{M}_+(\mathcal{X})$ and denote $\mathcal{X}_i = \text{supp}(\mu^i)$ for $i = 1, \ldots, J$. Consider random estimators $\hat{\mu}^i \in \mathcal{M}_+(\mathcal{X})$ derived from (8). Then,

$$\mathbb{E} \left[ \left| \sum_{i=1}^J \text{KR}_{p, C}^p(\mu^i, \mu) - \sum_{i=1}^J \text{KR}_{p, C}^p(\hat{\mu}^i, \mu) \right| \right] \leq \frac{2p \min\{diam(\mathcal{X}), C\}^{p-1}}{J} \sum_{i=1}^J \mathcal{E}_{\mathcal{P}, i, \mu_i}(C) \phi(t_i, s_i),$$

where $\phi$ is given by

$$\phi(t, s) = \begin{cases} \frac{2(1 - s)\mathbb{M}(\mu) + \frac{s}{\sqrt{J}} \sum_{x \in \mathcal{X}} \sqrt{x} \mu(x)}{J}, & \text{if } C \leq \frac{2h_{q, L}(L) \min_{x \neq x'} d(x, x')}{\sqrt{J}}; \\ \frac{1}{2s} \mathbb{M}(\mu) + \frac{1 - s}{\sqrt{J}} \sum_{x \in \mathcal{X}} \mu(x)^2, & \text{else.} \end{cases}$$

A more elaborate statement gives control over the set of empirical $(p, C)$-barycenters itself. This involves a related linear program that is presented in detail in Appendix C.

**Theorem 3.2.** Let $\mu^1, \ldots, \mu^J \in \mathcal{M}_+(\mathcal{X})$ and denote $\mathcal{X}_i = \text{supp}(\mu^i)$ for $i = 1, \ldots, J$. Consider random estimators $\hat{\mu}^i \in \mathcal{M}_+(\mathcal{X})$ derived from (8). Let $\mathcal{B}^*$ be the set of $(p, C)$-barycenters of $\mu^1, \ldots, \mu^J$ and $\mathcal{B}^*$ the set of $(p, C)$-barycenters of $\hat{\mu}^i \in \mathcal{M}_+(\mathcal{X})$. Then, for $p \geq 1$ it holds that

$$\mathbb{E} \left[ \sup_{\hat{\mu}^* \in \mathcal{B}^*} \inf_{\mu^* \in \mathcal{B}^*} \text{KR}_{p, C}^p(\mu^*, \mu^*) \right] \leq \frac{2p \min\{diam(\mathcal{X}), C\}^{p-1}}{V_p J} \sum_{i=1}^J \mathcal{E}_{\mathcal{P}, i, \mu_i}(C) \phi(t_i, s_i),$$

where $\phi$ is defined as in Theorem 3.1. The constant $V_p$ is strictly positive and given by

$$V_p := V_p(\mu^1, \ldots, \mu^J) := (J + 1)\text{diam}(\mathcal{X})^{-p} \min_{v \in V \setminus V^*} \frac{c^T v - f^*}{d_1(v, \mathcal{M})},$$

where $V$ is the set of feasible vertices from the linear program in Appendix C, $V^*$ is the subset of optimal vertices, $c$ is the cost vector of the program, $f^*$ is the optimal value, $\mathcal{M}$ is the set of minimisers of the linear program (19) and $d_1(x, \mathcal{M}) = \inf_{y \in \mathcal{M}} \|x - y\|_1.$
The proofs of Theorem 3.1 and Theorem 3.2 are deferred to Appendix D.

**Remark 3.3.** For $J = 1$ and any $p \geq 1, C > 0$ the $(p,C)$-barycenter of $\mu^1$ is just $\mu^1$. Thus, the optimal value of the Fréchet functional is zero and it holds

$$F(\hat{\mu}^*) - F(\mu^*) = KR_{p,C}^p(\mu^1, \hat{\mu}^1_t,s).$$

Consequently, it also holds

$$\sup_{\hat{\mu}^* \in B^*} \inf_{\mu^* \in B^*} KR_{p,C}^p(\mu^*, \hat{\mu}^*) = KR_{p,C}^p(\mu^1, \hat{\mu}^1_t,s).$$

Thus, the rate for the convergence of the $(p,C)$-barycenter of the empirical measures, can in general not be faster than the convergence rate of a single estimator. In particular, the rates in $t$ in Theorem 3.1 and Theorem 3.2 are sharp.

4 Simulations

In this section we investigate empirically the decay in the expected error for the Poisson model for measures within $X \subset [0,1]^2$. For the $(p,C)$-KRD we consider two measures $\mu, \nu \in M_+(X)$ and the relative $(p,C)$-KRD error

$$\mathbb{E} \left[ \frac{KR_{p,C}(\hat{\mu}_t,s, \hat{\nu}_t,s) - KR_{p,C}(\mu, \nu)}{KR_{p,C}(\mu, \nu)} \right].$$

For the setting of barycenters we consider the relative $(p,C)$-Fréchet error

$$\mathbb{E} \left[ \frac{F_{p,C}(\hat{\mu}^*) - F_{p,C}(\mu^*)}{F_{p,C}(\mu^*)} \right].$$

In both cases, the relative error allows for easier comparisons between models than the absolute error. Additionally, for the $(p,C)$-barycenter (17) is readily available from simulations, while numerically considering the quantity in Theorem 3.2 is difficult, as it requires all optimal solutions instead of a single one. All computations of the KRD and the $(p,C)$-barycenter in this section are performed using the methods available in the CRAN package **WSGeometry**.

4.1 Synthetic Datasets

We consider eight types of measures for our simulations. Let us fix some notation. Let $J \in \mathbb{N}$ be the number of measures generated. Let $U[0,1]^2$ denote the uniform distribution and let $\text{Poi}(\lambda)$ denote a Poisson distribution with intensity $\lambda$. In all eight settings considered below, the measures are of the form

$$\mu^i = \sum_{k=1}^{K_i} w_k^i \delta_{l_k^i}$$

for some weights $w_k^i$, locations $l_k^i$ and $K_i \in \mathbb{N}$. If $K_i = K_j$ for all $i,j = 1, \ldots, J$, then we omit the index and denote the number of points by $K$. Note, that all measures have been constructed to have their support included in $[0,1]^2$.

**Poisson Intensities on Uniform Positions (PI), see Figure 5 (a)**

Let $w_1^i, \ldots, w_K^i \sim \text{Poi}(\lambda)$ for some intensity $\lambda > 0$ and $l_1^i, \ldots, l_K^i \sim U[0,1]^2$ for $1 \leq i \leq J$. 

\[\text{We define } 0/0 := 0.\]
Poisson Intensities on a Grid (PIG), see Figure 5 (b)

Set $K = M^2$ for $M \in \mathbb{N}$ and let $w^1_i, \ldots, w^i_{M^2} \sim \text{Poi}(\lambda)$ and $l^1_i, \ldots, l^i_{M^2}$ be the location of an equidistant $M \times M$ grid in $[0,1]^2$ for $1 \leq i \leq J$.

Norm-based Intensities on Uniform Positions (NI), see Figure 6 (a)

Fix $J$ locations $l^1_0, \ldots, l^j_0 \in [0,1]^2$. Let $l^1_i, \ldots, l^i_K \sim U[0,1]^2$ and let $w^i_k = \|l^i_k - l^i_0\|_2$ for $1 \leq i \leq J$.

Norm-based Intensities on a Grid (NIG), see Figure 6 (b)

Let $K = M^2$ for $M \in \mathbb{N}$. Fix $J$ locations $l^1_0, \ldots, l^j_0 \in [0,1]^2$ and let $l^1_i, \ldots, l^i_{M^2}$ be the location of an equidistant $M \times M$ grid in $[0,1]^2$ for each $1 \leq i \leq J$. Set $w^i_k = \|l^i_k - l^i_0\|_2$ for $1 \leq i \leq J$.

Clustered Nested Ellipses (NEC), see Figure 7 (b)

Let $G^c_1, \ldots, G^c_J \sim \text{Poi}(\lambda^c)$ for $c = 1, \ldots, 5$. Let $\lambda_3 = 2$ and set $\lambda_c = 1$ else. Let $K_i = M \sum_{c=1}^5 G^c_i$. Set $w^i_k$ equal to 1 for $1 \leq k \leq K_i$ for $i = 1, \ldots, J$. Let $t_1, \ldots, t_M$ be a
discretisation of $[0, 2\pi]$. Let $U_1^i, \ldots, U_K^i, V_1^i, \ldots, V_K^i \sim U[0, 2, 1]$. Let $\alpha = (2, 12, 12, 22, 12)^T$ and $\beta = (12, 2, 12, 12, 22)^T$. Set for $c = 1, \ldots, 5$ and $j_i = 0, \ldots, G_i$

$$\hat{t}_M^{i}(\sum_{r=1}^{G_i} U_r^{i} + M(j_i-1)+k) = \frac{1}{24}((3^{-j} U_{M(j_i-1)+k} \sin(t_k) + \alpha_c, 3^{-j} V_{M(j_i-1)+k} \cos(t_k) + \beta_c))^T,$$

where we use the convention that a sum is zero if its last index is smaller than its first one.

Figure 7: (a) An example of $J = 8$ measures from the NE dataset with $M = 200$. (b) An example of $J = 8$ measures from the NEC dataset with $M = 95$.

Spirals of varying Length (SPI), Figure 8 (a)

Let $a_i \sim U[2, 4]$ and $b_i \sim U[3, 6]$ for $i = 1, \ldots, J$. Let $K_i = [b_i M]$ and let $t_1, \ldots, t_K$ be a discretisation of $[0, b\pi]$. Set $w_k^i = 1$ for $k = 1, \ldots, K_i$ and $i = 1, \ldots, J$. Set

$$l_k^i = a_i((t_k \sin(t_k) + 64)/140, (t_k \cos(t_k) + 70)/130)^T.$$

Clustered Spirals (SPIC), see Figure 8 (b)

Let $a_i^c \sim U[2, 4]$ and $b_i^c \sim U[3, 6]$ for $i = 1, \ldots, J$, $c = 1, \ldots, 5$. Let $K_i^c = [b_i^c M]$ and let $t_1, \ldots, t_K$ be a discretisation of $[0, b\pi]$. Set $w_k^i = 1$ for $k = 1, \ldots, K_i$ and $i = 1, \ldots, J$ and let $\alpha = (0, 3, 3, 6, 3)^T$ and $\beta = (3, 0, 3, 3, 6)^T$. Set

$$\hat{l}_k^i = \frac{1}{7}(((a_i^c t_k \sin(t_k) + 64)/140) + \alpha_c, (a_i^c t_k \cos(t_k) + 70)/130 + \beta_c)^T,$$

where we again use the convention that a sum is zero if its last index is smaller than its first one.

Figure 8: (a) An example of $J = 8$ measures from the SPI dataset with $M = 110$. (b) An example of $J = 8$ measures from the SPIC dataset with $M = 22$. 

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Figure 9: Expected relative $(2, C)$-KRD error for two measures in the Poisson sampling model for the NE class and different success probabilities $s$. For each pair of success probability $s$ and observation time $t$ the expectation is estimated from 1000 independent runs. Set $M = 100$. From top-left to bottom-right we have $C = 0.01, 0.1, 1, 10$, respectively.

Figure 10: As in Figure 9, but for the NEC class and $M = 75$. 

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4.2 Simulation Results for the $(2, C)$-Kantorovich-Rubinstein Distance

In the following, we discuss the results from our simulation studies for the Poisson model for the $(2, C)$-KRD between two measures within one of the eight classes of measures introduced above. Note, that for brevity the plots for some of the classes have been omitted to Appendix E and exemplary the classes PI, NE and NEC are discussed. The remaining plots in the Figures 20, 21, 22, 23 and 24 are found in Appendix E.

For the error of the NE class in Figure 9 it can be seen that the error is decreasing in $s$ and $t$, but increasing in $C$. Both of these behaviours are in line with the bound in Theorem 2.2. The decrease of the error for increasing $s$ and $t$ is immediately clear from our theoretical results. The increase of error for increasing $C$ is based on the fact that in the Poisson model the population total intensities of $\mu$ and $\nu$ are unknown and have to be estimated from the data. The $(p, C)$-KRD penalises mass deviation with a factor scaling with $C$, so naturally for increasing $C$, the errors in the estimation of the true difference of masses yields an increase in the expected relative $(p, C)$-KRD error. Notably, while the decrease in $s$ and $t$ is similar for the error of the NEC class in Figure 10, the error is no longer increasing in $C$. Instead the errors increase from $C = 0.01$ to $C = 0.1$, but then decrease going to $C = 1$. Afterwards they increase again at $C = 10$. This difference in behaviour is explained by the cluster structure of the measure in NEC. There is still the general trend of increasing error for increasing $C$, as present in the NE class, but now there is an additional change in behaviour based on the fact if transport occurs within clusters or between clusters. From $C = 0.1$ to $C = 1$, we pass the size of the clusters and the distance between the clusters. Thus, $C = 1$ is the first value in our simulation for which inter-cluster transports can occur. This causes a decrease in error, as the impact of the estimation of the total mass intensity of a measure within one cluster is decreased. After this point the usual increase in error for increasing $C$ due to the estimation of the total mass intensity occurs again. For the $(p, C)$-KRD error in the PI class in Figure 11 this effect is particularly strong. The error increases on average about two orders of magnitude from $C = 0.01$ to $C = 10$. This is explained by the fact that the total mass intensity in this class is significantly larger than for the classes NE and NEC, where each location in the support of the measures has mass one. This also causes an increase of the variance of the mass of the empirical measures at each location, which causes a faster increase of error for increasing $C$ at all scales of $C$. 

Figure 11: As in Figure 9, but for the PI class and $M = 450$. 

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Figure 12: Expected relative Fréchet error for the \((2, C)\)-barycenter for \(J = 5\) measures from the NE class in the Poisson sampling model with different success probabilities \(s\). For each pair of success probability \(s\) and observation time \(t\) the expectation is estimated from 100 independent runs. Set \(M = 100\). From left to right we have \(C = 0.1, 1, 10\), respectively.

Figure 13: As in Figure 12, but for the NEC class and \(M = 75\).

4.3 Simulation Results for the \((2, C)\)-Barycenter

It remains to discuss the results from our simulation studies for the Poisson model for the \((2, C)\)-barycenter between sets of measures within one of the eight classes of measures introduced above. We again exemplary discuss the classes NE, NEC and PI. The remaining plots in the Figures 25, 26, 27, 28 and 29 are found in Appendix E. We also restrict our analysis to the values of \(C = 0.1, 1, 10\), since for \(C = 0.01\) the \((p, C)\)-KRD is close to the TV distance. In particular, for all classes except PIG and NIG, where all measures share the same support grid, the \((2, C)\)-barycenter will be close or identical to the zero measure, since the measures in the other classes are almost surely disjoint. Additionally, if the barycenter of the population measures is the zero measure, any empirical barycenter has mass zero as well. Thus, there is little merit in simulating the barycenters in these cases. For the classes NIG and PIG the barycenters are essentially TV-barycenters for small \(C\) which removes any geometrically interesting features from the barycenter. Finally, for extremely small values of \(C\) the \((p, C)\)-barycenter computations tend to become numerically unstable due to either involving values close to machine accuracy and UOT plans for this values of \(C\) often being close to the zero measure. Hence, empirical simulations of the expected relative Fréchet error would also be less reliable in this regime of values for \(C\). In summary, empirical analysis of the properties of the \((p, C)\)-barycenter for values of \(C\) which are several orders of magnitude smaller than the diameter of \(\mathcal{Y}\) is inadvisable.

For the relative Fréchet errors we observe significant changes in behaviour compared to the relative \((p, C)\)-KRD before. Considering the error for the NE class in Figure 12, we note that for \(C = 0.1\) the behaviour in \(s\) and \(t\) is different than for the \((p, C)\)-KRD. Namely, for fixed \(s\), the error is in general not strictly decreasing in \(t\) and vice versa for fixed \(t\), the error is not always strictly decreasing in \(s\). This is an interesting effect arising for small values of the product \(st\). A point \(y \in \mathcal{Y}\) can only be a support point of a \((p, C)\)-barycenter if it is in the intersection of at least \(J/2\) balls of size \(Cp/2\) around support points of different measures (compare the construction of the centroid set in (5)). Now, for small \(s\) and \(t\) many support points of the population barycenter are not included in the support of the empirical one, since centroid set of the empirical measures is significantly smaller than the population level one. In particular, this can create situations where an increase in \(s\) or \(t\) on average adds support points to empirical barycenter, which cause the
relative error to increase, since placing mass zero at this location, for small $C$, is actually better than placing a potentially larger mass (since we assumed $(ts)^{-1}$ to be relatively small) at this location. Thus, while asymptotically, the rate in Theorem 3.1 is optimal, for certain, sufficiently small, values of $s$, $t$ and $C$, the behaviour of the relative Fréchet error might be counter-intuitive. For $C = 0.1$ and $C = 1$, the errors behave quite similarly to the $(p,C)$-KRD setting, though there is essentially no increase in error going from $C = 1$ to $C = 10$. This is explained by two points. First, the location of the $(p,C)$-barycenter tends to be more centred within the support of the measures (all measures are support on subsets of the unit square), so little transport between the barycenter and the $\mu_i$ occurs at a distance larger than one. Second, the key factor for the increasing error for increasing $C$ in the $(p,C)$-KRD case is the estimation error for the total mass intensities. However, for sufficiently large $C$ the mass of the $(p,C)$-barycenter is the median of the total masses of the $\mu_i$. Since, this quantity is significantly more stable under estimation than the individual total mass intensities, it is to be expected that the mass estimation has little effect on the relative Fréchet error. For the error of the NEC class in Figure 13 the results are similar to the NE case. We observe similar effects on the dependence of $s$ and $t$ for $C = 0.1$ and for $C = 1$ and $C = 10$, the errors look extremely similar. One notable distinction is the fact that from $C = 0.1$ to $C = 1$ the errors decrease on average. As before for the NEC class in the $(p,C)$-KRD setting, this can be explained by its cluster structure and $C = 1$ being the first value for which inter-cluster transport becomes possible in an UOT plan. This is therefore also the first value of $C$ which allows the $(p,C)$-barycenter to have mass between clusters. Finally, for the error of the PI class in Figure 14 the value of $C$ only has a minimal effect on the resulting errors. Notably and contrary to the two prior classes, we do not encounter any additional effects for $C = 0.1$. This is explained by the in general higher mass intensities of the measures in the PI class, which make the previously described effects due to low values of $s$ and $t$ less likely. Additionally, these measures do not possess any geometrical structures in their support, which could impact the behaviour on different scales. There is again little increase in error for increasing $C$, which is in stark contrast to the PI class in the $(p,C)$-KRD setting, where the error increased by multiple orders of magnitude. This is another strong indicator, that the Fréchet error is significantly more stable under $C$, due to the stability of total mass intensity of the empirical barycenter as opposed to the total mass intensity of the individual measures.

4.4 Real Data Example

In Figure 15 we consider the $(2,0.1)$-KRD between images which are an excerpt from STED microscopy of adult human dermal fibroblast cells (for the full dataset see Tameling et al. [2021]). The images in the Figures 15(a),(b) and Figures 15(c),(d) are visually similar, as they correspond to measurements taken based on two different markers (one at the inner mitochondrial membrane and one at the outer) in the same cells. The $(2,0.1)$-KRD captures this fact in the sense, that the pairwise distance between the measures are smallest for these pairs of images. Utilising UOT on this type of datasets is a potential way of quantifying dissimilarity between the respective measures and extending OT based
dissimilarity analysis to measures of unequal total intensity (the total mass intensities in this examples lies roughly between 6200 and 9500.

We further want to use this dataset to illustrate the performance of the randomised computational approach for the \((p, C)\)-KRD based on the multinomial model (recall (6)). The \(300 \times 300\) images here are specifically chosen such that the true distances can still be computed which allows to compare the expected error of the empirical \((p, C)\)-KRD for given sample sizes on this data set. We compare the results obtained from the resampling approach (i.e. the estimator from (6)) considered in the multinomial model to the subsampling approach (i.e. the estimator from (9)) obtained by sampling without replacement from the measures instead. In these simulations the maximum sample size is about \(1/5\) of the support sizes. This corresponds to a runtime of about 2.5% of the original problem size. While it is clear by construction that for sufficiently large sample sizes, subsampling yields a smaller error than the resampling (as the error approaches zero if the sample size approaches the support size), for smaller sample sizes the resampling can have a better performance. It yields a relative error below 5% at less than 10% of the original support size in all considered instances. This approximation can be achieved in around 0.5% of the original runtime. The subsampling approach does not reach this level of accuracy for the considered sample sizes. Thus, these simulations suggest that randomised computations based on the multinomial model allow for high accuracy approximations of the \((p, C)\)-KRD in real data applications at a significantly lower computational cost than the original problem and that for small sample sizes there are scenarios where the resampling approach yields significantly better performance than the subsampling one.

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Figure 15: (a)-(d): Excerpts of size $300 \times 300$ from the STED microscopy data of adult Human Dermal Fibroblasts in Tameling et al. [2021]. The images have on average about 25000 non-zero pixels. (a) and (c) have been labelled at MIC60 (a mitochondrial inner membrane complex); (b) and (d) have been labelled at TOM20 (translocase of the outer mitochondrial membrane).

(e)-(j): The relative error for the empirical $(2,0.1)$-KRD (obtained from resampling and subsampling) between the four filament structures in (a)-(d) considered as measures in $[0,1]^2$. (e) Between (a) and (b). (f) Between (a) and (c). (g) Between (a) and (d). (h) Between (b) and (c). (i) Between (b) and (d). (j) Between (c) and (d).
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A  Bounds for the Multinomial Model

In this section we provide results analogue to Theorem 2.2, Theorem 3.1 and Theorem 3.2 for the estimator in the multinomial model in (6). The proofs only differ in the way the respective expectations are bounded, so whenever suitable, we only provide these differences in the proofs.

**Lemma A.1 (Total Variation Bound).** Let $(\mathcal{X}, d)$ be a finite metric space and $\mu \in \mathcal{M}_+(\mathcal{X})$ with total mass $\mathcal{M}(\mu)$. Let $\hat{\mu}_N$ be the estimator from (6). Then, for any $p \geq 1$ it holds that

$$
\mathbb{E}\left[\text{KR}^p_{p,C}(\hat{\mu}_N, \mu)\right] \leq \left(\frac{Cp}{2} \sqrt{\mathcal{M}(\mu)} \sum_{x \in \mathcal{X}} \sqrt{\mu(x)}\right) N^{-\frac{1}{q}}.
$$

**Proof.** This proof is identical to the proof of Lemma 2.5 except for the bound on the expectation. For this, we note

$$
\mathbb{E}[\text{TV}(\hat{\mu}_N, \mu)] = \sum_{x \in \mathcal{X}} \mathbb{E}[|\hat{\mu}_N(x) - \mu(x)|]
$$

$$
= \frac{\mathcal{M}(\mu)}{N} \sum_{x \in \mathcal{X}} \mathbb{E}\left[\sum_{i=1}^N 1\{X_i = x\} - N \frac{\mu(x)}{\mathcal{M}(\mu)}\right]
$$

$$
\leq \frac{\mathcal{M}(\mu)}{N} \sum_{x \in \mathcal{X}} \sqrt{N} \frac{\mu(x)}{\mathcal{M}(\mu)} \left(1 - \frac{\mu(x)}{\mathcal{M}(\mu)}\right) \leq N^{-\frac{1}{q}} \sqrt{\mathcal{M}(\mu)} \sum_{x \in \mathcal{X}} \sqrt{\mu(x)},
$$

where the inequality follows from the fact the $X_i \sim \text{Ber}\left(\frac{\mu(x)}{\mathcal{M}(\mu)}\right)$ for $i = 1, \ldots, N$.  \[\square\]

**Theorem A.2.** Let $(\mathcal{X}, d)$ be a finite metric space and $\mu \in \mathcal{M}_+(\mathcal{X})$ with total mass $\mathcal{M}(\mu)$. Let $\hat{\mu}_N$ be the estimator from (6). Then, for any $p \geq 1$, resolution $q > 1$ and depth $L \in \mathbb{N}$ it holds that

$$
\mathbb{E}\left[\text{KR}^p_{p,C}(\hat{\mu}_N, \mu)\right] \leq \mathcal{E}^\text{Mult}_{p,\mathcal{X},\mu}(C)^{1/p} N^{-\frac{1}{q}}.
$$

For

$$
A_{q,p,L,\mathcal{X}}(l) := \text{diam}(\mathcal{X})^p 2^{p-1} \left(q^{-Lp} |\mathcal{X}|^{\frac{1}{2}} + \left(\frac{q}{q-1}\right)^p \sum_{j=1}^L q^{p-jp} |Q_j|^{\frac{1}{2}}\right),
$$

the constant is equal to

$$
\mathcal{E}^\text{Mult}_{p,\mathcal{X},\mu}(C, q, L) = \begin{cases} 
A_{q,p,L,\mathcal{X}}(1), & \text{if } C \geq 2h_{q,L}(0), \\
A_{q,p,L,\mathcal{X}}(l), & \text{if } 2h_{q,L}(l) \leq C < 2h_{q,L}(l - 1), \\
\frac{Cp}{2} \sqrt{\mathcal{M}(\mu)} \sum_{x \in \mathcal{X}} \sqrt{\mu(x)}, & \text{if } C \leq (2h_{q,L}(L) \lor \min_{x \neq x'} d(x, x')).
\end{cases}
$$

Furthermore, for $p = 1$ the factor $\frac{q}{(q-1)}$ in $A_{q,1,L,\mathcal{X}}(a, b, l)$ can be removed. Denote

$$
\mathcal{E}^\text{Mult}_{p,\mathcal{X},\mu}(C, q, L) := \inf_{L \in \mathbb{N}, q > 1} \mathcal{E}^\text{Mult}_{p,\mathcal{X},\mu}(C, q, L).
$$

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Proof. The proof of this result only differs from the proof of Theorem 2.2 by the upper bounds on the relevant expectations. By definition $\mathbb{E}[|\mathcal{M}(\hat{\mu}_N) - \mathcal{M}(\mu)|] = 0$. Furthermore, scaling the expectation by total mass

$$\mathbb{E}\left[\left|\hat{\mu}_N^L(C(x)) - \mu^L(C(x))\right|\right] = \mathcal{M}(\mu) \mathbb{E}\left[\left|\hat{\mu}_N^L(C(x)) - \frac{\mu^L(C(x))}{\mathcal{M}(\mu)}\right|\right],$$

we notice that $\frac{\hat{\mu}_N^L(C(x))}{\mathcal{M}(\mu)} \xrightarrow{D} \frac{1}{N} \sum_{i=1}^N X_i(x)$, where $X_1(x), \ldots, X_N(x) \overset{i.i.d.}{\sim} \text{Ber}(a(x))$ with $a(x) := \frac{\mu^L(C(x))}{\mathcal{M}(\mu)}$. Consequently, it holds that

$$\sum_{x \in Q_t} \mathbb{E}\left[\left|\hat{\mu}_N^L(C(x)) - \mu^L(C(x))\right|\right] = \mathcal{M}(\mu) \sum_{x \in Q_t} \mathbb{E}\left[\left|\frac{1}{N} \sum_{i=1}^N X_i(x) - a(x)\right|\right]
\leq \mathcal{M}(\mu) \sum_{x \in Q_t} \sqrt{\frac{a(x)(1 - a(x))}{N}}
\leq \mathcal{M}(\mu) \sqrt{\frac{|Q_t|}{N}}.
\qed

Notably, compared to $\mathcal{E}_{p,X,\mu}^\text{Pol}(C, q, L)$, the constant $\mathcal{E}_{p,X,\mu}^\text{Mult}(C, q, L)$ misses an additional summand for large $C$. This summand corresponds to the estimation error of the total mass intensity of $\hat{\mu}_N$ which is zero by assumptions of the model.

Remark A.3. If $C > \text{diam}(\mathcal{X})$ and $\mathcal{M}(\mu) = \mathcal{M}(\nu)$ UOT between $\mu$ and $\nu$ is equal to OT between these two measures. In particular, for $C > 2qL(0)$ we recover the respective deviation bounds for empirical optimal transport in Sommerfeld et al. [2019]. Since in the multinomial model for all $N \in \mathbb{N}$ it holds $\mathcal{M}(\hat{\mu}_N) = \mathcal{M}(\mu)$, this implies that for $C > \text{diam}(\mathcal{X})$ the $(p, C)$-KRD error is equal to the OT error. Since for empirical OT the parametric $N^{-\frac{1}{2}}$ rate is already known to be optimal [Fournier and Guillin, 2015], our rate in $N$ is sharp.

Theorem A.4. Let $\mu_1, \ldots, \mu_J \in \mathcal{M}_+(\mathcal{X})$ and denote $X_i = \text{supp}(\mu^i)$ for $i = 1, \ldots, J$. Consider random estimators $\hat{\mu}_N^1, \ldots, \hat{\mu}_N^J \in \mathcal{M}_+(\mathcal{X})$ derived from (6) and based on sample size $N_1, \ldots, N_J$, respectively. Then it holds for any barycenter $\mu^*$ of the population measures and any barycenter $\hat{\mu}^*$ of the estimators,

$$\mathbb{E}[|F_{p,C}(\mu^*) - F_{p,C}(\hat{\mu}^*)|] \leq \frac{2p \text{min}\{\text{diam}(\mathcal{Y}), C\}}{J} \sum_{i=1}^J \mathcal{E}_{1,X_i,\mu^i}^\text{Mult}(C) N_i^{-\frac{1}{2}}.$$

Theorem A.5. Let $\mu_1, \ldots, \mu_J \in \mathcal{M}_+(\mathcal{X})$ and denote $X_i = \text{supp}(\mu^i)$ for $i = 1, \ldots, J$. Consider random estimators $\hat{\mu}_N^1, \ldots, \hat{\mu}_N^J \in \mathcal{M}_+(\mathcal{X})$ derived from (6) and based on sample size $N_1, \ldots, N_J$, respectively. Let $\mathbf{B}^*$ be the set of $(p, C)$-barycenters of $\mu_1, \ldots, \mu_J$ and $\hat{\mathbf{B}}^*$ the set of $(p, C)$-barycenters of $\hat{\mu}_N^1, \ldots, \hat{\mu}_N^J$. Then, for $p \geq 1$ it holds that

$$\mathbb{E}\left[\sup_{\hat{\mu}^* \in \hat{\mathbf{B}}^*} \inf_{\mu^* \in \mathbf{B}^*} KR_{p,C}(\mu^*, \hat{\mu}^*)\right] \leq \frac{p \text{min}\{\text{diam}(\mathcal{Y}), C\}}{V_p J} \sum_{i=1}^J \mathcal{E}_{1,X_i,\mu^i}^\text{Mult}(C) N_i^{-\frac{1}{2}},$$

where the constant $V_p$ is defined as in Theorem 3.2.

The proofs of Theorem A.4 and Theorem A.5 are deferred to Appendix D.

Remark A.6. By the same argument as for the Poisson model, the approximation rate of the sampling estimator for the barycenter never decreases faster to zero than for a single measure. Thus, the $N^{-\frac{1}{2}}$ rate is sharp.
A.1 Explicit Bounds for Euclidean Spaces

Following the arguments in Section 2.4, we can also provide upper bounds on $d$-dimensional Euclidean spaces for the constant in Theorem A.2.

For $D < 2p$ and $L \to \infty$, it holds

$$
\mathcal{E}_{p,\mathcal{X},\mu}(C) \leq D^{p/2} \left\{ \begin{array}{ll}
     \text{diam}_{\infty}^p(\mathcal{X}) 2^{p-1} 2^{p-1/2} \frac{L}{1-2^{p/2}-p}, & \text{if } C \geq 2h_L(0), \\
     \text{diam}_{\infty}^p(\mathcal{X}) 2^{p-1} 2^{p(D/2-p)} \frac{L}{1-2^{p/2}-p}, & \text{if } 2h_L(l) \leq C < 2h_L(l - 1), \\
     \frac{C^p}{2} \sqrt{\mathcal{M}(\mu)} \sum_{x \in \mathcal{X}} \sqrt{\mu(x)}, & \text{if } C \leq (2h_L(L) \wedge \min_{x \neq x'} d_\infty(x, x')).
\end{array} \right.
$$

For $D = 2p$ and $L = \left\lfloor \frac{1}{2} \log_2(|\mathcal{X}|) \right\rfloor$, it holds

$$
\mathcal{E}_{p,\mathcal{X},\mu}(C) \leq D^{p/2} \left\{ \begin{array}{ll}
     \text{diam}_{\infty}^p(\mathcal{X}) 2^{p-1} (2^{2p} + D^{-1} \log_2(|\mathcal{X}|)), & \text{if } C \geq 2h_L(0), \\
     \text{diam}_{\infty}^p(\mathcal{X}) 2^{p-1} (2^{2p} + D^{-1} \log_2(|\mathcal{X}|) - l), & \text{if } 2h_L(l) \leq C < 2h_L(l - 1), \\
     \frac{C^p}{2} \sqrt{\mathcal{M}(\mu)} \sum_{x \in \mathcal{X}} \sqrt{\mu(x)}, & \text{if } C \leq (2h_L(L) \wedge \min_{x \neq x'} d_\infty(x, x')).
\end{array} \right.
$$

For $D > 2p$ and $L = \left\lfloor \frac{1}{2} \log_2(|\mathcal{X}|) \right\rfloor$, it holds

$$
\mathcal{E}_{p,\mathcal{X},\mu}(C) \leq D^{p/2} \left\{ \begin{array}{ll}
     \text{diam}_{\infty}^p(\mathcal{X}) 2^{p-1} |\mathcal{X}|^{1/p} \left( 1 + \frac{2^{p+D/2}}{2^{p/2} - p-1} \right), & \text{if } C \geq 2h_L(0), \\
     \text{diam}_{\infty}^p(\mathcal{X}) \left( |\mathcal{X}|^{1/p} + \frac{2^{p+D/2}}{2^{p/2} - p-1} \left( |\mathcal{X}|^{1/p} - 2^{p(D/2-p)(l-1)} \right) \right), & \text{if } 2h_L(l) \leq C < 2h_L(l - 1), \\
     \frac{C^p}{2} \sqrt{\mathcal{M}(\mu)} \sum_{x \in \mathcal{X}} \sqrt{\mu(x)}, & \text{if } C \leq (2h_L(L) \wedge \min_{x \neq x'} d_\infty(x, x')).
\end{array} \right.
$$

We stress that while these constants do not include the additional term for the estimation of the total mass intensity, their dependency on $|\mathcal{X}|$ is identical to that of the upper bounds on $\mathcal{E}_{p,\mathcal{X},\mu}(C)$. In particular, the phase transitions still occur depending on whether $D$ is larger than $2p$, smaller than $2p$ or equal to it.

A.2 Simulations

We repeat the simulations from Section 4 for the multinomial model. For the $(p, C)$-KRD the results (in Figure 16) slightly differ from the results in the Poisson model. Notably, for increasing $C$, the error is decreasing. This is explained by the fact that in the multinomial scheme, we do not have to estimate the total intensities of the measures and it is precisely this estimation error that drives the error for increasing $C$ in the Poisson model. Similarly to the Poisson scheme, we observe a decrease in error for the measure classes with clustered...
Figure 16: Expected relative $(2, C)$-KRD error for two measures in the multinomial model for the eight classes in Section 4. For each sampling size $N$ the expectation is estimated from 1000 independent runs. For each class the parameters are set, such that the measures have on average 300 support points. From top-left to bottom-right we have $C = 0.01, 0.1, 1, 10$, respectively.

Figure 17: Expected relative Fréchet error for the $(2, C)$-barycenter for $J = 5$ measures from the PI class for the multinomial model with different sample sizes $N$. For each sample size the expectation is estimated from 100 independent runs. For each class the parameters are set, such that the measures have on average 300 support points. From left to right we have $C = 0.1, 1, 10$, respectively.

support structures when $C$ surpasses the distance between two individual clusters. For the $(p, C)$-barycenters under the multinomial sampling model (in Figure 17) there is an initial increase in error for small sample sizes. Specifically, this occurs for $C = 0.1$ and the NEC and SPIC classes. This value of $C$ is below the cluster size. This effect is most likely for these measure classes. For increasing $C$ there is a significant reduction in estimation error. In particular, for some classes the error reduces by two orders of magnitude going from $C = 0.1$ to $C = 10$. Since the total mass intensities of the individual measures do not need to be estimated in this sampling model, we already observe a decrease in error for increasing $C$ for the $(p, C)$-KRD and naturally there is a similar effect for the Fréchet functional.

B Bounds for the Bernoulli Model

In this section we provide results analogue to Theorem 2.2, Theorem 3.1 and Theorem 3.2 for the estimator in the multinomial model in (7). The respective proofs only differ in the way the respective expectation are bounded, so whenever suitable, we only provide these differences in the proofs.
Lemma B.1 (Total Variation Bound). Let \((X, d)\) be a finite metric space and \(\mu \in \mathcal{M}_+(X)\) with \(\mu(x) \in \{0, 1\}\) for \(x \in X\). Let \(\hat{\mu}_{s_X}\) be the measure in (7). Then, for any \(p \geq 1\) it holds that

\[
\mathbb{E} \left[ KR_{p,C}^p(\hat{\mu}_{s_X}, \mu) \right] \leq C_p \sum_{x \in X} (1 - s_x).
\]

Proof. This proof is identical to the proof of Lemma 2.5 except for the bound on the expectation. For this, note that

\[
\mathbb{E} [\text{TV}(\hat{\mu}_{s_X}, \mu)] = \sum_{x \in X} \mathbb{E} \left[ \frac{1}{s_x} B_x - 1 \right] = \sum_{x \in X} (1 - s_x) + s_x \frac{1}{s_x} - 1 = 2 \sum_{x \in X} (1 - s_x),
\]

with \(B_x \sim \text{Ber}(s_x)\) for \(s_x \in [0, 1]\) for all \(x \in X\).

\[\square\]

Theorem B.2. Let \((X, d)\) be a finite metric space and \(\mu \in \mathcal{M}_+(X)\) with \(\mu(x) \in \{0, 1\}\) for \(x \in X\). Let \(\hat{\mu}_{s_X}\) be the measure in (7). Then, for any \(p \geq 1\), resolution \(q > 1\) and depth \(L \in \mathbb{N}\) it holds that

\[
\mathbb{E} [KR_{p,C}^p(\hat{\mu}_{s_X}, \mu)] \leq \mathcal{E}_{p,X,\mu}^{Ber}(C, q, L)^{1/p} \begin{cases} 
(2 \sum_{x \in X} (1 - s_x))^{1/p}, & \text{if } C \leq (2h_{q,L}(L) \vee \min_{x \neq x'} d(x, x')) \\
\left(\sum_{x \in X} \frac{1 - s_x}{s_x}\right)^{1/p}, & \text{else}.
\end{cases}
\]

The constant \(\mathcal{E}_{p,X,\mu}^{Ber}(C, q, L)\) is equal to \(\mathcal{E}_{p,X,\mu}^{Poi}(C, q, L)\) for all \(C > 0\), \(q > 1\) and \(L \in \mathbb{N}\). We denote

\[
\mathcal{E}_{p,X,\mu}^{Ber}(C) := \inf_{L \in \mathbb{N}, q > 1} \mathcal{E}_{p,X,\mu}^{Ber}(C, q, L).
\]

Proof. The proof of this result only differs from the proof of Theorem 2.2 by the upper bounds on the relevant expectations. Recall the estimator \(\hat{\mu}_{s_X}\) from (7) and let \(B_x \sim \text{Ber}(s_x)\) for \(s_x \in [0, 1]\) for all \(x \in X\). It holds that

\[
\sum_{x \in Q_t} \mathbb{E} \left[ |\hat{\mu}_{s_X}^L(C(x)) - \mu^L(C(x))| \right] = \sum_{x \in Q_t} \mathbb{E} \left[ \sum_{y \in C(x)} \frac{B_y}{s_y} - \sum_{y \in C(x)} s_y \right]
\leq \sum_{x \in Q_t} \sqrt{\text{Var} \left( \sum_{y \in C(x)} \frac{B_y}{s_y} \right)} = \sum_{x \in Q_t} \sqrt{\sum_{y \in C(x)} s_y^2 \text{Var}(B_y)}
= \sum_{x \in Q_t} \sqrt{\sum_{y \in C(x)} \frac{1 - s_y}{s_y}} \leq \sqrt{|Q_t|} \sqrt{\sum_{x \in X} \frac{1 - s_x}{s_x}}.
\]

The total mass can be bounded analogously as

\[
\mathbb{E} \left[ |\hat{\mu}_{s_X}^L(X) - \mu^L(X)| \right] \leq \sqrt{\sum_{x \in X} \frac{1 - s_x}{s_x}}.
\]

\[\square\]

Since the constants for the deviation bounds for this model coincide with those for the Poisson model we refer to the previous discussion on their properties.
Remark B.3. Consider $s_X$ such that $s_x = s$ for some $s \in [0,1]$ and all $x \in \mathcal{X}$. Note, that for sufficiently small $C$ the upper bound is an equality, since the $(p,C)$-KRD in this setting is proportional to the TV distance and that distance has a closed form solution here. For larger $C$, the expectation in the proof of Theorem B.2 amounts to bounding the mean absolute deviation of a binomial distribution. This has a closed form solution which scales as the standard deviation of the respective binomial for $s$ not too close to $0$ or $1$ [Berend and Kontorovich, 2013]. Hence, in this context the upper bound on the mean absolute deviation in the proof is sharp. So based on the presented approach for the deviation bounds, the upper bound is non-improvable.

Theorem B.4. Let $\mu^1, \ldots, \mu^J \in \mathcal{M}_+(\mathcal{X})$ and denote $\mathcal{X}_i = \text{supp}(\mu^i)$ for $i = 1, \ldots, J$. Consider (random) estimators $\hat{\mu}^1_{sX_1}, \ldots, \hat{\mu}^J_{sX_J} \in \mathcal{M}_+(\mathcal{X})$ derived from (7). Then,

$$\mathbb{E} \left[ |F_{p,C}(\mu^*) - F_{p,C}(\hat{\mu}^*)| \right] \leq 2p \min_{i \in \mathcal{X}} \left[ \text{diam}(\mathcal{X}_i), C \right] \sum_{i=1}^J \frac{1}{s_{X_i}} \mathbb{E}_{\text{Ber}}(C) \psi(s_{X_i}),$$

where $\psi$ is given by

$$\psi(s_{X_i}) = \begin{cases} 2 \sum_{x \in \mathcal{X}} (1 - s_x), & \text{if } C \leq \min_{x \neq x'} d(x, x') \\ \left( \sum_{x \in \mathcal{X}} \frac{1 - s_x}{s_x} \right)^{1/2}, & \text{else.} \end{cases}$$

Theorem B.5. Let $\mu^1, \ldots, \mu^J \in \mathcal{M}_+(\mathcal{X})$ and denote $\mathcal{X}_i = \text{supp}(\mu^i)$ for $i = 1, \ldots, J$. Consider (random) estimators $\hat{\mu}^1_{sX_1}, \ldots, \hat{\mu}^J_{sX_J} \in \mathcal{M}_+(\mathcal{X})$ derived from (7). Let $\mathbf{B}^*$ be the set of $(p,C)$-barycenters of $\mu^1, \ldots, \mu^J$ and $\hat{\mathbf{B}}^*$ the set of $(p,C)$-barycenters of $\hat{\mu}^1_{sX_1}, \ldots, \hat{\mu}^J_{sX_J}$. Then, for $p \geq 1$ it holds that

$$\mathbb{E} \left[ \sup_{\hat{\mu}^* \in \hat{\mathbf{B}}^*} \inf_{\mu^* \in \mathbf{B}^*} \text{KRD}^p_{p,C}(\mu^*, \hat{\mu}^*) \right] \leq p \min_{i \in \mathcal{X}} \left[ \text{diam}(\mathcal{X}_i), C \right] \sum_{i=1}^J \frac{1}{s_{X_i}} \mathbb{E}_{\text{Ber}}(C) \psi(s_{X_i}),$$

where $\psi$ is defined as in Theorem B.4 and $V_p$ is defined as in Theorem 3.1.

The proofs of Theorem B.4 and Theorem B.5 are deferred to Appendix D.

B.1 Simulations

To construct a reasonable framework for the simulations, we fix $s^0 \in \mathbb{R}_+$ and assume that

$$s_x = \frac{s^0}{\|x - (0.5, 0.5)^T\|_2 + s_0}.$$  

Intuitively, the success probability at a given point $x$ is larger, if $x$ is closer to the centre of $[0,1]^2$ and smaller if it is further away from the centre. However, it still holds that for $s^0 \to \infty$ the success probability at each location converges to one. For the simulations, we now consider the error as a function of $s^0$. Note that in this simulation study only the classes of measures with mass one at each support point are considered in accordance with the Bernoulli model in (7). One notable observation for the empirical $(p,C)$-KRD (in Figure 18) is that the error of the SPIC class is significantly higher than for the NEC class, even though they share the same cluster locations. This can be explained by the fact that, by construction, the measures in the NEC class have a higher proportion of their mass in their central clusters, which is close to $(0.5, 0.5)^T$ and thus has a high probability of being observed. This effect also carries over to the $(p,C)$-barycenter (in Figure 19). In general, for the $(p,C)$-KRD the error in this model is increasing in $C$ (which is again explained by the estimation error for the true total mass intensity). However, the effect is
Figure 18: Expected relative $(2, C)$-KRD error for two measures in the Bernoulli Model for the measure classes from Section 4. For each pair of success probability $s$ and observation time $t$ the expectation is estimated from 1000 independent runs. The parameters are chosen such that the measures have on average 300 support points. From top-left to bottom-right we have $C = 0.01, 0.1, 1, 10$, respectively.

Figure 19: Expected relative Fréchet error for the $(2, C)$-barycenter for $J = 5$ measures from the PI class for the Bernoulli model with different success vectors $s_X$. For each sample size the expectation is estimated from 100 independent runs. The parameters are set such that the measures in all classes have on average 300 support points. From left to right we have $C = 0.1, 1, 10$, respectively.

less pronounced than in the Poisson model. For the clustered data types a small decrease of error for increasing $C$ over the cluster size can again be noted. Though, also this effect is less significant than in the other models. For the $(p, C)$-barycenter a decrease in error in $C$ can be observed which is consistent with the previous results for the Poisson model and again explained by the increased stability of the total mass intensity of the barycenter compared to the individual ones.

C Lifts to Balanced Optimal Transport Problems

A key tool in establishing properties of the $(p, C)$-KRD and the $(p, C)$-barycenter is the lift of these problems to the space of probability measures by augmenting the space $X$ with a dummy point having a fixed distance to all points in $X$. For a fixed parameter $C > 0$, consider a dummy point $d$ and define the augmented space $\tilde{X} := X \cup \{d\}$ with
According to Heinemann et al. [2022a], the augmented measure \( p,C \) defined on the centroid set \( \tilde{X} \) is the minimiser of the \( p,C \)-Fréchet functional \( \tilde{F}_{p,C}(\mu) \) over the set \( \Pi_{\pm}(\mu, \nu) \) of couplings \( \pi \in \Pi_{\pm}(\mu, \nu) \) with \( \mu \) and \( \nu \) non-negative measures whose total mass is bounded by \( B \). Setting \( \tilde{\mu} := \mu + (B - M(\mu))\delta_0 \), any measure \( \mu \in M_+(X) \) defines an augmented measure \( \tilde{\mu} \) on \( X \) such that \( M(\tilde{\mu}) = B \). For any \( \mu, \nu \in M_+(X) \) and their augmented versions \( \tilde{\mu}, \tilde{\nu} \in M_+(X) \) it holds

\[
KR_{C,p}(\mu, \nu) = \tilde{OT}_p(\tilde{\mu}, \tilde{\nu}).
\]

Here, \( \tilde{OT}_p \) denotes the \( p \)-OT distance defined for measures \( \mu, \nu \) on \( (\tilde{X}, \tilde{d}) \) with \( M(\mu) = M(\nu) \) as

\[
\tilde{OT}_p^p(\mu, \nu) := \min_{\pi \in \Pi_{\pm}(\mu, \nu)} \sum_{x, x' \in \tilde{X}} d^p(x, x') \pi(x, x'),
\]

where the set of couplings \( \Pi_{\pm}(\mu, \nu) \) is the set \( \Pi_{\pm}(\mu, \nu) \) with inequalities replaced by equalities. Similarly, the \((p, C)\)-barycenter problem can be augmented. For this, let \( \tilde{Y} := Y \cup \{0\} \) and augment the \( (p, C) \)-barycenter problem in \( (18) \) (replace \( X \) by \( Y \) and recall that \( X \subset Y \)) and augment the measures \( \mu_1, \ldots, \mu_J \) to \( \tilde{\mu}_1, \ldots, \tilde{\mu}_J \) where \( \tilde{\mu}_i = \mu_i + \sum_{j \neq i} \delta_j \) for \( 1 \leq i \leq J \). In particular, it holds \( M(\tilde{\mu}_i) = \sum_{i=1}^J M(\mu^i) \) and the augmented \( p \)-Fréchet functional is defined as

\[
\tilde{F}_{p,C}(\mu) := \frac{1}{J} \sum_{i=1}^J \tilde{OT}_p^p(\tilde{\mu}_i, \mu).
\]

Any minimiser of \( \tilde{F}_{p,C} \) is referred to as augmented \((p, C)\)-barycenter.

**LP-Formulation for the \((p, C)\)-Barycenter**

According to Heinemann et al. [2022a], the augmented \((p, C)\)-barycenter problem can be rewritten as a linear program based on the centroid set \( \tilde{C}_{KR}(J, p, C) = C_{KR}(J, p, C) \cup \{0\} \) (recall \( 5 \) for the definition of \( C_{KR}(J, p, C) \)) of the augmented measures. This yields

\[
\min_{\pi^{(1)}, \ldots, \pi^{(J)}, c} \frac{1}{J} \sum_{j=1}^J \sum_{i=1}^J |\tilde{C}_{KR}(J, p, C)| \pi^{(j)}_i c_{jk}
\]

s.t.

\[
\begin{align*}
\sum_{k=1}^{M_i} \pi^{(i)}_k &= a_j, & & \forall i = 1, \ldots, J, \forall j = 1, \ldots, |\tilde{C}_{KR}(J, p, C)|, \\
\sum_{j=1}^J \pi^{(j)}_i &= b_k, & & \forall i = 1, \ldots, J, \forall k = 1, \ldots, M_i, \\
\pi^{(i)}_j &\geq 0, & & \forall i = 1, \ldots, J, \forall j = 1, \ldots, |\tilde{C}_{KR}(J, p, C)|, \forall k = 1, \ldots, M_i,
\end{align*}
\]

where \( M_i = |\tilde{X}| \) for each \( 1 \leq i \leq J \) is the cardinality of the support of the augmented measure \( \tilde{\mu}_i \). Here, \( c_{jk} \) denotes the distance between the \( j \)-th point of \( |\tilde{C}_{KR}(J, p, C)| \) and the \( k \)-th point in the support of \( \tilde{\mu}_i \), while \( b^i \) is the vector of masses corresponding to \( \tilde{\mu}_i \).
\[|KR_{p,C}^p(\mu^1,\mu^3) - KR_{p,C}^p(\mu^2,\mu^3)| = |\hat{\theta}_p^p(\hat{\mu}^1,\hat{\mu}^3) - \hat{\theta}_p^p(\hat{\mu}^2,\hat{\mu}^3)| \]
\[\leq \text{diam}(\tilde{\mathcal{Y}})^{p-1} p \hat{\theta}_1(\hat{\mu}^1,\hat{\mu}^3) \]
\[= \min\{\text{diam}(\mathcal{Y}), C\}^{p-1} p K R_{1,C}(\mu^1,\mu^2),\]

where the inequality follows from Sommerfeld and Munk [2018]. Taking expectation and applying the previous display together with Theorem 2.2 yields

\[\mathbb{E}[|F_{p,C}(\mu) - \tilde{F}_{p,C}(\mu)|] \leq \frac{1}{J} \sum_{j=1}^{J} \mathbb{E}[|KR_{p,C}^p(\mu^j,\mu) - KR_{p,C}^p(\hat{\mu}^j,\mu)|] \]
\[\leq p \min\{\text{diam}(\mathcal{Y}), C\}^{p-1} \frac{1}{J} \sum_{j=1}^{J} \mathbb{E}[KR_{1,C}(\mu^j,\hat{\mu}^j)] \]
\[\leq p \min\{\text{diam}(\mathcal{Y}), C\}^{p-1} \frac{1}{J} \sum_{j=1}^{J} \mathcal{E}_{\mu^j}(C) \theta_i.\]

Let \(\mu^*\) and \(\hat{\mu}^*\) be minimizers of their respective \(p\)-Fréchet functional \(F_{p,C}\) and \(\tilde{F}_{p,C}\). Then, it follows that

\[\mathbb{E}[|F_{p,C}(\hat{\mu}^*) - F_{p,C}(\mu^*)|]\]
\[= \mathbb{E} \left[ F_{p,C}(\hat{\mu}^*) - \tilde{F}_{p,C}(\mu^*) + \tilde{F}_{p,C}(\mu^*) - F_{p,C}(\mu^*) \right] \]
\[\leq \mathbb{E} \left[ F_{p,C}(\hat{\mu}^*) - \tilde{F}_{p,C}(\mu^*) \right] + \mathbb{E} \left[ \tilde{F}_{p,C}(\mu^*) - F_{p,C}(\mu^*) \right] \]
\[\leq \mathbb{E} \left[ F_{p,C}(\hat{\mu}^*) - \tilde{F}_{p,C}(\mu^*) \right] + p \min\{\text{diam}(\mathcal{Y}), C\}^{p-1} \frac{1}{J} \sum_{i=1}^{J} \mathcal{E}_{\mu^i}(C) \theta_i \]
\[\leq \mathbb{E} \left[ F_{p,C}(\hat{\mu}^*) - \tilde{F}_{p,C}(\mu^*) \right] + p \min\{\text{diam}(\mathcal{Y}), C\}^{p-1} \frac{1}{J} \sum_{i=1}^{J} \mathcal{E}_{\mu^i}(C) \theta_i \]
\[\leq p \min\{\text{diam}(\mathcal{Y}), C\}^{p-1} \frac{2}{J} \sum_{i=1}^{J} \mathcal{E}_{\mu^i}(C) \theta_i,\]

where the fourth inequality follows from \(\hat{\mu}^*\) being a minimiser of \(\tilde{F}_{p,C}\).

**Proof of Theorem 3.2, Theorem A.5 and Theorem B.5.** Let \(\hat{\mu}^1,\ldots,\hat{\mu}^J\), \(\mathcal{E}_{\mu^1,\ldots,\mu^J}(C)\) and \(\theta_i\) for all \(i = 1,\ldots,J\) as in the previous proof. Let \(\mathcal{B}\) be the set of \((p,C)\)-barycenters of the measures \(\mu^1,\ldots,\mu^J\) and define \(\mathcal{B}\) as the set of \(\text{OT}_p\)-barycenters of the augmented measures \(\tilde{\mu}^1,\ldots,\tilde{\mu}^J\). Similar, we denote \(\mathcal{B}\) the set of \((p,C)\)-barycenters of the estimated measures \(\hat{\mu}^1,\ldots,\hat{\mu}^J\) and let \(\mathcal{B}\) be the set of \(p\)-barycenters of their augmented versions. Define the
lift of a measure $\mu \in \mathcal{M}_+(\mathcal{Y})$ to a measure $\tilde{\mu} \in \mathcal{M}(\tilde{\mathcal{Y}})$ by

$$
\phi_{\mu^1,\ldots,\mu^J}(\mu) = \mu + \left( \sum_{i=1}^J \mathbb{M}(\mu^i) - \mathbb{M}(\mu) \right) \delta_0.
$$

If $\mu \in \mathcal{B}$ then it follows by Lemma 3.3 in Heinemann et al. [2022a] that $\phi_{\mu^1,\ldots,\mu^J}(\mu) \in \hat{\mathcal{B}}$. Conversely, for any $\tilde{\mu} \in \hat{\mathcal{B}}$ it holds that $\phi^{-1}_{\mu^1,\ldots,\mu^J}(\tilde{\mu}) \in \mathcal{B}$. We denote by $\phi(\mathcal{B}) := \{\phi_{\mu^1,\ldots,\mu^J}(\mu)|\mu \in \mathcal{B}\}$ and analogously $\phi^{-1}(\hat{\mathcal{B}}) := \{\phi^{-1}_{\mu^1,\ldots,\mu^J}(\tilde{\mu})|\tilde{\mu} \in \hat{\mathcal{B}}\}$. With this we have

$$
\mathbb{E} \left[ \sup_{\hat{\mu} \in \hat{\mathcal{B}}} \inf_{\bar{\mu} \in \mathcal{B}} \Theta_{p,C}(\mu, \hat{\mu}) \right] = \mathbb{E} \left[ \sup_{\hat{\mu} \in \hat{\mathcal{B}}} \inf_{\bar{\mu} \in \mathcal{B}} \Theta_{p,C}(\mu, \hat{\mu}) \right]
$$

$$
= \mathbb{E} \left[ \sup_{\hat{\mu} \in \hat{\mathcal{B}}} \inf_{\bar{\mu} \in \mathcal{B}} \Theta_{p,C}(\mu, \hat{\mu}) \right] \geq \Theta_{p,C}(\mathcal{B}) - \Theta_{p,C}(\hat{\mu}) + \Theta_{p,C}(\hat{\mu}) \geq 2V_P \Theta_{p,C}(\hat{\mu}, \tilde{\mu}),
$$

where $V_P$ is the constant from Theorem 3.2.

Invoking Lemma D.1 with $\mu \in \hat{\mathcal{B}}$ and applying Theorem 3.1 yields

$$
\frac{2\theta}{J} \sum_{i=1}^J \mathcal{E}_{1,\mathcal{X},\mu^i}(C) \min\{\text{diam}(\mathcal{X}), C\}^{p-1} \geq \mathbb{E} \left[ \Theta_{p,C}(\hat{\mu}) - \Theta_{p,C}(\tilde{\mu}) \right]
$$

$$
\geq \mathbb{E} \left[ 2V_P \sup_{\hat{\mu} \in \hat{\mathcal{B}}} \inf_{\bar{\mu} \in \mathcal{B}} \Theta_{p,C}(\hat{\mu}, \bar{\mu}) \right]
$$

$$
= \mathbb{E} \left[ 2V_P \sup_{\hat{\mu} \in \hat{\mathcal{B}}} \inf_{\bar{\mu} \in \mathcal{B}} \Theta_{p,C}(\mu, \bar{\mu}) \right],
$$

where the equality follows from (20) and hence

$$
\frac{\theta}{J} \sum_{i=1}^J \mathcal{E}_{1,\mathcal{X},\mu^i}(C) \min\{\text{diam}(\mathcal{X}), C\}^{p-1} \geq \mathbb{E} \left[ \sup_{\hat{\mu} \in \hat{\mathcal{B}}} \inf_{\bar{\mu} \in \mathcal{B}} \Theta_{p,C}(\mu, \bar{\mu}) \right].
$$

\qed
E Additional Figures for the Poisson Sampling

E.1 Distance

Figure 20: As in Figure 9, but for the NI class and $M = 22$.

Figure 21: As in Figure 20, but for the NI class and $M = 300$.

Figure 22: As in Figure 20, but for the NIG class and $M = 17$. 
Figure 23: As in Figure 20, but for the SPI class and $M = 65$.

Figure 24: As in Figure 20, but for the SPIC class and $M = 12$.

E.2 Barycenter

Figure 25: Expected relative Fréchet error for the $(2,C)$-barycenter for $J = 5$ measures from the PIG class in the Poisson sampling model with different success probabilities $s$. For each pair of success probability $s$ and observation time $t$ the expectation is estimated from 1000 independent runs. Set $M = 22$. From top-left to bottom-right we have $C = 0.1, 1, 10$, respectively.

Figure 26: As in Figure 25, but for the NI class and $M = 300$. 
Figure 27: As in Figure 25, but for the NIG class and $M = 17$.

Figure 28: As in Figure 25, but for the SPI class and $M = 65$.

Figure 29: As in Figure 25, but for the SPIC class and $M = 12$. 

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