Empirical optimal transport on countable metric spaces: Distributional limits and statistical applications

Carla Tameling * Max Sommerfeld † Axel Munk ‡

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Abstract

We derive distributional limits for empirical transport distances between probability measures supported on countable sets. Our approach is based on sensitivity analysis of optimal values of infinite dimensional mathematical programs and a delta method for non-linear derivatives. A careful calibration of the norm on the space of probability measures is needed in order to combine differentiability and weak convergence of the underlying empirical process. Based on this we provide a sufficient and necessary condition for the underlying distribution on the countable metric space for such a distributional limit to hold. We give an explicit form of the limiting distribution for ultra-metric spaces. Finally, we apply our findings to optimal transport based inference in large scale problems. An application to nanoscale microscopy is given.

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1 Introduction

Optimal transport based distances between probability measures (see e.g., Rachev and Rüschendorf (1998) or Villani (2009) for a comprehensive treatment), e.g., the Wasserstein distance (Vasershtein, 1969), which is also known as Earth Movers distance (Rubner et al., 2000), Kantorovich-Rubinstein distance (Kantorovich and Rubinstein, 1958) or Mallows distance (Mallows, 1972), are of...
fundamental interest in probability and statistics, with respect to both theory and practice. The $p$-th Wasserstein distance (WD) between two probability measures $\mu$ and $\nu$ on a Polish metric space $(\mathcal{X}, d)$ is given by

$$W_p(\mu, \nu) = \left( \inf \int_{\mathcal{X} \times \mathcal{X}} d(x, y)^p d\pi(x, y) \right)^{1/p}$$

(1)

for $p \in [1, \infty)$, the infimum is taken over all probability measures $\pi$ on the product space $\mathcal{X} \times \mathcal{X}$ with marginals $\mu$ and $\nu$.

The WD metrizes weak convergence of a sequence of probability measures on $(\mathcal{X}, d)$ together with convergence of its first $p$ moments and has become a standard tool in probability, e.g., to study limit laws (e.g., Johnson and Samworth (2005); Rachev and Rüschendorf (1994); Shorack and Wellner (1986)), to derive bounds for Monte Carlo computation schemes such as MCMC (e.g., Eberle (2014); Rudolf and Schweizer (2015)), for point process approximations (Barbour and Brown, 1992; Schuhmacher, 2009) or bootstrap convergence (Bickel and Freedman, 1981). Besides of its theoretical importance, the WD is used in many applications as a measure to compare complex objects, e.g., in image retrieval (Rubner et al., 2000), deformation analysis (Panaretos and Zemel, 2016), meta genomics (Evans and Matsen, 2012), computer vision (Ni et al., 2009), goodness-of-fit tests (Munk and Czado, 1998; del Barrio et al., 2000), finance (Rachev et al., 2011) and machine learning (Rolet et al., 2016).

In such applications the WD has to be estimated from a finite sample of the underlying measures. This raises the question how fast the empirical Wasserstein distance (EWD), i.e., when either $\mu$ or $\nu$ (or both) are estimated by the empirical measures $\hat{\mu}_n = \frac{1}{n} \sum_{i=1}^n \delta_{X_i}$ (and $\hat{\nu}_m = \frac{1}{m} \sum_{i=1}^m \delta_{Y_i}$) approaches WD. Ajtai et al. (1984) investigated the rate of convergence of EWD for the uniform measure on the unit square, Talagrand (1992) and Talagrand (1994) extended this to higher dimensions. Horowitz and Karandikar (1994) provided non-asymptotic bounds for the average speed of convergence for the empirical 2-Wasserstein distance. There are several refinements of these results, e.g., Boissard and Gouic (2014) and Fournier and Guillin (2014).

As a natural extension of such results, there is a long standing interest in distributional limits for EWD, in particular motivated from statistical applications. Most of this work is restricted to the univariate case $\mathcal{X} \subset \mathbb{R}$. Munk and Czado (1998) derived central limit theorems for a trimmed WD on the real line when $\mu \neq \nu$ whereas del Barrio et al. (1999a,b) consider the empirical Wasserstein distance when $\mu$ belongs to a parametric family of distributions, e.g., for a Gaussian location scale family, for the assessment of goodness of fit. In a similar spirit del Barrio et al. (2005) provided asymptotics for a weighted version of the empirical 2-Wasserstein distance in one dimension and Freitag and Munk (2005) derive limit laws for semiparametric models, still restricted to the univariate case. There are also several results for dependent data in one dimension, e.g., Dede (2009), Dedecker and Merlevede (2015). For a recent survey we refer to Bobkov and Ledoux (2014) and Mason (2016) and references.
therein. A major reason of the limitation to dimension $D = 1$ is that only for $X \subset \mathbb{R}$ (or more generally a totally ordered space) the coupling which solves (1) is known explicitly and can be expressed in terms of the quantile functions $F^{-1}$ and $G^{-1}$ of $\mu$ and $\nu$, respectively, as $\pi = (F^{-1} \times G^{-1})\#L$, where $L$ is the Lebesgue measure on $[0,1]$ (see Mallows (1972)). All the above mentioned work relies essentially on this fact. For higher dimensions only in specific settings such a coupling can be computed explicitly and then can be used to derive limit laws (Rippl et al., 2016). Already for $D = 2$ Ajtai et al. (1984) indicate that the scaling rate for the limiting distribution of $W_1(\hat{\mu}_n, \mu)$ when $\mu$ is the uniform measure on $X = [0,1]^2$ (if it exists) must be of complicated nature as it is bounded from above and below by a rate of order $\sqrt{n \log(n)}$.

Recently, del Barrio and Loubes (2017) gave distributional limits for the quadratic EWD in general dimension with a scaling rate $\sqrt{n}$. This yields a (non-degenerate) normal limit in the case $\mu \neq \nu$, i.e., when the data generating measure is different from the measure to be compared with (extending Munk and Czado (1998) to $D > 1$). Their result centers the EWD with an expected EWD (whose value is typically unknown) instead of the true WD and requires $\mu$ and $\nu$ to have a positive Lebesgue density on the interior of their convex support. Their proof uses the uniqueness and stability of the optimal transportation potential (i.e., the minimizer of the dual transportation problem, see Villani (2003) for a definition and further results) and the Efron-Stein variance inequality. However, in the case $\mu = \nu$, their distributional limit degenerates to a point mass at 0, underlining the fundamental difficulty of this problem again.

An alternative approach has been advocated recently in Sommerfeld and Munk (2016) who restrict to finite spaces $X = \{x_1, \ldots, x_N\}$. They derive limit laws for the EWD for $\mu = \nu$ (and $\mu \neq \nu$), which requires a different scaling rate. In this paper we extend their work to measures $r = (r_x)_{x \in X}$ that are supported on countable metric spaces $(X, d)$, linking the asymptotic distribution of the EWD on the one hand to the issue of weak convergence of the underlying multinomial process associated with $\hat{\mu}_n$ with respect to a weighted $\ell^1$-norm

$$||r||_{\ell^1(d\nu)} = \sum_{x \in X} d^p(x, x_0) |r_x| + |r_{x_0}|$$

and on the other hand to infinite dimensional sensitivity analysis. Here, $x_0 \in X$ is fixed, but arbitrary. Notably, we obtain a necessary and sufficient condition for such a limit law, which sheds some light on the limitation to approximate the WD between continuous measures for $D \geq 2$ by discrete random variables.

The outline of this paper is a follows. In Section 2 we give distributional limits for the EWD of measures that are supported on a countable metric space. In short, this limit can be characterized as the optimal value of an infinite dimensional linear program applied to a Gaussian process over the set of dual solutions. The main ingredients of the proof are the directional Hadamard differentiability of the Wasserstein distance on countable metric spaces and the delta method for non-linear derivatives. We want to emphasize that the delta method for non-linear derivatives is not a standard tool (see Shapiro (1991);
Moreover, for the delta method to work here weak convergence in the weighted $\ell^1$-norm (2) of the underlying empirical process $\sqrt{n}(\hat{r}_n - r)$ is required as the directional Hadamard differentiability is proven w.r.t. this norm. We find that the well known summability condition

$$\sum_{x \in \mathcal{X}} d^p(x, x_0) \sqrt{r_x} < \infty$$

is necessary and sufficient for weak convergence. This condition is known to be necessary and sufficient for the discrete empirical process $\sqrt{n}(\hat{\mu}_n - \mu)$ to be Donsker according to the Borisov-Durst Theorem (see Dudley (2014)) and was originally introduced in a more general way by Jain (1977). Furthermore, we examine (3) in a more detailed way. We give examples and counterexamples for (3) and discuss whether the condition holds in case of an approximation of continuous measures. Further, we examine under which assumptions it follows that (3) holds for all $p' \leq p$ if it is fulfilled for $p$, and put it in relation to its one-dimensional counterpart, see del Barrio et al. (1999b).

In Section 3 we specify the case where the metric structure on the ground space is given by a rooted tree with weighted edges. In this case we can provide a simplified limiting distribution and use its explicit formula to derive a distributional upper bound for general metric spaces.

In Section 4 we combine this with a well known lower bound (Pele and Werman, 2009) to derive a computationally efficient strategy to test for the equality of two measures $r$ and $s$ on a countable metric space. Furthermore, we derive an explicit formula of the upper bound from Section 3 in the case of $\mathcal{X}$ being a regular grid.

An application of our results to data from single marker switching microscopy imaging is given in Section 5. As the number of pixels typically is of magnitude $10^5 - 10^6$ this challenges the assumptions of a finite space underlying the limit law in Sommerfeld and Munk (2016) and our work provides the theoretical justification to perform EWD based inference in such a case. Finally, we stress that our results can be extended to many other situations, e.g., the comparison of $k$ samples and when the underlying data are dependent, as soon as a weak limit of the underlying empirical process w.r.t. the weighted $\ell^1$-norm (2) can be shown.

2 Distributional Limits

2.1 Wasserstein distance on countable metric spaces

To be more specific, let $\mathcal{X} = \{x_1, x_2, \ldots\}$ be a countable metric space equipped with a metric $d: \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}_+$. The probability measures on $\mathcal{X}$ are infinite dimensional vectors $r$ in

$$\mathcal{P}(\mathcal{X}) = \left\{ r = (r_x)_{x \in \mathcal{X}} : r_x \geq 0 \quad \forall x \in \mathcal{X} \text{ and } \sum_{x \in \mathcal{X}} r_x = 1 \right\}.$$
The $p$-th Wasserstein distance ($p \geq 1$) then becomes

$$W_p(r, s) = \left\{ \inf_{w \in \Pi(r, s)} \sum_{x, x' \in \mathcal{X}} d^p(x, x') w_{x, x'} \right\}^{1/p},$$

(4)

where

$$\Pi(r, s) = \left\{ w \in \mathcal{P}(\mathcal{X} \times \mathcal{X}) : \sum_{x \in \mathcal{X}} w_{x, x'} = r_x \right\}$$

is the set of all couplings between $r$ and $s$. Furthermore, let

$$\mathcal{P}_p(\mathcal{X}) = \left\{ r \in \mathcal{P}(\mathcal{X}) : \sum_{x \in \mathcal{X}} d^p(x, x_0) r_x < \infty \right\}$$

be the set of probability measures on the countable metric space $\mathcal{X}$ with finite $p$-th moment w.r.t. $d$. Here, $x_0 \in \mathcal{X}$ is arbitrary and we want to mention that the space is independent of the choice of $x_0$. The weighted $\ell^1$-norm (2) can be extended in the following way to $\mathcal{P}_p(\mathcal{X} \times \mathcal{X})$

$$\|w\|_{\ell^1(d^p)} = \sum_{x, x' \in \mathcal{X}} d^p(x_0, x) |w_{x, x'}| + |w_{x_0, x'}|$$

$$+ \sum_{x, x' \in \mathcal{X}} d^p(x, x_0) |w_{x, x'}| + |w_{x, x_0}|.$$

2.2 Main Results

Before we can state the main results we need a few definitions.

Define the empirical measure generated by i.i.d. random variables $X_1, \ldots, X_n$ from the measure $r$ as

$$r_n = (\hat{r}_{n, x})_{x \in \mathcal{X}}, \text{ where } \hat{r}_{n, x} = \frac{1}{n} \sum_{k=1}^{n} \mathbf{1}\{X_k = x\},$$

(5)

and $s_m$ defined in the same way by $Y_1, \ldots, Y_m \overset{i.i.d.}{\sim} s$. In the following we will denote weak convergence by $\overset{w}{\to}$ and furthermore, let

$$\ell^\infty(\mathcal{X}) = \left\{ (a_x)_{x \in \mathcal{X}} \in \mathbb{R}^\mathcal{X} : \sup_{x \in \mathcal{X}} |a_x| < \infty \right\}$$

and

$$\ell^1(\mathcal{X}) = \left\{ (a_x)_{x \in \mathcal{X}} \in \mathbb{R}^\mathcal{X} : \sum_{x \in \mathcal{X}} |a_x| < \infty \right\}.$$
Finally, we also require a weighted version of the $\ell_\infty$-norm to characterize the set of dual solutions:

$$\|a\|_{\ell_\infty(1/d^p)} = \max \left( |a_{x_0}|, \sup_{x \neq x_0 \in \mathcal{X}} |d^{-p}(x,x_0)a_x| \right),$$

for $p \geq 1$. The space $\ell_\infty_{d^{-p}}(\mathcal{X})$ contains all elements which have a finite $\|\cdot\|_{\ell_\infty(1/d^p)}$-norm.

For $r, s \in \mathcal{P}_p(\mathcal{X})$ we define the following convex sets

$$S^*(r,s) = \left\{ (\lambda, \mu) \in \ell_{d^{-p}}(\mathcal{X}) \times \ell_{d^{-p}}(\mathcal{X}) : \langle r, \lambda \rangle + \langle s, \mu \rangle = W_p(r,s), \lambda_x + \mu_{x'} \leq d^p(x,x') \ \forall x, x' \in \mathcal{X} \right\} \quad (6)$$

and

$$S^* = \left\{ \lambda \in \ell_{d^{-p}}(\mathcal{X}) : \lambda_x - \lambda_{x'} \leq d^p(x,x') \ \forall x, x' \in \mathcal{X} \right\}. \quad (7)$$

For our limiting distributions we define the following (multinomial) covariance structure

$$\Sigma(r) = \begin{cases} r_x(1-r_x) & \text{if } x = x', \\ -r_xr_{x'} & \text{if } x \neq x'. \end{cases} \quad (8)$$

**Theorem 2.1.** Let $(\mathcal{X}, d)$ be a countable metric space and $r, s \in \mathcal{P}_p(\mathcal{X})$, $p \geq 1$, and $\hat{r}_n$ be generated by i.i.d. samples $X_1, \ldots, X_n \sim r$. Furthermore, let $G \sim \mathcal{N}(0, \Sigma(r))$ be a Gaussian process with $\Sigma$ as defined in (8). Assume (3) for some $x_0 \in \mathcal{X}$. Then

a) $$n^{\frac{1}{2p}}W_p(\hat{r}_n,r) \overset{d}{\rightarrow} \left\{ \max_{\lambda \in S^*} \langle G, \lambda \rangle \right\}^{\frac{1}{p}}, \text{ as } n \to \infty. \quad (9)$$

b) In the case where $r \neq s$ it holds for $n \to \infty$

$$n^{\frac{1}{p}}(W_p(\hat{r}_n,s) - W_p(r,s)) \overset{d}{\rightarrow} \frac{1}{p} W_p^{-1}r(s) \left\{ \max_{(\lambda,\mu) \in S^*(r,s)} \langle G, \lambda \rangle \right\}. \quad (10)$$

**Remark 2.2.** a) Note, that in the case $r \neq s$ in the one sample case (10) the objective function is independent of the second component $\mu$ of the feasible set $S^*(r,s)$. This is due to the fact that the second measure $s$ is deterministic in this case.

b) We will comment on condition (3), known from the Borisov-Durst Theorem (see Dudley (2014), Thm. 7.9), in Section 2.3.
c) Observe, that the limit in (10) is normally distributed if the set $S^*(r, s)$ is a singleton. In the case of finite $X$ conditions for $S^*(r, s)$ to be a singleton are known (Hung et al., 1986; Klee and Witzgall, 1968).

d) Parallel to our work del Barrio and Loubes (2017) showed asymptotic normality of EWD in general dimensions for the case $r \neq s$. Their results require the measures to have moments of order $4+\delta$ for some $\delta > 0$ and positive density on their convex support. Their proof relies on a Stein-identity.

e) We emphasize that our distributional limit also holds for $p \in (0, 1)$ even if $W_p$ is no longer a distance in this case.

f) The limiting distribution in the case $r = s$ can also be written as

$$\left\{ \max_{\lambda \in S^*} (G, \lambda) \right\}^{1/p} = W_p(G^+, G^-),$$

where $G^+$ and $G^-$ are the (pathwise) Jordan-decomposition of the Gaussian process $G$, such that $G = G^+ - G^-$. For more details see Appendix A.2.

For statistical applications it is also interesting to consider the two sample case, extensions to $k$-samples, $k \geq 2$ being obvious then.

**Theorem 2.3.** Under the same assumptions as in Thm. 2.1 and with $\hat{s}_m$ generated by $Y_1, \ldots, Y_m \stackrel{iid}{\sim} s$, independently of $X_1, \ldots, X_n$ and $H \sim \mathcal{N}(0, \Sigma(s))$, which is independent of $G$, and the extra assumption that $s$ also fulfills (3) the following holds.

a) Let $\rho_{n,m} = (nm/(n+m))^{1/2}$. If $r = s$ and $\min(n, m) \to \infty$ such that $m/(n+m) \to \alpha \in [0, 1]$ we have

$$\rho_{n,m}^{-1/p} W_p(\hat{r}_n, \hat{s}_m) \xrightarrow{\phi} \left\{ \max_{\lambda \in S^*} (G, \lambda) \right\}^{1/p}. \tag{11}$$

b) For $r \neq s$ and $n,m \to \infty$ such that $\min(n, m) \to \infty$ and $m/(n+m) \to \alpha \in [0, 1]$ we have

$$\rho_{n,m} W_p(\hat{r}_n, \hat{s}_m) - W_p(r, s) \xrightarrow{\phi} \frac{1}{p} W_p^{-1-p}(r, s) \left\{ \max_{(\lambda, \mu) \in S^*(r, s)} \sqrt{\alpha}(G, \lambda) + \sqrt{1-\alpha}(H, \mu) \right\}. \tag{12}$$

Note, that we obtain different scaling rates under equality of measures $r = s$ (null-hypothesis) and the case $r \neq s$ (alternative), which has important statistical consequences. For $r \neq s$ we are in the regime of the standard C.L.T. $\sqrt{n}$, but for $r = s$ we get the rate $n^{1/p}$, which is strictly slower for $p > 1$. According to Bobkov and Ledoux (2014) Thm. 7.11 in the one dimensional case this rate is optimal since the support of a probability measure on a countable metric space is not connected.
Remark 2.4. In the case of dependent data the results from Thm. 2.1 and 2.3 can also be applied, if one shows the weak convergence of the empirical process w.r.t. the $\| \cdot \|_{\ell_1(D^p)}$-norm. All other steps of the proof remain unchanged.

The rest of this subsection is devoted to the proofs of Theorem 2.1 and Theorem 2.3.

Proof of Thm. 2.1 and Thm. 2.3. To prove these two theorems we use the delta method A.2. Therefore, we need to verify (1.) directional Hadamard differentiability of $W_p(\cdot, \cdot)$ and (2.) weak convergence of $\sqrt{n}(\hat{r}_n - r)$. We mention that the delta method required here is not standard as the directional Hadamard derivative is not linear (see Römisch (2004), Shapiro (1991) or Dümbgen (1993)).

1. In Appendix A.1, Theorem A.3 directional Hadamard differentiability of $W_p$ is shown with respect to the $\| \cdot \|_{\ell_1(D^p)}$-norm (2).

2. The weak convergence of the empirical process w.r.t. the $\| \cdot \|_{\ell_1(D^p)}$-norm is addressed in the following lemma.

Lemma 2.5. Let $X_1, \ldots, X_n \sim r$ be i.i.d. taking values in a countable metric space $(X,d)$ and let $\hat{r}_n$ be the empirical measure as defined in (5). Then

$$\sqrt{n}(\hat{r}_n - r) \xrightarrow{D} G$$

with respect to the $\| \cdot \|_{\ell_1(D^p)}$-norm, where $G$ is a Gaussian process with mean 0 and covariance structure

$$\Sigma(r) = \begin{cases} r_x(1 - r_x) & \text{if } x = x', \\ -r_x r_{x'} & \text{if } x \neq x', \end{cases}$$

as given in (8) if and only if condition (3) is fulfilled.

Proof of Lemma. The weighted $\ell^1$-space $\ell^1_\text{dip}$ is according to Prop. 3, Maulney (1973) of cotype 2, hence $\sqrt{n}(\hat{r}_n - r)$ converges weakly w.r.t. the $\ell^1_\text{dip}$-norm by Corollary 1 in Jain (1977) if and only if the summability condition (3) is fulfilled.

Theorem 2.1 a) is now a straight forward application of the delta method A.2 and the continuous mapping theorem for $f(x) = x^{1/p}$.

For Theorem 2.1 b) we use again the delta method, but this time in combination with the chain rule for directional Hadamard differentiability (Prop. 3.6 (i), Shapiro (1990)).
The proof of Theorem 2.3 works analogously. Note, that under the assumptions of the theorem it holds \((r = s)\)

\[
\rho_{n,m}(\hat{r}_n, \hat{s}_m) - (r, s) = \left( \sqrt{\frac{m}{n+m}} \sqrt{n}(\hat{r}_n - r), \sqrt{\frac{n}{n+m}} \sqrt{m}(\hat{s}_m - s) \right) \xrightarrow{D} (\sqrt{\alpha} G, \sqrt{1 - \alpha} G')
\]

(13)

with \(G' \equiv G\).

2.3 Examination of the summability condition (3)

According to Lemma 2.5 condition (3) is necessary and sufficient for the weak convergence with respect to the \(\| \cdot \|_{\ell_1(d\nu)}\)-norm (2). As this condition is crucial for our main theorem and we are not aware of a comprehensive discussion, we will provide such in this section.

The following question arises. "If the condition holds for \(p\) does it then also hold for all \(p' \leq p\)?" This is not true in general, but it is true if \(\mathcal{X}\) has no accumulation point (i.e., is discrete in the topological sense).

**Lemma 2.6.** Let \(\mathcal{X}\) be a space without an accumulation point. If condition (3) holds for \(p\), then it also holds for all \(p' \leq p\).

*Proof.* Let \(\mathcal{X}\) be a space without an accumulation point, i.e., there exists \(\epsilon > 0\) such that \(d(x, x_0) > \epsilon\) for all \(x \neq x_0 \in \mathcal{X}\). Then,

\[
\sum_{x \in \mathcal{X}} q^p(x_0, x) \sqrt{T_x} = \epsilon^p \sum_{x \in \mathcal{X}} \left( \frac{d(x_0, x)}{\epsilon} \right)^p \sqrt{T_x} \\
\geq \epsilon^p \sum_{x \in \mathcal{X}} \left( \frac{d(x_0, x)}{\epsilon} \right)^{p'} \sqrt{T_x} \\
= \epsilon^{p/p'} \sum_{x \in \mathcal{X}} q^{p'}(x_0, x) \sqrt{T_x}.
\]

\(\square\)

**Exponential families** As we will see, condition (3) is fulfilled for many well known distributions including the Poisson distribution, geometric distribution or negative binomial distribution with the euclidean distance as the ground measure \(d\) on \(\mathcal{X} = \mathbb{N}\).

**Theorem 2.7.** Let \((P_\eta)_{\eta}\) be an \(s\)-dimensional standard exponential family (SEF) (see Lehmann and Casella (1998), Sec. 1.5) of the form

\[
r_\eta^x = h_x \exp \left( \sum_{i=1}^s \eta_i T_i^x - A(\eta) \right).
\]

The summability condition (3) is fulfilled if \((P_\eta)_{\eta}\) satisfies
1.) \( h_x \geq 1 \) for all \( x \in \mathcal{X} \),

2.) the natural parameter space \( \mathcal{N} \) is closed with respect to multiplication with \( \frac{1}{2} \), i.e., \( \sum_{x \in \mathcal{X}} r_x^\eta < \infty \Rightarrow \sum_{x \in \mathcal{X}} r_x^{\eta/2} < \infty \),

3.) the \( p \)-th moment w.r.t. the metric \( d \) on \( \mathcal{X} \) exists, i.e., \( \sum_{x \in \mathcal{X}} d^p(x, x_0)r_x < \infty \) for some arbitrary, but fixed \( x_0 \in \mathcal{X} \).

Proof. For the SEF in (14) condition (3) reads

\[
\sum_{x \in \mathcal{X}} d^p(x_0, x) \sqrt{\exp \left( \frac{1}{2} \sum_{i=1}^{s} \eta_i T_i x - A(\eta) \right)} h_x
\]

\[
= \frac{1}{\sqrt{\lambda(\eta)}} \sum_{x \in \mathcal{X}} d^p(x_0, x) \exp \left( \frac{1}{2} \sum_{i=1}^{s} \eta_i T_i x \right) \sqrt{h_x}
\]

\[
\leq \frac{\lambda(\frac{1}{2} \eta)}{\sqrt{\lambda(\eta)}} \sum_{x \in \mathcal{X}} d^p(x_0, x) \exp \left( \frac{1}{2} \sum_{i=1}^{s} \eta_i T_i x \right) h_x < \infty,
\]

where \( \lambda(\eta) \) denotes the Laplace transform. The first inequality is due to the fact that \( h_x \geq 1 \) for all \( x \in \mathcal{X} \) and the second is a result of the facts that the natural parameter space is closed with respect to multiplication with \( \frac{1}{2} \) and that the \( p \)-th moment w.r.t. \( d \) exist.

The following examples show, that all three conditions in Theorem 2.7 are necessary.

Example 2.8. Let \( \mathcal{X} \) be the countable metric space \( \mathcal{X} = \{ \frac{1}{k} \}_{k \in \mathbb{N}} \) and let \( r \) be the measure with probability mass function

\[ r_{1/k} = \frac{1}{\zeta(\eta)} \frac{1}{k^n} \]

with respect to the counting measure. Here, \( \zeta(\eta) \) denotes the Riemann zeta function. This is an SEF with natural parameter \( \eta \), natural statistic \( -\log(k) \) and natural parameter space \( \mathcal{N} = (1, \infty) \). We choose the euclidean distance as the distance \( d \) on our space \( \mathcal{X} \) and set \( x_0 = 1 \). It holds

\[
\sum_{k=1}^{\infty} \left| 1 - \frac{1}{k} \right|^p \frac{1}{\zeta(\eta)} \frac{1}{k^n} \leq \sum_{k=1}^{\infty} \frac{1}{\zeta(\eta)} \frac{1}{k^n} = 1 < \infty \quad \forall \eta \in \mathcal{N}
\]

and hence all moments exist for all \( \eta \) in the natural parameter space. Furthermore, \( h_{1/k} \equiv 1 \). However, the natural parameter space is not closed with respect to multiplication with \( \frac{1}{2} \) and therefore,

\[
\sum_{k=1}^{\infty} \left| 1 - \frac{1}{k} \right|^p \frac{1}{\zeta(\eta)} \frac{1}{k^{n/2}} \geq \sum_{k=2}^{\infty} \frac{1}{2^p} \sum_{k=2}^{\infty} \frac{1}{\sqrt{\zeta(\eta)}} \frac{1}{k^{n/2}} = \infty \quad \forall \eta \in (1, 2],
\]

i.e., condition (3) is not fulfilled.
The next example shows, that we cannot omit condition 1.) in Thm. 2.7.

**Example 2.9.** Consider $X = \mathbb{N}$ with the metric $d(k,l) = \sqrt{|k|! - |l|!}$. The family of Poisson distributions constitute an SEF with natural parameter space $\mathcal{N} = (-\infty, \infty)$ which satisfies condition 2.) in Thm. 2.7, i.e., closed with respect to multiplication with $\frac{1}{2}$. The first moment with respect to this metric exists and $h_k < 1$ for all $k \geq 2$. Condition (3) for $p = 1$ with $x_0 = 0$ reads

$$\sum_{k=1}^{\infty} \sqrt{k!} \left[ \frac{\eta^k}{k!} \exp(-\eta) \right] = \sum_{k=1}^{\infty} \eta^{k/2} \exp(-\eta/2) = \infty$$

for all $\eta > 1$, i.e., the summability condition (3) is not fulfilled.

If the $p$-th moment does not exist, it is clear that condition (3) cannot be fulfilled as $\sqrt{x} \geq x$ for $x \in [0,1]$.

### 2.4 Approximation of continuous distributions

In this section we investigate to what extent we can approximate continuous measure by its discretization such that condition (3) remains valid. Let $\mathcal{X} = (\frac{k}{M})_{k \in \mathbb{Z}}$ be a discretization of $\mathbb{R}$ and $X$ a real-valued random variable with c.d.f. $F$ which is continuous and has a Lebesgue density $f$. We take $d$ to be the euclidean distance and $x_0 = 0$. For $k \in \mathbb{Z}$ we define

$$r_k := F\left(\frac{k+1}{M}\right) - F\left(\frac{k}{M}\right).$$

Now, (3) can be estimated as follows.

$$\sum_{k=-\infty}^{\infty} \left| \frac{k}{M} \right|^p \sqrt{F\left(\frac{k+1}{M}\right) - F\left(\frac{k}{M}\right)}$$

$$= \sum_{k=-\infty}^{\infty} \left| \frac{k}{M} \right|^p \frac{1}{\sqrt{M}} M^{k+1/M} \int_{k/M}^{k+1/M} f(x)dx$$

$$\geq \sum_{k=-\infty}^{\infty} \left| \frac{k}{M} \right|^p \sqrt{M} \int_{k/M}^{k+1/M} \sqrt{f(x)}dx$$

$$\geq \sqrt{M} \sum_{k=-\infty}^{\infty} \frac{1}{2^p} \int_{k/M}^{k+1/M} |x|^p \sqrt{f(x)}dx$$

$$= \sqrt{M} \frac{1}{2^p} \int_{\mathbb{R}} |x|^p \sqrt{f(x)}dx,$$

where the first inequality is due to Jensen’s inequality. As the r.h.s. tends to infinity with rate $\sqrt{M}$ as $M \to \infty$, condition (3) does not hold in the limit. Consequently, we are not able to derive distributional limits for continuous measures from our results.
The one-dimensional case \( D = 1 \) For the rest of this Section we consider \( \mathcal{X} = \mathbb{R} \) and want to put condition (3) in relation to the condition (del Barrio et al., 1999b)

\[
\int_{-\infty}^{\infty} \sqrt{F(t)(1 - F(t))} dt < \infty, \tag{17}
\]

where \( F(t) \) denotes the cumulative distribution function, which is sufficient and necessary for the empirical 1-Wasserstein distance on \( \mathbb{R} \) to satisfy a limit law (see also Corollary 1 in Jain (1977) in a more general context). Condition (3) is stronger than (17) as the following shows. Let \( \mathcal{X} \) be a countable subset of \( \mathbb{R} \) and index the elements \( x_i \) for \( i \in \mathbb{Z} \) such that they are ordered. Furthermore, let \( d(x, y) = |x - y| \) be the euclidean distance on \( \mathcal{X} \). For any measure \( r \) with cumulative distribution function \( F \) on \( \mathcal{X} \) it holds

\[
\int_{-\infty}^{\infty} \sqrt{F(t)(1 - F(t))} dt \\
= \sum_{k \in \mathbb{Z}} d(x_k, x_{k+1}) \sqrt{\sum_{j \leq k} r_j} \sqrt{\sum_{j > k} r_j} \\
\leq \sum_{k=0}^{\infty} d(x_k, x_{k+1}) \sqrt{\sum_{j > k} r_j} + \sum_{k=-\infty}^{1} d(x_k, x_{k+1}) \sqrt{\sum_{j \leq k} r_j} \\
\leq \sum_{k=0}^{\infty} d(x_k, x_{k+1}) \sum_{j > k} \sqrt{r_j} + \sum_{k=-\infty}^{1} d(x_k, x_{k+1}) \sum_{j \leq k} \sqrt{r_j} \\
= \sum_{k=0}^{\infty} d(x_0, x_k) \sqrt{r_k} + \sum_{k=-\infty}^{1} d(x_0, x_k) \sqrt{r_k}.
\]

Hence, if condition (3) holds, (17) is also fulfilled. However, the conditions are not equivalent as the following example shows.

**Example 2.10.** Let \( \mathcal{X} = \mathbb{N} \) and \( d(x, y) = |x - y| \) the euclidean distance and \( r \) a power-law, i.e., \( r_n = \frac{1}{\zeta(s)} \frac{1}{n^s} \), where \( \zeta(s) \) is the Riemann zeta function. In this case (17) reads

\[
\int_{-\infty}^{\infty} \sqrt{F(t)(1 - F(t))} dt = \frac{1}{\zeta(s)} \sum_{k=1}^{\infty} \left( \frac{1}{j^s} \sum_{j=k+1}^{\infty} \frac{1}{j^s} \right) \\
\leq \frac{1}{\zeta(s)} \sum_{k=1}^{\infty} \left( \frac{1}{j^s} \sum_{j=k+1}^{\infty} \frac{1}{j^s} \right) \leq \frac{1}{\zeta(s)} \sum_{k=1}^{\infty} \left( \frac{1}{k^s} \right) \\
\]

and this is finite for all \( s > 3 \). On the other hand, condition (3) reads as

\[
\sum_{k=1}^{\infty} (k - 1) \frac{1}{\zeta(s)} \frac{1}{k^s} \leq \frac{1}{\sqrt{\zeta(s)}} \sum_{k=1}^{\infty} \frac{1}{k^{s/2 - 1}}.
\]
This is finite for all $s > 4$. Hence, condition (17) is fulfilled for $s \in (3,4]$, but not (3).

For $p=2$ in dimension $D=1$ there is no such easy condition anymore in the case of continuous measures, see del Barrio et al. (2005). Already for the normal distribution one needs to subtract a term that tends sufficiently fast to infinity to get a distributional limit (which was originally proven by de Wet and Venter (1972)). Nevertheless, for a fixed discretization of the normal distribution via binning as in (16) condition (3) is fulfilled and Theorems 2.1 and 2.3 are valid.

3 Limiting Distribution for Tree Metrics

3.1 Explicit limits

In this subsection we give an explicit expression for the limiting distribution in (9) and (11) in the case $r = s$ when the metric is generated by a weighted tree. This extends Thm. 5 in Sommerfeld and Munk (2016) for finite spaces to countable spaces $\mathcal{X}$. In the following we recall their notation.

Assume that the metric structure on the countable space $\mathcal{X}$ is given by a weighted tree, that is, an undirected connected graph $\mathcal{T} = (\mathcal{X}, E)$ with vertices $\mathcal{X}$ and edges $E \subset \mathcal{X} \times \mathcal{X}$ that contains no cycles. We assume the edges to be weighted by a function $w : E \to \mathbb{R}_+$. Without imposing any further restriction on $\mathcal{T}$, we assume it to be rooted at $\text{root}(\mathcal{T}) \in \mathcal{X}$, say. Then, for $x \in \mathcal{X}$ and $x \neq \text{root}(\mathcal{T})$ we may define parent$(x) \in \mathcal{X}$ as the immediate neighbour of $x$ in the unique path connecting $x$ and root$(\mathcal{T})$. We set parent$(\text{root}(\mathcal{T})) = \text{root}(\mathcal{T})$. We also define children$(x)$ as the set of vertices $x' \in \mathcal{X}$ such that there exists a sequence $x' = x_1, \ldots, x_n = x \in \mathcal{X}$ with parent$(x_j) = x_{j+1}$ for $j = 1, \ldots, n - 1$. Note that with this definition $x \in \text{children}(x)$. Furthermore, observe that children$(x)$ can consist of countably many elements, but the path joining $x$ and $x' \in \text{children}(x)$ is still finite as explained below.

For $x, x' \in \mathcal{X}$ let $e_1, \ldots, e_n \in E$ be the unique path in $\mathcal{T}$ joining $x$ and $x'$, then the length of this path,

$$d_\mathcal{T}(x, x') = \sum_{j=1}^{n} w(e_j),$$

defines a metric $d_\mathcal{T}$ on $\mathcal{X}$. This metric is well defined, since the unique path joining $x$ and $x'$ is finite as we show in the following. Let $A_0 = \{x \in \mathcal{X} : x = \text{root}(\mathcal{T})\}$ and $A_k = \{x \in \mathcal{X} : \text{parent}(x) \in A_{k-1}\}$ for $k \in \mathbb{N}$. By the definition of the $A_k$, these sets are disjoint and it follows $\bigcup_{k=0}^{\infty} A_k = \mathcal{X}$. Now let $x, x' \in \mathcal{X}$, then there exist $k_1$ and $k_2$ such that $x \in A_{k_1}$ and $x' \in A_{k_2}$. Then, there is a sequence of $k_1 + k_2 + 1$ vertices connecting $x$ and $x'$. Hence, the unique path joining $x$ and $x'$ has at most $k_1 + k_2$ edges.
Additionally, define
\[(S_T u)_x = \sum_{x' \in \text{children}(x)} u_{x'}\]
and
\[Z_{T,p}(u) = \left\{ \sum_{x \in X} |(S_T u)_x| d_T(x, \text{parent}(x))^p \right\}^{\frac{1}{p}} \tag{18}\]
for \(u \in \mathbb{R}^X\) and we set w.l.o.g. \(x_0 = \text{root}(T)\).

The main result of this section is the following.

**Theorem 3.1.** Let \(r \in \mathcal{P}_p(X)\), defining a probability distribution on \(X\) that fulfils condition (3) and let the empirical measures \(\hat{r}_n\) and \(\hat{s}_m\) be generated by independent random variables \(X_1, \ldots, X_n\) and \(Y_1, \ldots, Y_m\), respectively, all drawn from \(r = s\).

Then, with a Gaussian vector \(G \sim N(0, \Sigma(r))\) with \(\Sigma(r)\) as defined in (8) we have the following.

a) **(One sample)** As \(n \to \infty\),
\[n^{\frac{1}{p}} W_p(\hat{r}_n, r) \xrightarrow{D} Z_{T,p}(G) \tag{19}\]

b) **(Two sample)** If \(n \wedge m \to \infty\) and \(n/(n + m) \to \alpha \in [0, 1]\) we have
\[\left( \frac{nm}{n + m} \right)^{\frac{1}{p}} W_p(\hat{r}_n, \hat{s}_m) \xrightarrow{D} Z_{T,p}(G) \tag{20}\]

A rigorous proof of Thm. 3.1 is given in Appendix A.3.

The same result was derived in Sommerfeld and Munk (2016) for finite spaces. For \(X\) countable we require a different technique of proof. Simplifying the set of dual solutions in the same way, the second step of rewriting the target function with a summation and difference operator does not work in the case of measures with countable support, since the inner product of the operators applied to the parameters is no longer well defined. For this setting we need to introduce a new basis in \(\ell^1_{dp}(X)\) and for each element \(\mu \in \ell^1_{dp}(X)\) a sequence which has only finitely many non-zeros that converges to \(\mu\) in order to obtain an upper bound on the optimal value. Then, we define a feasible solution for which this upper bound is attained.

### 3.2 Distributional Bound for the Limiting Distribution

In this section we use the explicit formula on the r.h.s. of (19) for the case of tree metrics to stochastically bound the limiting distribution.

This is based on the following simple observation: Let \(T\) be a spanning tree of \(X\) and \(d_T\) the tree metric generated by \(T\) and the weights \((x, x') \mapsto d(x, x')\)
as described in Section 3.1. Then for any \( x, x' \in X \) we have \( d(x, x') \leq d_T(x, x') \). Let \( S^* \) denote the set defined in (7) with the metric \( d_T \) instead of \( d \). Then \( S^* \subset S^*_T \) and hence
\[
\max_{\lambda \in S^*} \langle v, \lambda \rangle \leq \max_{\lambda \in S^*_T} \langle v, \lambda \rangle
\]
for all \( v \in \mathbb{R}^X \). It follows that
\[
\max_{\lambda \in S^*} \langle v, \lambda \rangle \leq Z_{T,p}(v) \quad (21)
\]
for all \( v \in \mathbb{R}^X \) and this proves the following main result of this subsection.

**Theorem 3.2.** Let \( r, s \in \mathcal{P}_p(X) \), assume that \( r, s \) fulfil condition (3) and let \( \hat{r}_n, \hat{s}_m \) be generated by i.i.d. \( X_1, \ldots, X_n \sim r \) and \( Y_1, \ldots, Y_m \sim s \), respectively. Let further \( T \) be a spanning tree of \( X \). Then, under the null hypothesis \( r = s \), we have, as \( n \) and \( m \) approach infinity such that \( n \wedge m \to \infty \) and \( n/(n + m) \to \alpha \), that
\[
\limsup_{n,m \to \infty} P \left[ \left( \frac{nm}{n + m} \right)^{1/p} W_p(\hat{r}_n, \hat{s}_m) \geq z \right] \leq P \left[ Z_{T,p}(G) \geq z \right], \quad (22)
\]
where \( G \sim \mathcal{N}(0, \Sigma(r)) \) with \( \Sigma(r) \) as defined in (8).

**Remark 3.3.** While the stochastic bound of the limiting distribution \( Z_{T,p} \) is very fast to compute as it is explicitly given, the Wasserstein distance \( W_p(\hat{r}_n, \hat{s}_m) \) in (22) is a computational bottleneck. Classical general-purpose approaches, e.g., the simplex algorithm (Luenberger and Ye, 2008) for general linear programs or the auction algorithm for network flow problems (Bertsekas, 1992, 2009) were found to scale rather poorly to very large problems such as image retrieval (Rubner et al., 2000).

Attempts to solve this problem include specialized algorithms (Gottschlich and Schuhmacher, 2014) and approaches leveraging additional geometric structure of the data (Ling and Okada, 2007; Schmitzer, 2016). However, many practical problems still fall outside the scope of these methods (Schrieber et al., 2017), prompting the development of numerous surrogate quantities which mimic properties of optimal transport distances and are amenable to efficient computation. Examples include Pele and Werman (2009); Shirdhonkar and Jacobs (2008); Bonneel et al. (2015) and the particularly successful entropically regularized transport distances (Cuturi, 2013; Solomon et al., 2015).

In the next section we will discuss how to approximate the countable space \( X \) by a finite collection of points. Here, we want to mention that the distributional bound also holds on a finite collection of points.

## 4 Computational strategies for simulating the limit laws

If we want to simulate the limiting distributions in Thm. 2.1 and 2.3 we need to restrict to a finite number \( N \) of points, i.e., we choose a subset \( I \) of \( X \) such
that \( \#I = N \). Let \( r \in \mathcal{P}_p(X) \) fulfilling (3) and \( G \sim \mathcal{N}(0, \Sigma(r)) \), we define \( G^I = (G^I)_x = G_x \mathbb{1}_{\{x \in I\}} \). An upper bound for the difference between the exact limiting distribution and the limiting distribution on the finite set \( I \) in the one sample case for \( r = s \) is given as (see (21))

\[
\left| \max_{\lambda \in S^*} (G^I, \lambda) - \max_{\lambda \in S^*} (G, \lambda) \right| \leq \max_{\lambda \in S^*_T} |G^I - G, \lambda| \\
= \max \left\{ \max_{\lambda \in S^*_T} (G^I - G, \lambda), \max_{\lambda \in S^*_T} (G - G^I, \lambda) \right\} \\
= \sum_{x \in \mathcal{X}} |(S_T(G^I - G))_x| d_T(x, \text{parent}(x))^p \\
= \sum_{x \notin I} |G_x| d_T(x, \text{root}(T))^p.
\]

For the last equality one needs to construct the tree as follows: Choose \( I \) such that \( x_0 \) from condition (3) is an element of \( I \) and choose \( x_0 \) to be the root of the tree and let all other elements of \( X \) be direct children of the root, i.e., \( \text{children}(x) = x \) for all \( x \neq \text{root}(T) \in X \). The upper bound can be made stochastically arbitrarily small as

\[
E \left[ \sum_{x \notin I} |G_x| d_T(x, \text{root}(T))^p \right] \leq \sum_{x \notin I} d_T(x, \text{root}(T))^p \sqrt{r_x(1 - r_x)}, \tag{23}
\]

where we used Hölder’s inequality and the definition of \( \Sigma(r) \). As the root was chosen to be \( x_0 \), the sum above is finite as \( r \) fulfills condition (3) and becomes arbitrarily small for \( I \) large enough. Hence, (23) details that the speed of approximation by \( G^I \) depends on the decay of \( r \) and suggests to choose \( I \) such that most of the mass of \( r \) is concentrated on it.

However, the computation of \( \max_{\lambda \in S^*} \langle G^I, \lambda \rangle \) is a linear program with \( N^2 \) constraints and \( N \) variables and hence as difficult as the computation of the WD between two measures supported on \( I \), i.e., on \( N \) points. This renders a naive Monte-Carlo approach to obtain quantiles computational infeasible for large \( N \). In the following subsections we therefore discuss possibilities to make the computation of the limit more accessible.

### 4.1 Thresholded Wasserstein distance

Following Pele and Werman (2009) we define for a thresholding parameter \( t \geq 0 \) the thresholded metric

\[
d_t(x, x') = \min \{ d(x, x'), t \}. \tag{24}
\]
Then, \(d_t\) is again a metric. Let \(W_p^t(r, s)\) be the Wasserstein distance with respect to \(d_t\). Since \(d_t(x, x') \leq d(x, x')\) for all \(x, x' \in \mathcal{X}\) we have that \(W_p^t(r, s) \leq W_p(r, s)\) for all \(r, s \in \mathcal{P}(\mathcal{X})\) and all \(t \geq 0\).

**Theorem 4.1.** The limiting distribution from Thm. 2.1 with the thresholded ground distance \(d_t\) instead of \(d\) can be computed in \(O(N^2 \log N)\) time with \(O(N)\) memory requirement, if each point in \(\mathcal{X}\) has \(O(1)\) neighbours with distance smaller or equal to \(t\). The limiting distribution can be calculated as the optimal value of the following network flow problem:

\[
\min_{w \in \mathbb{R}^{X \times X}_+} \sum_{x, x' \in \mathcal{X}} d_p^t(x, x')w_{x,x'}
\]

subject to \(\sum_{x \neq x' \in \mathcal{X}} w_{x,x} - \sum_{x' \neq x \in \mathcal{X}} w_{x,x'} = G_x,\)

where \(G = (G_x)_{x \in \mathcal{X}}\) is a Gaussian process with mean zero and covariance structure as defined in (8).

**Proof.** If we take the thresholded distance as the ground distance similar as in Theorem 2.1 we obtain the limiting distribution as

\[
\left\{ \max_{\lambda \in \mathbb{R}^X} (G, \lambda) \right\}^{1/p},
\]

where now \(S^t_p = \{ \lambda \in \mathbb{R}^X : \lambda_x - \lambda_{x'} \leq d_p^t(x, x') \}\). The \(p\)-th power of the limiting distribution is again a finite dimensional linear program and since there is strong duality in this case, it is equivalent to solve (25). As the linear program (25) is a network flow problem, we can redirect all edges with length \(t\) through a virtual node without changing the optimal value. From the assumption that each point has \(O(1)\) neighbours with distance not equal to \(t\), we can deduce that the number of edges \((N^2\) in the original problem) is reduced to \(O(N)\). According to Pele and Werman (2009) the new linear program with the virtual node can be solved in \(O(N^2 \log N)\) time with \(O(N)\) memory requirement.

**Remark 4.2.**

a) In contrast to the computation of the limiting distribution for the thresholded Wasserstein distance in Thm. 4.1, general purpose network flow algorithms such as the auction algorithm, Orlin’s algorithm or general purpose LP solvers are required for the computation of the limiting distribution with a generic ground distance (that is, not thresholded). These algorithms have at least cubic worst case complexity (Bertsekas, 1981; Orlin, 1993) and quadratic memory requirement and perform much worse than \(O(N^2)\) empirically (Gottschlich and Schuhmacher, 2014).

b) The resulting network flow problem can be tackled with existing efficient solvers (Bertsekas, 1992) or commercial solvers like CPLEX (https://www.ibm.com/jp-en/marketplace/ibm-ilog-cplex) which exploit the network structure.
c) For the distributional bound (22) one can also use the thresholded Wasserstein distance $W_t^p$ instead of $W^p$ to be computationally more efficient. A large threshold $t$ will result in a better approximation of the true Wasserstein distance, but will also require more computation time.

4.2 Regular Grids

In this section we are going to derive an explicit formula for the distributional bound from Section 3.2, when $X$ is a regular grid. In this case a spanning tree can be constructed from a dyadic partition. Let $D$ be a positive integer, $L$ a power of two and $X$ the regular grid of $L^D$ points in the unit hypercube $[0,1]^D$. The general case is analogous, but it is cumbersome. For $0 \leq l \leq l_{\text{max}}$ with

$$l_{\text{max}} = \log_2 L$$

let $P_l$ be the natural partition of $X$ into $2^{Dl}$ squares of each $L^D/2^{Dl}$ points.

**Theorem 4.3.** Under the assumptions described above, (22) reads

$$Z_{T,p}(u) = \left\{ \sum_{l=0}^{l_{\text{max}}} D^{p/2} 2^{-p(l+1)} \sum_{F \in P_l} |S_F u| \right\}^{1/p}.$$  \hspace{1cm} (26)

This expression can be evaluated efficiently and used with Theorem 3.2 to obtain a stochastic bound of the limiting distribution on regular grids.

**Proof.** Define $X'$ by adding to $X$ all center-points of sets in $P_l$ for $0 \leq l < l_{\text{max}}$. We identify center points of $P_{l_{\text{max}}}$ with the points in $X$. A tree with vertices $X'$ can now be build using the inclusion relation of the sets $\{P_l\}_{0 \leq l \leq l_{\text{max}}}$ as ancestry relation. More precisely, the leaves of the tree are the points of $X'$ and the parent of the center point of $F \in P_l$ is the center point of the unique set in $P_{l-1}$ that contains $F$.

If we use the Euclidean metric to define the distance between neighboring vertices we get

$$d_T(x, \text{parent}(x)) = \sqrt{D^2 2^{-l}},$$

if $x \in P_l$.

A measure $r$ on $X$ naturally extends to a measure on $X'$ if we give zero mass to all inner vertices. We also denote this measure by $r$. Then, if $x \in X'$ is the center point of the set $F \in P_l$ for some $0 \leq l \leq l_{\text{max}}$, we have that $(S_T r)_x = S_F r$ where $S_F r = \sum_{x \in F} r_x$. Inserting this two formulas into (22) yields (26). \hfill $\square$

5 Application: Single-Marker Switching Microscopy

Single Marker Switching (SMS) Microscopy (Betzig et al., 2006; Rust et al., 2006; Egner et al., 2007; Heilemann et al., 2008; Fölling et al., 2008) is a living
cell fluorescence microscopy technique in which fluorescent markers which are
tagged to a protein structure in the probe are stochastically switched from a no-
signal giving (off) state into a signal-giving (on) state. A marker in the on state
emits a bunch of photons some of which are detected on a detector before it is
either switched off or bleached. From the photons registered on the detector,
the position of the marker (and hence of the protein) can be determined. The
final image is assembled from all observed individual positions recorded in a
sequence of time intervals (frames) in a position histogram, typically a pixel
grid.

SMS microscopy is based on the principle that at any given time only a
very small number of markers are in the on state. As the probability of switch-
ing from the off to the on state is small for each individual marker and they
remain in the on state only for a very short time (1-100ms). This allows SMS mi-
croscopy to resolve features below the diffraction barrier that limits conventional
far-field microscopy (see Hell (2007) for a survey) because with overwhelming
probability at most one marker within a diffraction limited spot is in the on
state (Aspelmeier et al., 2015). At the same time this requires quite long ac-
quisition times (1min-1h) to guarantee sufficient sampling of the probe. As a
consequence, if the probe moves during the acquisition, the final image will be
blurred.

Correcting for this drift and thus improving image quality is an area of active
research (Geisler et al., 2012; Deschout et al., 2014; Hartmann et al., 2016). In
order to investigate the validity of such a drift correction method we introduce a
test of the Wasserstein distance between the image obtained from the first half of
the recording time and the second half. This test is based on the distributional
upper bound of the limiting distribution which was developed in Section 3.2 in
combination with a lower bound of the Wasserstein distance (Pele and Werman,
2009). In fact, there is no standard method for problems of this kind and we
argue that the (thresholded) Wasserstein distance is particular useful in such
a situation as the specimen moves between the frames without loss of mass,
ence the drift induces a transport structure between successive frames. In the
following we compare the distribution from the first half of frames with the
distribution from the second half scaled with the sample sizes (as in (20)). We
reject the hypothesis that the distributions from the first and the second half are
the same, if our test statistic is larger than the $1-\alpha$ quantile of the distributional
bound of the limiting distribution in (22). If we have statistical evidence that
the tresholded Wasserstein distance is not zero, we can also conclude that there
is a significant difference in the Wasserstein distance itself.

Statistical Model

It is common to assume the bursts of photons registered
on the detector as independent realizations of a random variable with a density
that is proportional to the density of markers in the probe (Aspelmeier et al.,
2015). As it is expected that the probe drifts during the acquisition this density
will vary over time. In particular, the positions registered at the beginning of
the observation will follow a different distribution than those observed at the
end.

Data and Results  We consider an SMS image of a tubulin structure presented in Hartmann et al. (2016) to assess their drift correction method. This image is recorded in 40,000 single frames over a total recording time of 10 minutes (i.e., 15 ms per frame). We compare the aggregated sample collected during the first 50% (= 20,000 frames) of the total observation time with the aggregated sample obtained in the last 50% on a 256 × 256 grid for both the original uncorrected values and for the values where the drift correction of Hartmann et al. (2016) was applied. Heat maps of these four samples are shown in the left hand side of Figure 1 (no correction) and Figure 2 (corrected), respectively.

The question we will address is: "To what extend has the drift been properly removed by the drift correction?" In addition, from the application of the thresholded Wasserstein distance for different thresholds we expect to obtain detailed understanding for which scales the drift has been removed. As Hartmann et al. (2016) have corrected with a global drift function one might expect that on small spatial scales not all effects have been removed.

We compute the thresholded Wasserstein distance $W^t_1$ between the two pairs
Figure 2: Left: Aggregated samples of the first (first row) and the last (second row) 50% of the observation time as heat maps of relative frequency with correction for the drift of the probe. Magnifications of a small area are shown to highlight the drift correction of the picture. Right: Empirical distribution function of a sample from the upper bound (tree approximation) of the limiting distribution. The red dot (line) indicates the scaled thresholded Wasserstein distance after drift correction for $t = 6/256$. The difference between the first and the second 50% is no longer significant.
of samples as described in Section 4.1 with different thresholds $t \in \{2, 3, \ldots, 14\}/256$. We compare these values with a sample from the stochastic upper bound for the limiting distribution on regular grids obtained as described in Section 4.2. This allows us to obtain a test for the null hypothesis ‘no difference’ based on Theorem 3.2. To visualize the outcomes of these tests for different thresholds $t$ we have plotted the corresponding p-values in Figure 3. The red line indicates the magnitude of the drift over the total recording time. As the magnitude is approximately $6/256$, we plot in the right hand side of Figure 1 and Figure 2 the empirical distribution functions of the upper bound (22) and indicate the value of the test-statistic for $t = 6/256$ with a red dot without the drift correction and with the correction, respectively.

As shown in Figure 3 the differences caused by the drift of the probe are recognized as highly statistically significant ($p \leq 0.05$) for thresholds larger than $t = 4/256$. After the drift correction method is applied, the difference is no longer significant for thresholds smaller than $t = 14/256$. The estimated shift during the first and the second 50% of the observations is three pixels in x-direction and one pixel in y-direction. That shows that the significant difference that is detected when comparing the images without drift correction for $t \in \{5, 6, 7, 8, 9, 10\}/256$ is caused in fact by the drift. The fact that there is still a significant difference for large thresholds ($t \geq 14$) in the corrected pictures
suggests further intrinsic and local inhomogeneous motion of the specimen or non-polynomial drift that is not captured by the drift model used in Hartmann et al. (2016) and bleaching effects of fluorescent markers.

In summary, this example demonstrates that our strategy of combining a lower bound for the Wasserstein distance with a stochastic bound of the limiting distribution is capable of detecting subtle differences in a large $N$ setting.

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A Proofs

A.1 Hadamard directional differentiability

In this section we follow mainly Shapiro (1991) and Römisch (2004). Let \( \mathcal{U} \) and \( \mathcal{Y} \) be normed spaces.

Definition A.1 (cf. Shapiro (1991), Römisch (2004)). A mapping \( f : D_f \subset \mathcal{U} \to \mathcal{Y} \) is said to be Hadamard directionally differentiable at \( u \in \mathcal{U} \) if for any sequence \( h_n \) that converges to \( h \) and any sequence \( t_n \searrow 0 \) such that \( u + t_nh_n \in D_f \) for all \( n \) the limit

\[
    f'_u(h) = \lim_{n \to \infty} \frac{f(u + t_nh_n) - f(u)}{t_n}
\]

exist.

Note that this derivative is not required to be linear in \( h \), but it is still positively homogeneous. Moreover, the directional Hadamard derivative \( f'_u(\cdot) \) is continuous if \( u \) is an interior point of \( D_f \) (Römisch, 2004).

An extension of this definition is the Hadamard directional differentiability tangentially to a set. Let \( K \) be a subset of \( \mathcal{U} \), \( f \) is directionally differentiable tangentially to \( K \) in the sense of Hadamard at \( x \) if the limit (27) exists for all
sequences $h_n$ that converge to $h$ of the form $h_n = t_n^{-1}(k_n - u)$ where $k_n \in K$ and $t_n \searrow 0$. This derivative is defined on the contingent (Bouligand) cone to $K$ at $x$

$$T_K(u) = \left\{ h \in \mathcal{X} : h = \lim_{n \to \infty} t_n^{-1}(k_n - u), k_n \in K, t_n \searrow 0 \right\}.$$ 

The delta method for mappings that are directionally Hadamard differentiable tangentially to a set reads the following:

**Theorem A.2** (Römisch (2004), Theorem 1). Let $K$ be a subset of $\mathcal{U}$, $f : K \to \mathcal{Y}$ a mapping and assume that the following two conditions are satisfied:

i) The mapping $f$ is Hadamard directionally differentiable at $u \in K$ tangentially to $K$ with derivative $f'_u(\cdot) : T_K(u) \to \mathcal{Y}$.

ii) For each $n$, $X_n : \Omega_n \to K$ are maps such that $a_n(X_n - u) D \to X$ for some sequence $a_n \to +\infty$ and some random element $X$ that takes values in $T_K(u)$.

Then we have $a_n(f(X_n) - f(u)) D \to f'_u(X)$.

**Hadamard directional differentiability of the Wasserstein distance on countable metric spaces** For $r, s \in \mathcal{P}_p(\mathcal{X})$ the $p$-th power of the $p$-th Wasserstein distance is the optimal value of an infinite dimensional linear program. We use this fact to verify that the $p$-th power of the Wasserstein distance (4) on countable metric spaces is directionally Hadamard differentiable with methods of sensitivity analysis of optimal values.

The $p$-th power of the Wasserstein distance on countable metric spaces is the optimal value of the following infinite dimensional linear program

$$\min_{w \in \mathbb{R}^{X \times X}} \sum_{x,x' \in \mathcal{X}} d^p(x,x')w_{x,x'}$$

subject to

$$\sum_{x' \in \mathcal{X}} w_{x,x'} = r_x, \quad \forall x \in \mathcal{X},$$

$$\sum_{x \in \mathcal{X}} w_{x,x'} = s_{x'}, \quad \forall x' \in \mathcal{X},$$

$$w_{x,x'} \geq 0, \quad \forall x, x' \in \mathcal{X}. \tag{28}$$

**Theorem A.3.** $W^p_p$ as a map from $(\mathbb{R}^X, \| \cdot \|_{c^0(d^p)})$ to $\mathbb{R}$, $(r, s) \mapsto W^p_p(r, s)$ is Hadamard directionally differentiable and the directional derivative is given by

$$(d_1, d_2) \mapsto \sup_{(\lambda, \mu) \in S^*(r, s)} -\langle \lambda, d_1 \rangle + \langle \mu, d_2 \rangle, \tag{29}$$

where $S^*(r, s)$ is set of optimal solutions of the dual problem which is defined in (6). Recall, that definition

$$S^*(r, s) = \left\{ (\lambda, \mu) \in \ell^\infty_{d^p}(\mathcal{X}) \times \ell^\infty_{d^p}(\mathcal{X}) : \langle r, \lambda \rangle + \langle s, \mu \rangle = W^p_p(r, s), \right\}$$

$$\lambda_x + \mu_{x'} \leq d^p(x, x') \quad \forall x, x' \in \mathcal{X} \right\}.$$
The set of dual solutions $S^*$ is convex and the limiting distribution is again an infinite dimensional linear program. Hence, the maximum is attained at the boundary of $S^*$.

**Proof.** We will use Theorem 4.24 from Bonnans and Shapiro (2000). Therefore, we need to check the following four assumptions.

1. Problem (28) is convex, since the cost function $\sum_{x,x' \in X} d_p(x,x')w_{x,x'}$ is convex, the constraint set $K = \mathbb{R}^{X \times X} \times \{0\} \times \{0\}$, where $\mathbb{R}^{X \times X}$ are the matrices that have only non-negative entries, is convex. It remains to show that the constraint function $G(w,r,s) = \begin{pmatrix} w \\ w^T 1 - r \\ w 1 - s \end{pmatrix}$, is convex with respect to $-K$, i.e. $\psi((w,(r,s)),(\tilde{w},(\tilde{r},\tilde{s}))) = I_K(G((w,(r,s))) + (\tilde{w},(\tilde{r},\tilde{s})))$ is convex.

Let $(w_1,r_1,s_1,\tilde{w}_1,\tilde{r}_1,\tilde{s}_1)$ and $(w_2,r_2,s_2,\tilde{w}_2,\tilde{r}_2,\tilde{s}_2)$ be in $\mathbb{R}^{X \times X} \times \mathbb{R}^X \times \mathbb{R}^{X \times X} \times \mathbb{R}^X \times \mathbb{R}^X \times \mathbb{R}^X$ such that $G(w_1,(r_1,s_1)) + (\tilde{w}_1,\tilde{r}_1,\tilde{s}_1)$ and $G(w_2,(r_2,s_2)) + (\tilde{w}_2,\tilde{r}_2,\tilde{s}_2)$ are in $K$. This yields for $i=1,2$ that

$$w_i + \tilde{w}_i \geq 0,$$

$$w_i^T 1 - r_i + \tilde{r}_i = 0,$$

$$w_i 1 - s_i + \tilde{s}_i = 0.$$ (30)

And therefore the convex combination of $G(w_1,(r_1,s_1)) + (\tilde{w}_1,\tilde{r}_1,\tilde{s}_1)$ and $G(w_2,(r_2,s_2)) + (\tilde{w}_2,\tilde{r}_2,\tilde{s}_2)$ is also in $K$.

2. We want to show that the set of optimal solutions is non-empty. Since $X$ is countable, the space is separable. If we take the discrete topology on $X$ that is induced by the discrete metric

$$d_D(x,y) = \begin{cases} 0 & \text{if } x = y, \\ 1 & \text{if } x \neq y, \end{cases}$$

our space is complete and hence, $X$ is a Polish space. By Thm. 4.1 in Villani (2009) with $a,b \equiv 0$ the set of optimal solutions of (28) is nonempty for each right hand side of constraints $(r,s)$.

3. Set for some direction $(d_1,d_2) \in \mathbb{R}^X \times \mathbb{R}^X$

$$\bar{G}(w,t) = (w, w^T 1 - r + td_1, w 1 - s + td_2, t).$$

We are going to show that the following directional regularity condition in a direction $(d_1,d_2) \in \mathbb{R}^X \times \mathbb{R}^X$

$$0 \in \text{int} \left\{ \bar{G}(w_0,0) + D_2 \bar{G}(w_0,0)\mathbb{R}^{X \times X} \times \{0\} - K \times \mathbb{R} \right\},$$

30
holds for all optimal solutions \( w_0 \).

For an optimal solution \( w_0 \) it is

\[
\bar{G}(w_0, 0) = (w_0, 0, 0, 0).
\]

Since \( \bar{G}(w, t) \) is linear in \( w \) and bounded \( D_w \bar{G}(w_0, 0) \mathbb{R}^X \times \mathcal{X} \times \{0\} = \bar{G}(w, 0) \) and the directional regularity condition reads

\[
0 \in \text{int} \left\{(w_0, 0, 0, 0) + (w, w^T 1 - r, w(1 - s), 0) - K \times \mathbb{R}\right\}.
\]

This is fulfilled because \( w \in \mathbb{R}^{X \times \mathcal{X}} \).

4. We aim to verify the stability of the optimal solution. Let \( (r_w \) with all other rows. In this manner, we obtain a subsequence of \( \mathcal{X} \) and we can extract a convergent subsequence and proceed the same way.

The remaining elements of the second row form again a bounded sequence. We delete the columns that are not in this subsequence from the scheme.

Since it holds for \( l \) large enough such that \( \bar{G}(w, 0) \) is bounded and hence, \( \bar{G}(X) \) together with the \( \ell^1(d^p) \)-norm is complete.

Let \( (r_k)_{k \in \mathbb{N}} \) be a sequence that converges to \( r \) and \( (s_k)_{k \in \mathbb{N}} \) a sequence that converges to \( s \), let \( (w_k)_{k \in \mathbb{N}} \in \Pi(r_k, s_k) \), where \( \Pi(r_k, s_k) \) is the set of all transport plans between \( r_k \) and \( s_k \).

1. Step: Prove that \( (w_k)_{k \in \mathbb{N}} \) has a convergent subsequence.

Let \( A_1 \subset A_2 \subset A_3 \cdots \subset \mathcal{X} \) be such that \( \mathcal{X} = \bigcup_{n \in \mathbb{N}} A_n \) and \( |A_n| < \infty \) \( \forall n \in \mathbb{N} \), this is possible since \( \mathcal{X} \) is countable. Now write

\[
\begin{align*}
(w_1|_{A_1 \times A_1}) & \quad (w_2|_{A_1 \times A_1}) & \quad (w_3|_{A_1 \times A_1}) & \quad (w_4|_{A_1 \times A_1}) & \quad \ldots \\
(w_1|_{A_2 \times A_2}) & \quad (w_2|_{A_2 \times A_2}) & \quad (w_3|_{A_2 \times A_2}) & \quad (w_4|_{A_2 \times A_2}) & \quad \ldots \\
\vdots & \quad \vdots & \quad \vdots & \quad \vdots & \quad \ldots \\
(w_1|_{A_l \times A_l}) & \quad \ldots
\end{align*}
\]

Since all \( w_k \)’s are probability measures, the \( \| \cdot \|_{\ell^1(d^p)} \) of each row is bounded and therefore, we are able to extract a convergent subsequence.

We delete the columns that are not in this subsequence from the scheme. The remaining elements of the second row form again a bounded sequence and we can extract a convergent subsequence and proceed the same way with all other rows. In this manner, we obtain a subsequence of \( (w_k) \) (which, for notational convenience, we also denote by \( (w_k) \)) such that \( w_k|_{A_l \times A_l} \) is convergent for any fixed \( l \in \mathbb{N} \).

Now we want to prove that \( (w_k) \) is a Cauchy-sequence in \( \mathcal{P}_p(X) \times \mathcal{P}_p(X) \). Since it holds for \( r \in \mathcal{P}_p(X) \) that \( \|r\|_{\ell^1(d^p)} \) is a convergent series and therefore we can choose \( l \) large enough such that \( \|r|_{A_l^C} \|_{\ell^1(d^p)} < \epsilon \).

\[
(A_l \times A_l)^C = \mathcal{X} \times A_l^C \cup A_l^C \times \mathcal{X}
\]
and hence
\[ \|w_k|_{(A_l \times A_l)^c} \|_{\ell^1(d\nu)} \leq \|w_k|_{X \times A_l^c} \|_{\ell^1(d\nu)} + \|w_k|_{A_l \times X} \|_{\ell^1(d\nu)} \]
\[ = \|r_k|_{A_l^c} \|_{\ell^1(d\nu)} + \|s_k|_{A_l^c} \|_{\ell^1(d\nu)} < 2\epsilon. \]

For all \( m, k \geq k_0 \) it holds
\[ \|w_k - w_m\|_{\ell^1(d\nu)(X \times X)} = \|w_k - w_m\|_{\ell^1(d\nu)(A_l \times A_l)} + \|w_k - w_m\|_{\ell^1(d\nu)((A_l \times A_l)^c)} \xrightarrow{k_0 \to \infty} 0. \]

Hence there exists a convergent subsequence of \((w_k)\) by the completeness of \(P_p(X)\) with \(\|\cdot\|_{\ell^1(d\nu)}\), that will also be denoted by \((w_k)\) such that \(w_k \to w\) as \(k \to \infty\).

2. Step: It remains to show that \(w\) is an optimal transport plan of \(r\) and \(s\). For this, we need the definition of \(c\)-cyclical monotonicity.

**Definition A.4** (Cyclical Monotonicity, Def. 5.1 Villani (2009)). Let \(X\) and \(Y\) be arbitrary sets and \(c : X \times Y \to (-\infty, +\infty]\) be a function. A subset \(\Gamma \subset X \times Y\) is said to be \(c\)-cyclically monotone if for any \(N \in \mathbb{N}\) and any family \((x_1, y_1), \ldots, (x_N, y_N)\) of points in \(\Gamma\) holds the inequality
\[ \sum_{i=1}^{N} c(x_i, y_i) \leq \sum_{i=1}^{N} c(x_i, y_{i+1}), \]
where \(y_{N+1} = y_1\). A transport plan is said to be \(c\)-cyclically monotone if it is concentrated on a \(c\)-cyclically monotone set.

We take again \(X\) with the discrete topology and \(a = b \equiv 0\). Since all \(w_k\) are optimal and the optimal cost is finite, since we restricted ourselves to \(P_p(X)\), they are by Thm. 5.10 (ii) in Villani (2009) \(d^p\)-cyclically monotone. Therefore, \(w_k^{\otimes N} = \bigotimes_{i=1}^{N} w_k\) is concentrated on
\[ C(N) = \left\{ (x_1, y_1), \ldots, (x_N, y_N) \in (X \times X)^N \mid \sum_{i=1}^{N} d^p(x_i, y_i) \leq \sum_{i=1}^{N} d^p(x_i, y_{i+1}) \right\}. \]

For fixed \(N\) this set is closed since it is determined by a continuous function.
This implies that \(w^{\otimes N}\) is also concentrated on \(C(N)\) and hence \(w\) is \(d^p\)-cyclically monotone. It follows from Thm. 5.10 (ii) in Villani (2009) that \(w\) is optimal.
Step 1 and step 2 give the stability of the optimal solution.
A.2 Rewriting the limiting distribution under equality of measures

First, observe that for the case \( r = s \) the set of dual solutions \( S^* \) (7) can be rewritten in the following way:

\[
S^* = S^*(r, r) = \left\{ (\lambda, \mu) \in \ell^\infty_{d-p}(X) \times \ell^\infty_{d-p}(X) : \langle r, \lambda \rangle + \langle r, \mu \rangle = 0, \right. \\
\left. \lambda_x + \mu_{x'} \leq d^p(x, x') \quad \forall x, x' \in X \right\} \\
= \left\{ (\lambda, \mu) \in \ell^\infty_{d-p}(X) \times \ell^\infty_{d-p}(X) : \lambda = -\mu, \lambda_x + \mu_{x'} \leq d^p(x, x') \quad \forall x, x' \in X \right\}.
\]

We decompose the Gaussian process \( G \) with mean zero and covariance structure as defined in (8) into \( G = G^+ - G^- \) with \( G^+, G^- \) non-negative, then the limiting distribution in (9) can be rewritten as follows:

\[
\max_{\lambda \in S^*} \langle G, \lambda \rangle = \max_{\lambda \in S^*} \langle G^+, \lambda \rangle - \langle G^-, \lambda \rangle = \max_{(\lambda, \mu)} \langle G^+, \lambda \rangle + \langle G^-, \mu \rangle \\
\text{s.t. } \lambda_x + \mu_{x'} \leq d^p(x, x') \quad \forall x, x' \in X,
\]

for the second equality we used that \( \lambda = -\mu \). The maximization problem in the last line is the dual of the \( p \)-th power of the \( p \)-Wasserstein distance between \( G^+ \) and \( G^- \) and as Kantrovich duality holds this equals \( W_p^p(G^+, G^-) \).

A.3 Proof of Theorem 3.1

Simplify the set of dual solutions \( S^* \) As a first step, we rewrite the set of dual solutions \( S^* \) given in definition (7) in our tree notation as

\[
S^* = \{ \lambda \in \ell^\infty_{d-p}(X) : \lambda_x - \lambda_{x'} \leq d_T(x, x')^p, \quad x, x' \in X \}. \tag{31}
\]

The key observation is that in the condition \( \lambda_x - \lambda_{x'} \leq d_T(x, x')^p \) we do not need to consider all pairs of vertices \( x, x' \in X \), but only those which are joined by an edge. To see this, assume that only the latter condition holds. Let \( x, x' \in X \) arbitrary and \( x = x_1, \ldots, x_n = x' \) the sequence of vertices defining the unique path joining \( x \) and \( x' \), such that \( (x_j, x_{j+1}) \in E \) for \( j = 1, \ldots, n - 1 \). That this path contains only a finite number of edges, was proven in Section 3. Then

\[
\lambda_x - \lambda_{x'} = \sum_{j=1}^{n-1} (\lambda_{x_j} - \lambda_{x_{j+1}}) \leq \sum_{j=1}^{n-1} d_T(x_j, x_{j+1})^p \leq d_T(x, x')^p,
\]

such that (31) is satisfied for all \( x, x' \in X \). Noting that if two vertices are joined by an edge then one has to be the parent of the other, we can write the set of dual solutions as

\[
S^* = \{ \lambda \in \ell^\infty_{d-p}(X) : |\lambda_x - \lambda_{\text{parent}(x)}| \leq d_T(x, \text{parent}(x))^p, \quad x \in X \}. \tag{32}
\]
Rewrite the target function. To rewrite the target function we need to make several definitions. Let
\[ \tilde{e}_y^{(x)}(x, x_0) = \begin{cases} \frac{1}{d^p(x, x_0)} & \text{if } y = x, \\ -\frac{1}{d^p(x, x_0)} & \text{if } y = \text{parent}(x), \\ 0 & \text{else}. \end{cases} \]
Furthermore, we define for \( \mu \in \ell_1^{d^p}(X) \)
\[ \eta_x = \sum_{x' \in \text{children}(x)} d^p(x, x_0) \mu_{x'} \]
and
\[ \mu_n = \sum_{x \in A \leq n \setminus \text{root}(T)} \eta_x \tilde{e}^{(x)} = \mu I_{A \leq n} + \sum_{x \in A = n} \frac{1}{d^p(x, x_0)} \eta_x e(x), \]
here \( A_{\leq n} = \{ x \in X : \text{level of } x \leq n, x \text{ is within the first } n \text{ vertices of its level} \} \), \( A_n = \{ x \in X : \text{level of } x = n, x \text{ is within the first } n \text{ vertices of its level} \} \), \( A_{> n} = \{ x \in X : \text{level of } x > n \text{ or } x \text{ is not within the first } n \text{ vertices of its level} \} \) and \( e(x) \) the sequence 1 at \( x \) and 0 everywhere else. For this sequence \( \mu_n \) it holds
\[ \| \mu - \mu_n \|_{\ell_1^{d^p}} = \sum_{x \in X} d^p(x, x_0) \left| \mu_{A_{\leq n}} - \sum_{x \in A_n} \frac{1}{d^p(x, x_0)} \eta_x e(x) \right| \]
\[ \leq \| \mu_{A_{> n}} \|_{\ell_1^{d^p}} + \left| \sum_{x \in A_n} \eta_x \right|. \]
As \( n \to \infty \), the first part tends to zero as \( \mu \in \ell_1^{d^p}(X) \), and
\[ \left| \sum_{x \in A_n} \eta_x \right| \leq \sum_{x \in A_n} \sum_{x' \in \text{children}(x)} |\mu_{x'}| d^p(x', x_0) \leq \sum_{x \in A_n} |\mu_x| d^p(x, x_0) \to 0. \]
Hence, our target function for \( \mu \in \ell_1^{d^p}(X) \) and \( \lambda \in \ell_\infty^{d-p}(X) \) can be rewritten in the following way
\[ \langle \mu, \lambda \rangle = \lim_{n \to \infty} \langle \mu_n, \lambda \rangle \]
\[ = \lim_{n \to \infty} \sum_{x \in A_{\leq n}} \eta_x \langle \tilde{e}^{(x)}, \lambda \rangle \]
\[ = \lim_{n \to \infty} \sum_{x \in A_{\leq n}} \sum_{x' \in \text{children}(x)} \mu_{x'} (\lambda_x - \lambda_{\text{parent}(x)}) \]
\[ \leq \lim_{n \to \infty} \sum_{x \in A_{\leq n}} \sum_{x' \in \text{children}(x)} \mu_{x'} \left| \lambda_x - \lambda_{\text{parent}(x)} \right| \]
\[ = \lim_{n \to \infty} \sum_{x \in A_{\leq n}} \left| (\mathcal{S}_T \mu)_x \right| \left| \lambda_x - \lambda_{\text{parent}(x)} \right| \]
(33)
Observe that for $\lambda \in S^*$ it holds
\[ |\lambda_x - \lambda_{\text{parent}(x)}| \leq d^p(x, \text{parent}(x)). \tag{34} \]

By condition (3) $G \sim \mathcal{N}(0, \Sigma(r))$ is an element of $\ell_{d^p}(\mathcal{X})$. For $\lambda \in S^*$ we get with (33) and (34) that
\[ \langle G, \lambda \rangle \leq \lim_{n \to \infty} \sum_{x \in A \leq n} |(S^r G)_x| d_T(x, \text{parent}(x))^p. \tag{35} \]

Therefore, $\max_{\lambda \in S^*} \langle G, \lambda \rangle$ is bounded by $\lim_{n \to \infty} \sum_{x \in A \leq n} |(S^r G)_x| d_T(x, \text{parent}(x))^p$. We can define the sequence $\nu \in \ell^\infty_{d^p}(\mathcal{X})$ by
\[ \nu_{\text{root}} = 0 \]
\[ \nu_x - \nu_{\text{parent}(x)} = \text{sign}((S^r G)_x) d_T(x, \text{parent}(x))^p \tag{36} \]

From (32) and the fact that $d^p(x, \text{parent}(x)) \leq d^p(x, \text{root}(T))$ we see that $\nu \in S^*$ and by plugging $\nu$ into equation (35) we can conclude that $\langle G, \nu \rangle$ attains the upper bound in (35).

As the last step of our proof, we verify that the limit in (35) exists. Therefore, we rewrite condition (3) in terms of the edges and recall that $x_0 = \text{root}(T)$.
\[ \sum_{x \in \mathcal{X}} d_T(x, x_0)^p \sqrt{r_x} \geq \sum_{x \in \mathcal{X}} \sum_{x' \in \text{children}(x)} d_T(x, \text{parent}(x))^p \sqrt{r_{x'}}. \tag{37} \]

The first moment of the limiting distribution can be bounded in the following way:
\[
\mathbb{E} \left[ \sum_{x \neq \text{root}(T)} |(S^r G)_x| d_T(x, \text{parent}(x))^p \right] \\
\leq \sum_{x \in \mathcal{X}} d_T(x, \text{parent}(x))^p \sqrt{r_x (1 - (S^r r)_x)} \\
\leq \sum_{x \in \mathcal{X}} \sum_{x' \in \text{children}(x)} d_T(x, \text{parent}(x))^p \sqrt{r_{x'}} \\
< \infty
\]
due to Hölder’s inequality and (37). This bound shows that the limit in (35) is almost surely finite and hence, concludes the proof.