

A NEWTON ALGORITHM FOR SEMIDISCRETE OPTIMAL  
TRANSPORT WITH STORAGE FEES\*MOHIT BANSIL<sup>†</sup> AND JUN KITAGAWA<sup>‡</sup>

**Abstract.** We introduce and prove convergence of a damped Newton algorithm to approximate solutions of the semidiscrete optimal transport problem with storage fees, corresponding to a problem with hard capacity constraints. This is a variant of the optimal transport problem arising in queue penalization problems and has applications to data clustering. Our result is novel, as it is the first numerical method with proven convergence for this variant problem; additionally, the algorithm applies to the classical semidiscrete optimal transport problem but does not require any connectedness assumptions on the support of the source measure, in contrast with existing results. Furthermore we find some stability results of the associated Laguerre cells. All of our results come with quantitative rates. We also present some numerical examples.

**Key words.** optimal transport, numerical analysis, calculus of variations

**AMS subject classifications.** 49Q22, 49M15, 49M25, 65K10

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## 1. Introduction.

**1.1. Semidiscrete optimal transport with storage fees.** In this paper, we deal with the following problem. Let  $X \subset \mathbb{R}^n$ ,  $n \geq 2$ , be compact and  $Y := \{y_i\}_{i=1}^N \subset \mathbb{R}^n$  be a finite collection of fixed points, along with a *cost function*  $c : X \times Y \rightarrow \mathbb{R}$  and a *storage fee function*  $F : \mathbb{R}^N \rightarrow \mathbb{R}$ . We also fix a Borel probability measure  $\mu$  with  $\text{spt } \mu \subset X$  and assume  $\mu$  is absolutely continuous with respect to Lebesgue measure. The *semidiscrete optimal transport with storage fees* is then to find a pair  $(T, \lambda)$  with  $\lambda = (\lambda^1, \dots, \lambda^N) \in \mathbb{R}^N$  and  $T : X \rightarrow Y$  measurable satisfying  $T_\# \mu = \sum_{i=1}^N \lambda^i \delta_{y_i}$ , such that

$$(1.1) \quad \int_X c(x, T(x)) d\mu + F(\lambda) = \min_{\tilde{\lambda} \in \mathbb{R}^N, \tilde{T}_\# \mu = \sum_{i=1}^N \tilde{\lambda}^i \delta_{y_i}} \int_X c(x, \tilde{T}(x)) d\mu + F(\tilde{\lambda}).$$

In [BK19], the authors have shown under appropriate conditions the existence of solutions to the problem with storage fees, along with a dual problem with strong duality, and a characterization of dual maximizers and primal minimizers. It is not difficult to see that an optimal  $T$  can be constructed via a  $\mu$ -a.e. partition of the domain  $X$  which is induced by a maximizing dual potential. The cells forming such a partition are known as *Laguerre cells* (see Definition 2.3).

To contrast, the classical (semidiscrete) optimal transport problem would be to fix a discrete probability measure  $\nu$  supported on  $Y$ , and to find a measurable mapping  $T : X \rightarrow Y$  such that  $T_\# \mu(E) := \mu(T^{-1}(E)) = \nu(E)$  for any measurable  $E \subset Y$ , and

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$T$  satisfies

$$(1.2) \quad \int_X c(x, T(x)) d\mu = \min_{\tilde{T} \# \mu = \nu} \int_X c(x, \tilde{T}(x)) d\mu,$$

and it is easy to see that the classical problem is a special case of the problem with storage fees above (see the paragraph below).

In this paper, we propose and show convergence of a damped Newton algorithm, when the storage fee function is of the form

$$(1.3) \quad F(\lambda) = F_w(\lambda) := \begin{cases} 0, & \lambda \in \prod_{i=1}^N [0, w^i], \\ +\infty & \text{else,} \end{cases}$$

where  $w = (w^1, \dots, w^N) \in \mathbb{R}^N$  is some fixed vector with nonnegative components. The minimization (1.1) with this choice of  $F$  corresponds to a problem where the  $i$ th target point has a hard capacity constraint given by  $w^i$  with no other associated cost of storage. It is clear that if  $w$  satisfies  $\sum_{i=1}^N w^i = 1$ , the solution of the problem with storage fees solves the classical optimal transport problem with target measure  $\nu = \sum_{i=1}^N w^i \delta_{y_i}$ , and hence this variant includes the classical case.

**1.2. Contributions of the paper.** The major novelties of our algorithm are mainly the following three aspects. First, this is the first algorithm available for problems with storage fees. Second, our method applies to classical optimal transport where the source measure does not satisfy a Poincaré–Wirtinger inequality, which is a crucial condition in existing results such as [KMT19]. Third, we give explicit errors on the geometric structures arising in the approximations generated by our algorithm.

We introduce some preliminary notions in section 2 to state our damped Newton algorithm; as such, we defer the precise statements of our main theorems to section 2, along with the outline for the remainder of the paper. In Theorem 2.6, we show that the above-mentioned damped Newton algorithm has global linear convergence and local superlinear convergence. The algorithm applies to a relaxed version of the original problem depending on two parameters  $h$  and  $\epsilon > 0$ . We note that the rates of convergence and basin of attraction for the local superlinear convergence depend on these parameters and degenerate as they approach 0. In Theorems 2.11 and 2.14, we utilize the results of [BK20] to show explicit convergence rates for the Laguerre cells in terms of both the  $\mu$  symmetric difference and the Hausdorff distance. This convergence is shown in terms of these parameters  $h$  and  $\epsilon$ . Our result is a significant improvement over [KMT19] by the second author, in that the algorithm applies to the wider class of problems with storage fees, but also because the convergence of the algorithm is shown without a connectedness assumption on the support of the source measure (see Remark 2.13 below). It should also be noted that the convergence proof is not a straightforward application of the analysis in [KMT19].

**1.3. Literature analysis.** Optimal transport with storage fees first appears in [CJP09] in urban planning related to the queue penalization problem. The problem also corresponds to the “lower level problem” in the bilevel location problem which is well studied in logistics and operations research; see, for example, [WZZ06, LOE12, MPdN17]. This interpretation is also related to a problem of monopolistic pricing analyzed in [CM18]. Additionally, the “lower level problem” can be seen as a toy model for data clustering, where the set of data is very large and approximated by an absolutely continuous measure, and each cluster has a hard upper bound on size. These are a few of the potential applications of the optimal transport problem with

storage fees, and we emphasize that this paper provides the first numerical method for this problem.

For the classical optimal transport problem (see [PC19] for an excellent overview), there are now many numerical methods. We briefly mention three popular approaches: entropic regularization, discretization schemes for solving the Monge–Ampère equation with the second boundary value condition, or approximation of a semidiscrete problem.

Entropic regularization is accomplished by adding the *relative (Shannon) entropy* with respect to the tensor product of the source and target measures to the objective functional in the measure valued (Kantorovich) problem, to act as a regularizing term. Numerically, the problem can be solved using the Sinkhorn algorithm (first done for optimal transport by Cuturi [Cut13]). This is generally a fast and parallelizable method: when transporting between two discrete measures supported on  $N$  points each, the Sinkhorn algorithm finds approximations with total transport cost within  $\epsilon$  of the true value in  $O(\frac{N^2 \log N}{\epsilon^3})$  operations (see [AWR17]). However, the entropic regularization method has the disadvantage that solutions of the regularized problem are only known to converge in a weak sense to the true solution (weak convergence of measures; see [CDPS17]) with no explicit convergence rates. Although our proposed method here differs in the exact mechanism, it shares a kindred spirit with entropic regularization in the following sense: both methods are based on adding a barrier term to the original functional, which turns the problem into a strictly convex one and simultaneously adds a constraint shrinking the feasible domain for the objective functional. In the case of entropic regularization, transport plans that are singular with respect to the reference measure are forbidden, while in our case, plans where the second marginal exceeds some bound on the mass are forbidden.

For absolutely continuous source and target measures, the solution of the optimal transport problem can be constructed by solving a PDE of Monge–Ampère type with the *second boundary value* condition. Finite difference schemes for the Monge–Ampère operator with these boundary conditions have been investigated by Benamou, Froese, and Oberman; in [Obe08, FO11a, FO11b, BFO14], they show that various schemes are monotone, stable, and consistent, and hence approximations converge uniformly to a viscosity solution of the PDE (via Barles and Souganidis [BS91]). This approach applies to problems with absolutely continuous measures, and some of the schemes mentioned are robust for singular solutions of the PDE. However, no explicit convergence rates are available for these methods in the optimal transport case ([NZ19] gives quantitative rates for the Dirichlet problem assuming higher regularity of solutions). Also, stencils need to be modified near the boundary for these schemes, which is difficult for complicated geometries. Last, convexity of solutions is essential, and hence these schemes are limited to the “classical” Monge–Ampère case,  $c(x, y) = \|x - y\|^2$ .

The method we use is based on the duality theory for semidiscrete transport problems. By Brenier’s theorem [Bre91], solutions of the semidiscrete optimal transport problem can be constructed from a finite envelope of a certain family of functions depending on the cost (when  $c(x, y) = \|x - y\|^2$ , the family is affine functions). For the classical Monge–Ampère equation, this construction goes back to Aleksandrov [Ale05]. The papers [CKO99, Kit14, AG17] propose a non-Newton type iterative method, the last result being applicable to *generated Jacobian equations*, a class more general than optimal transport. These results give an upper bound on the number of iterations necessary but are slower with a bound of  $O(\frac{N^4}{\epsilon})$  steps for an error  $\epsilon > 0$  with target measure supported on  $N$  points.

The first use of a Newton method with this envelope construction appears to be [OP88] for a semidiscrete Monge–Ampère equation with a Dirichlet boundary condition; there, local convergence is proved, and global convergence was later shown in [Mir15], their setting is for weak solutions of *Aleksandrov* type, generally different from optimal transport solutions. For the classical optimal transport problem, the authors of [AHA98] observed that finding the optimal map is equivalent to extremizing the so-called Kantorovich functional; [Mér11] observed good empirical behavior of Newton type methods for this problem (but without convergence proofs). A damped Newton method is used for the quadratic cost on the torus in [LR05, SAK15] with proofs of convergence based on regularity theory of the Monge–Ampère equation due to Caffarelli [Caf92]. In [KMT19], a damped Newton algorithm is proposed that applies to a wider class of cost functions, and global linear and local superlinear convergence for Hölder continuous source measures is proved. A key assumption is that the source measure satisfies a Poincaré–Wirtinger inequality, a quantitative connectivity assumption on the support (see also [MMT18]). Advantages of the semidiscrete approach is that it produces exact solutions to some transport problem, and some methods can be applied to a wide variety of cost functions other than the quadratic distance cost. Additionally, directly solving a semidiscrete problem has one advantage over considering a sequence of purely discrete approximations, as it is currently not well known how much error is introduced in optimal transport problems by discretization of the source measure. It is true that Newton based methods generally require the computation of associated *Laguerre cells* (see Definition 2.3), which is a computationally difficult problem. In the case when  $c(x, y) = \|x - y\|^2$ , there are efficient methods available (see, for example, [Lév15]). Outside of this quadratic cost function, the choice of cost  $c(x, y) = -\log(1 - \langle x, y \rangle)$  on  $\mathbb{S}^2 \times \mathbb{S}^2$  yields Laguerre cells which are intersections of quadratic cells with the unit sphere, and hence the method of [Lév15] can also be used to efficiently calculate the associated Laguerre cells; this cost function satisfies the structural conditions (Reg), (Twist), and (QC), which are crucial for proving convergence of Newton methods, and arises when modeling the far-field reflector problem in geometric optics [Wan04].

Finally, we mention that there is some relation to the unbalanced optimal transport problem first introduced in [KMV16, LMS16, CPSV18b]. In [CPSV18a, Corollary 5.9], a formulation of the unbalanced optimal transport metric is given which has some resemblance to the optimal transport problem with storage fees, where essentially the storage fee function is replaced by the Kullback–Leibler divergence of the marginals of the coupling under consideration against the source and target measures. See also [LMS18].

**1.4. Strategy of proof and obstacles.** For our algorithm, we first replace the storage fee  $F_w$  by a uniformly convex regularization. Then we apply a damped Newton method to a function that is related to (but not exactly equal to) the gradient of the associated dual problem. One reason that we do not apply Newton directly to the gradient of the dual problem is to keep better track of the error introduced by our regularization; see Remarks 2.7 and 2.15 for more details.

We try here to explain how we originally arrived at this formulation. There are a number of difficulties that prevent a direct translation of the damped Newton algorithm from [KMT19] to the problem with storage fees. First, in the classical case one fixes a discrete target measure  $\nu = \sum_{i=1}^N \lambda^i \delta_{y_i}$ , and the Newton algorithm is used to approximate the weight vector  $\lambda = (\lambda^1, \dots, \lambda^N)$ . However, in our problem with storage fees, the weight vector  $\lambda$  itself must be chosen as part of the minimization and

hence is not fixed, and thus it is not even a priori clear what quantity to approximate with a Newton algorithm. Additionally, unlike the classical problem, it is possible that  $\lambda^i = 0$  for one or more of the entries in an optimal choice for the weight vector, but the algorithm from [KMT19] uses the assumption that all  $\lambda^i$  have strictly positive lower bounds in a crucial way to obtain the convergence. To remedy these issues, we will first approximate the storage function  $F_w$ : we will use the characterization for solutions found in [BK19] to find approximating storage functions  $\tilde{F}_w$ , along with minimizers of the problem (1.1) with  $F = \tilde{F}_w$ . However, a second difficulty arises as the functions of the form  $F_w$  have both highly singular behavior in their subdifferentials at the boundary of their effective domains, while being nonstrictly convex everywhere. Thus, we will further replace functions of this form with uniformly convex, smooth approximations. This procedure turns out to have a regularizing effect on the problem, which allows us to obtain convergence without the aforementioned connectedness assumption as in [KMT19] (see also Remark 2.7). At this point, we found that fixing one particular regularization, we were unable to control the error introduced by the magnitude of the regularization. However, we discovered that we can also keep track of this error by allowing the regularization itself to vary and be updated over the course of our Newton method, which led to the final incarnation of Algorithm 1.

Concerning the proof of the convergence of the Laguerre cells, we first prove Lemma A.1 on the strong convexity of a functional associated to the semidiscrete optimal transport problem. We note that the lemma does not require any connectivity assumption on the support of the source measure. This lemma is then used to control the difference of the Laguerre cells of the problems associated to  $\tilde{F}_w$  and those of our uniformly convex, smooth approximations. From here we are able to apply the results of [BK20] to obtain the desired convergence.

## 2. Setup.

**2.1. Notation and conventions.** Here we gather notation and conventions to be used in the remainder of the paper. As mentioned above, we fix positive integers  $N$  and  $n$  and a collection  $Y := \{y_i\}_{i=1}^N \subset \mathbb{R}^n$ . The standard  $N$ -simplex will be denoted by

$$\Lambda := \left\{ \lambda \in \mathbb{R}^N \mid \sum_{i=1}^N \lambda^i = 1, \lambda^i \geq 0 \right\},$$

and to any vector  $\lambda \in \Lambda$  we associate the discrete measure  $\nu_\lambda := \sum_{i=1}^N \lambda^i \delta_{y_i}$ . The notation  $\mathbf{1}$  will refer to the vector in  $\mathbb{R}^N$  whose components are all 1. We also reserve the notation  $\|V\| := \sqrt{\sum_{i=1}^N |V^i|^2}$  for the Euclidean ( $\ell^2$ ) norm of a vector  $V \in \mathbb{R}^N$ , while  $\|V\|_1 := \sum_{i=1}^N |V^i|$  and  $\|V\|_\infty := \max_{i \in \{1, \dots, N\}} |V^i|$  will respectively stand for the  $\ell^1$  and  $\ell^\infty$  norms. We also write  $\|M\|$  for the operator norm of a matrix  $M$ . The distinction from the Euclidean norm of a vector should be clear from the context.

Given any set  $A$ , we write

$$\delta(\lambda \mid A) := \begin{cases} 0, & \lambda \in A, \\ +\infty, & \lambda \notin A, \end{cases}$$

for the *indicator function* of the set  $A$ , and for any vector  $w \in \mathbb{R}^N$  with nonnegative entries, we denote  $F_w(\lambda) := \sum_{i=1}^N \delta(\lambda^i \mid [0, w^i]) = \delta(\lambda \mid \prod_{i=1}^N [0, w^i])$ . We will also

use  $\mathcal{L}$  to denote the  $n$ -dimensional Lebesgue measure and  $\mathcal{H}^k$  for the  $k$ -dimensional Hausdorff measure.

Regarding the cost function  $c$ , we will generally assume the following standard conditions from optimal transport theory:

$$\begin{aligned} (\text{Reg}) \quad & c(\cdot, y_i) \in C^2(X) \quad \forall i \in \{1, \dots, N\}, \\ (\text{Twist}) \quad & \nabla_x c(x, y_i) \neq \nabla_x c(x, y_k) \quad \forall x \in X, i \neq k. \end{aligned}$$

We also assume the following condition, originally studied by Loeper in [Loe09].

**DEFINITION 2.1.** *We say  $c$  satisfies Loeper's condition if for each  $i \in \{1, \dots, N\}$  there exist a convex set  $X_i \subset \mathbb{R}^n$  and a  $C^2$  diffeomorphism  $\exp_i^c(\cdot) : X_i \rightarrow X$  such that*

(QC)

$$\forall t \in \mathbb{R}, 1 \leq k, i \leq N, \{p \in X_i \mid -c(\exp_i^c(p), y_k) + c(\exp_i^c(p), y_i) \leq t\} \text{ is convex.}$$

See Remark 2.4 below for a discussion of these conditions.

We also say that a set  $\tilde{X} \subset X$  is  $c$ -convex with respect to  $Y$  if  $(\exp_i^c)^{-1}(\tilde{X})$  is a convex set for every  $i \in \{1, \dots, N\}$ .

It will be convenient to also introduce  $c$ -convex functions and the  $c$ - and  $c^*$ -transforms. In the semidiscrete case, the  $c^*$ -transform of a function defined on  $X$  will be a vector in  $\mathbb{R}^N$ , while the  $c$ -transform of a vector in  $\mathbb{R}^N$  will be a function whose domain is  $X$ .

**DEFINITION 2.2.** *If  $\varphi : X \rightarrow \mathbb{R} \cup \{+\infty\}$  ( $\varphi \not\equiv +\infty$ ) and  $\psi \in \mathbb{R}^N$ , their  $c$ - and  $c^*$ -transforms are a vector  $\varphi^c \in \mathbb{R}^N$  and a function  $\psi^{c^*} : X \rightarrow \mathbb{R} \cup \{+\infty\}$ , respectively, defined by*

$$(\varphi^c)^i := \sup_{x \in X} (-c(x, y_i) - \varphi(x)), \quad (\psi^{c^*})(x) := \max_{i \in \{1, \dots, N\}} (-c(x, y_i) - \psi^i).$$

*If  $\varphi : X \rightarrow \mathbb{R} \cup \{+\infty\}$  is the  $c^*$ -transform of some vector in  $\mathbb{R}^N$ , we say  $\varphi$  is a  $c$ -convex function. A pair  $(\varphi, \psi)$  with  $\varphi : X \rightarrow \mathbb{R} \cup \{+\infty\}$  and  $\psi \in \mathbb{R}^N$  is a  $c$ -conjugate pair if  $\varphi = \psi^{c^*}$  and  $\psi = \varphi^c$ .*

**DEFINITION 2.3.** *For any  $\psi \in \mathbb{R}^N$  and  $i \in \{1, \dots, N\}$ , we define the  $i$ th Laguerre cell associated to  $\psi$  as the set*

$$\text{Lag}_i(\psi) := \{x \in X \mid -c(x, y_i) - \psi^i = \psi^{c^*}(x)\}.$$

We also define the function  $G : \mathbb{R}^N \rightarrow \Lambda$  and the set  $\mathcal{K}^\epsilon$  for any  $\epsilon \geq 0$  by

$$\begin{aligned} G(\psi) &:= (G^1(\psi), \dots, G^N(\psi)) = (\mu(\text{Lag}_1(\psi)), \dots, \mu(\text{Lag}_N(\psi))), \\ \mathcal{K}^\epsilon &:= \{\psi \in \mathbb{R}^N \mid G^i(\psi) > \epsilon \ \forall i \in \{1, \dots, N\}\}. \end{aligned}$$

**Remark 2.4.** The above conditions (Reg), (Twist), and (QC) are the same ones assumed in [KMT19]. As also mentioned there, (Reg) and (Twist) are standard in the existence theory of optimal transport, while (QC) holds if  $Y$  is a finite set sampled from a continuous space, and  $c$  is a  $C^4$  cost function satisfying what is known as the *Ma-Trudinger-Wang* condition (along with an additional convexity assumption on the domain of  $c$ , which we do not detail here). In such a setting, the maps  $\exp_i^c(\cdot)$  from (QC) can be taken as the inverses of the mappings  $x \mapsto -\nabla_x c(x, y_i)$ . The strong

Ma–Trudinger–Wang condition was first introduced in [MTW05] and in [TW09] in a weaker form. The condition is also *necessary* for the regularity theory of the Monge–Ampère type equation arising in optimal transport; see [Loe09]. The Ma–Trudinger–Wang condition is known to hold for a relatively large class of cost functions, which include  $\|x - y\|^2$  and, as mentioned above, the cost  $-\log(1 - \langle x, y \rangle)$  appearing in the far-field reflector problem. For more examples, see [MTW05, section 6] and [TW09, section 8].

If  $\mu$  is absolutely continuous with respect to Lebesgue measure, under (Twist) the Laguerre cells associated to different indices are disjoint up to sets of  $\mu$ -measure zero. Then by the generalized Brenier’s theorem [Vil09, Theorem 10.28], for any vector  $\psi \in \mathbb{R}^N$  it is known that the  $\mu$ -a.e. single valued map  $T_\psi : X \rightarrow Y$  defined by  $T_\psi(x) = y_i$  whenever  $x \in \text{Lag}_i(\psi)$  is a minimizer in the classical optimal transport problem (1.2), where the source measure is  $\mu$  and the target measure is defined by  $\nu = \nu_{G(\psi)}$ .

In order to introduce the damped Newton algorithm, we will analyze our problem (1.1). We must introduce a few more pieces of notation. The motivations for  $g$  and  $w_{h,\epsilon}^i$  will be explained in detail in the following section; the set  $\mathcal{W}^{\epsilon_0}$  is to ensure nondegeneracy of the derivative  $Dw_{h,\epsilon}$ , while  $\Sigma_{w,h,\epsilon}$  is a normalization to obtain compactness of our parameter space. These two are related to the fact that the map  $G$  is invariant under translation by multiples of  $\mathbf{1}$  while the map  $w_{h,\epsilon}$  as defined below is not.

**DEFINITION 2.5.** For  $h > 0$  and  $\epsilon \geq 0$ , define  $g : \mathbb{R} \rightarrow \mathbb{R}$  and  $w_{h,\epsilon} : \mathbb{R}^N \rightarrow \mathbb{R}^N$  by

$$g(t) := 2 \left( 1 + t^2 - t\sqrt{1+t^2} \right), \quad w_{h,\epsilon}^i(\psi) := (G^i(\psi) - \epsilon)g\left(\frac{\psi^i}{h}\right).$$

Also, we write for any  $\epsilon_0 > 0$  and  $w \in \mathbb{R}^N$  with nonnegative entries,

$$\begin{aligned} \mathcal{W}^{\epsilon_0} &:= \{\psi \in \mathbb{R}^N \mid w_{h,\epsilon}^i(\psi) \geq \epsilon_0 \ \forall i \in \{1, \dots, N\}\}, \\ \Sigma_{w,h,\epsilon} &:= \left\{ \psi \in \mathcal{K}^\epsilon \mid \sum_{i=1}^N w^i = \sum_{i=1}^N w_{h,\epsilon}^i(\psi) \right\}. \end{aligned}$$

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**Algorithm 1** Damped Newton’s algorithm.

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**Parameters** Fix  $h, \epsilon > 0$ , and  $w \in \mathbb{R}^N$  such that  $\sum_{i=1}^N w^i \geq 1$ ,  $w^i \in [0, 1]$ .

**Input** A tolerance  $\zeta > 0$  and an initial  $\psi_0 \in \mathbb{R}^N$  such that

$$(2.1) \quad \epsilon_0 := \frac{1}{2} \min \left[ \min_i w_{h,\epsilon}^i(\psi_0), \ \min_i w^i \right] > 0.$$

**While**  $\|w_{h,\epsilon}(\psi_k) - w\| \geq \zeta$

**Step 1** Compute  $\vec{d}_k = -[Dw_{h,\epsilon}(\psi_k)]^{-1}(w_{h,\epsilon}(\psi_k) - w)$ .

**Step 2** For each  $\ell \in \mathbb{N}$ , let  $r_\ell \in \mathbb{R}$  be such that  $\psi_{k+1,\ell} := \psi_k + 2^{-\ell} \vec{d}_k + r_\ell \mathbf{1}$  satisfies  $\psi_{k+1,\ell} \in \Sigma_{w,h,\epsilon}$ .

**Step 3** Determine the minimum  $\ell \in \mathbb{N}$  such that  $\psi_{k+1,\ell}$  satisfies

$$\begin{cases} \min_i w_{h,\epsilon}^i(\psi_{k+1,\ell}) \geq \epsilon_0, \\ \|w_{h,\epsilon}(\psi_{k+1,\ell}) - w\| \leq (1 - 2^{-(\ell+1)})\|w_{h,\epsilon}(\psi_k) - w\|. \end{cases}$$

**Step 4** Set  $\psi_{k+1} = \psi_k + 2^{-\ell} \vec{d}_k + r_\ell \mathbf{1}$  and  $k \leftarrow k + 1$ .

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We now use the above notation to propose the following damped Newton algorithm to approximate solutions of (1.1). Note that below we do not lose any generality in assuming  $w^i \leq 1$  for each  $i$ , as  $\mu$  is a probability measure.

We note that there is a unique choice of number  $r_\ell$  in Step 2 above (see Proposition 4.1). In the implementation that we have used to demonstrate examples in section 6, we use a bisection method on the function  $\Phi(\psi, \cdot)$  appearing in the proof of Proposition 4.1 to determine  $r_\ell$ .

We now give some heuristics on our algorithm. For  $h, \epsilon \geq 0$  fixed, define for any  $t_0 \geq 0$  the function  $\sigma_{t_0, h} : \mathbb{R} \rightarrow \mathbb{R}$  by

$$(2.2) \quad \sigma_{t_0, h}(t) = \begin{cases} -h\sqrt{t(t_0 - t)} & \text{if } t \in [0, t_0], \\ +\infty & \text{else} \end{cases}$$

and for any  $w \in \mathbb{R}^N$ ,  $w^i \geq 0$ , the function  $F_{w, h, \epsilon} : \mathbb{R}^N \rightarrow \mathbb{R} \cup \{+\infty\}$  by

$$(2.3) \quad \begin{aligned} F_{w, h, \epsilon}(\lambda) &= \sum_{i=1}^N \sigma_{w^i, h}(\lambda^i - \epsilon) + \delta(\lambda \mid \Lambda) \\ &= \begin{cases} -h \sum_{i=1}^N \sqrt{(\lambda^i - \epsilon)(w^i - \lambda^i + \epsilon)}, & \lambda \in \Lambda \cap \prod_{i=1}^N [\epsilon, w^i + \epsilon], \\ +\infty & \text{else.} \end{cases} \end{aligned}$$

It can be seen that  $F_{w, h, \epsilon}$  is a uniformly convex approximation to  $F_w = F_{w, 0, 0}$  when  $h, \epsilon > 0$ . Detailed calculations will be deferred to Proposition 3.2 in the following section, but if  $\psi \in \mathbb{R}^N$  is a vector such that  $w_{h, \epsilon}(\psi) = w$ , using the results of [BK19] it can be seen for the map  $T_\psi$  defined as in Remark 2.4 that the pair  $(T_\psi, G(\psi))$  is the unique solution to the minimization problem (1.1) with storage fee function given by  $F_{w, h, \epsilon}$ . Thus the algorithm generates a vector  $\psi$  and a storage fee function  $\tilde{F}$  approximating the original  $F_w$ , such that  $(T_\psi, G(\psi))$  solves the optimal transport problem with storage fee  $\tilde{F}$ . The normalization  $\psi \in \Sigma_{w, h, \epsilon}$  at each step in Algorithm 1 is necessary in order to ensure that the magnitude of the error vector  $w_{h, \epsilon}(\psi_k) - w$  will actually go to zero.

The main theorem of our paper is the following on convergence of the above algorithm. Also, see Definition 2.8 below for the notion of a universal constant.

**THEOREM 2.6.** *Suppose  $c$  satisfies (Reg), (Twist), and (QC). Also suppose  $X$  is a bounded set that is  $c$ -convex with respect to  $Y$ ,  $\mu = \rho dx$  for some density  $\rho \in C^{0, \alpha}(X)$  for some  $\alpha \in (0, 1]$ , and  $\text{spt } \mu \subset X$ . Then if  $h \in (0, 1]$ ,  $\epsilon \in (0, \frac{1}{2N})$ , and  $\sum_{i=1}^N w^i \geq 1$ , Algorithm 1 converges globally with a linear rate and locally with superlinear rate  $1 + \alpha^2$ .*

*Specifically, the iterates of Algorithm 1 satisfy*

$$\|w_{h, \epsilon}(\psi_{k+1}) - w\| \leq (1 - \bar{\tau}_k/2) \|w_{h, \epsilon}(\psi_k) - w\|,$$

where

$$\bar{\tau}_k := \min \left( \frac{\epsilon_0^{\frac{1}{\alpha^2}} \kappa^{\frac{1+\alpha}{\alpha^2}}}{(6N^{3/2} L \tilde{L}^{1+\alpha})^{\frac{1}{\alpha^2}} \|w_{h, \epsilon}(\psi_k) - w\| N^{\frac{1}{\alpha^2}}}, 1 \right),$$

where  $L$  and  $\kappa$  are as in Proposition 3.3, and  $\tilde{L} \leq \frac{C}{h^{18} \epsilon^9}$  for some universal constant  $C$ .

In addition, as soon as  $\bar{\tau}_k = 1$  we have

$$\|w_{h,\epsilon}(\psi_{k+1}) - w\| \leq \frac{2L\tilde{L}^{1+\alpha}\sqrt{N}\|w_{h,\epsilon}(\psi_k) - w\|^{1+\alpha^2}}{\kappa^{1+\alpha^2}}.$$

*Remark 2.7.* In [KMT19], the goal is to find a root of the mapping  $G - \beta$  which is in fact the gradient of the concave dual functional in the Kantorovich problem. In contrast, our mapping  $w_{h,\epsilon} - w$  is not the gradient of any scalar function (seen easily, as  $Dw_{h,\epsilon}$  is not symmetric). However, there is a connection between the choice of  $w_{h,\epsilon}$  and the *dual problem* of our optimal transport problem with storage fees. The authors have shown in [BK19] that a natural dual problem for (1.1) is to maximize

$$(2.4) \quad \mathbb{R}^N \ni \psi \mapsto - \int_X \max_i (-c(x, y_i) - \psi^i) d\mu(x) - F^*(\psi),$$

where  $F^*$  is the Legendre transform of  $F$ . This function is convex, and using [KMT19, Theorem 1,1], formally the first order condition for a maximum reads as  $G(\psi) \in \partial F^*(\psi)$ , or equivalently  $\psi \in \partial F(G(\psi))$ . Under mild conditions, this first order condition actually characterizes optimality; see [BK19, Theorem 4.7]. This choice of  $w_{h,\epsilon}$  is exactly what guarantees that a root of  $w_{h,\epsilon} - w$  satisfies this first order condition when  $F = F_{w,h,\epsilon}$  (see Proposition 3.2). See also Remark 2.15 below for further comments related to this dual problem.

In what follows, it will be possible in theory to obtain the exact dependence of constants on various quantities involving the storage fee function, the cost function, the domain, and the density of the source measure by tracing these bounds through the results of [KMT19]. However, we are most interested in the dependencies on the parameters  $h$  and  $\epsilon$ , and thus in the interest of brevity we will introduce the following terminology. The constants below are the same as those introduced in [KMT19, Remark 4.1].

**DEFINITION 2.8.** Suppose  $c$  satisfies (Reg) and (Twist),  $X$  is a bounded set,  $c$ -convex with respect to  $Y$ ,  $\mu = \rho dx$  for some density  $\rho \in C^{0,\alpha}(X)$  for some  $\alpha \in (0, 1]$ , and  $\text{spt } \mu \subset X$ . Then we will say that a positive, finite constant is universal if it has bounds away from zero and infinity depending only on the following quantities:  $\alpha$ ,  $n$ ,  $N$ ,  $\|\rho\|_{C^{0,\alpha}(X)}$ ,  $\mathcal{H}^{n-1}(\partial X)$ ,  $\max_{i \in \{1, \dots, N\}} \|c(\cdot, y_i)\|_{C^2(X)}$ , and

$$\begin{aligned} \epsilon_{\text{tw}} &:= \min_{x \in X} \min_{i,j \in \{1, \dots, N\}, i \neq j} \|\nabla_x c(x, y_i) - \nabla_x c(x, y_j)\|, \\ C_\nabla &:= \max_{x \in X, i \in \{1, \dots, N\}} \|\nabla_x c(x, y_i)\| \\ C_{\text{exp}} &:= \max_{i \in \{1, \dots, N\}} \max \left\{ \|\exp_i^c\|_{C^{0,1}((\exp_i^c)^{-1}(X))}, \|(\exp_i^c)^{-1}\|_{C^{0,1}(X)} \right\}, \\ C_{\text{cond}} &:= \max_{i \in \{1, \dots, N\}} \max_{p \in (\exp_i^c)^{-1}(X)} \text{cond}(D \exp_i^c(p)), \\ C_{\text{det}} &:= \max_{i \in \{1, \dots, N\}} \|\det(D \exp_i^c)\|_{C^{0,1}((\exp_i^c)^{-1}(X))}, \end{aligned}$$

where  $\text{cond}$  is the condition number of a linear transformation.

*Remark 2.9.* Apart from sections 3 and 4, we have written all estimates to keep as explicit track of  $N$  as possible. However, in these two sections doing so is a tedious exercise; in particular, it would require careful book-keeping of exactly what norms are being used. We comment that if the collection  $\{y_1, \dots, y_N\}$  is constructed by sampling

from a continuous domain  $Y$ , and  $c$  is a cost function on  $X \times Y$  satisfying (Reg), (Twist), and the Ma–Trudinger–Wang condition (along with appropriate convexity conditions on  $X$  and  $Y$ , which we will not detail here), then of the constants introduced in Definition 2.8, only  $\epsilon_{\text{tw}}$  will depend on  $N$ . In particular, if this is the case, the dependencies of all universal constants that arise in the paper (apart from that of  $\epsilon_{\text{tw}}$ ) can be seen to be polynomial in  $N$ .

Since Algorithm 1 only produces solutions to an approximating problem, we are concerned with how close these solutions might be to the solutions of our original problem. The second and third theorems of our paper show that solutions of (1.1) with the choice  $F = F_{\tilde{w}, h, \epsilon}$  are in fact close to the solution of the problem with  $F_w$  if  $\tilde{w} = w_{h, \epsilon}(\psi)$  for some dual variable  $\psi$ ,  $\tilde{w}$  is close to  $w$ , and  $h, \epsilon$  are small.

**DEFINITION 2.10.** *If  $A, B \subset \mathbb{R}^n$  are Borel sets, the  $\mu$ -symmetric distance between them is*

$$(2.5) \quad \Delta_\mu(A, B) := \mu((A \setminus B) \cup (B \setminus A)).$$

The following theorem gives quantified closeness for Laguerre cells of the approximating problems to those of the original problem in terms of the  $\mu$ -symmetric distance.

**THEOREM 2.11.** *Suppose  $c$  satisfies (Reg) and (Twist) and that  $\mu$  is absolutely continuous. Also suppose  $h > 0$ ,  $\epsilon \in (0, \frac{1}{2N})$ , and  $w \in \mathbb{R}^N$  with  $\sum_{i=1}^N w^i \geq 1$ ,  $w^i \geq 0$ . Then if  $\psi_{h, \epsilon} \in \mathcal{K}^\epsilon$  and  $(T, \lambda)$  is a pair minimizing (1.1) with the storage fee function  $F_w$ ,*

$$(2.6) \quad \|G(\psi_{h, \epsilon}) - \lambda\|_1 \leq 2(N\epsilon + \|w_{h, \epsilon}(\psi_{h, \epsilon}) - w\|_1 + 2N\sqrt{2C_L h})$$

and

$$(2.7) \quad \sum_{i=1}^N \Delta_\mu(\text{Lag}_i(\psi_{h, \epsilon}), T^{-1}(\{y_i\})) \leq 8N(N\epsilon + \|w_{h, \epsilon}(\psi_{h, \epsilon}) - w\|_1 + 2N\sqrt{2C_L h}),$$

where  $C_L > 0$  is the universal constant from Lemma A.1.

The above theorem shows the  $\mu$ -symmetric distance between the Laguerre cells generated along the iterates of our algorithm and those of the true, unregularized problem is controlled by  $h, \epsilon$ , and the error  $\|w_{h, \epsilon}(\psi_{h, \epsilon}) - w\|_1$  which is being minimized in Algorithm 1.

The final theorem below shows that when a Laguerre cell associated to the problem with the unregularized problem has nonzero Lebesgue measure, the above closeness can be measured in the Hausdorff distance, under an additional connectedness assumption. Before stating this result, we recall the following definition.

**DEFINITION 2.12.** *If  $1 \leq q \leq \infty$ , a probability measure  $\mu$  on  $X$  satisfies a  $(q, 1)$ -Poincaré–Wirtinger (PW) inequality if there is a constant  $C_{pw} > 0$  such that for any  $f \in C^1(X)$ ,*

$$\left\| f - \int_X f d\mu \right\|_{L^q(\mu)} \leq C_{pw} \|\nabla f\|_{L^1(\mu)}.$$

We will say “ $\mu$  satisfies a  $(q, 1)$ -PW inequality.”

*Remark 2.13.* Recall that some kind of connectedness condition on  $\text{spt } \mu$  is necessary in order to obtain invertibility of the derivative of the map  $G$  in nontrivial directions (see the discussion immediately preceding [KMT19, Definition 1.3]), and a Poincaré–Wirtinger inequality can be viewed as a quantitatively strengthened version of connectivity which is sufficient for our purposes. In particular, if  $\text{spt } \mu$  is not connected,  $\mu$  *cannot* satisfy a PW inequality of any kind, and thus the removal of this condition in Theorem 2.6 represents a significant expansion of admissible measures compared to [KMT19].

If  $\rho$  is bounded away from zero on  $\text{spt } \rho$  and the support is connected, it satisfies an  $(\frac{n}{n-1}, 1)$ -PW inequality. By scaling,  $q = \frac{n}{n-1}$  is the largest possible value of  $q$ . We will only use the case of  $q > 1$  in order to obtain quantitative bounds on the Hausdorff convergence of Laguerre cells, namely for Theorem 2.14. We also remark that in Theorem 2.14, we can make do with  $q = 1$  if all of the Laguerre cells of the limit problem have nonzero measure. Below,  $d_{\mathcal{H}}$  is the Hausdorff distance between subsets of  $\mathbb{R}^n$ .

**THEOREM 2.14.** *Suppose that  $c$  and  $\mu$  satisfy the same conditions as Theorem 2.6 and that  $\mu$  satisfies a  $(q, 1)$ -PW inequality for some  $q \geq 1$ . Also suppose  $h > 0$ ,  $\epsilon \in (0, \frac{1}{2N})$ , and  $w \in \mathbb{R}^N$  with  $\sum_{i=1}^N w^i > 1$ ,  $w^i \geq 0$ , and  $(T, \lambda)$  being a pair minimizing (1.1) with the storage fee function  $F_w$ , and  $\psi \in \mathbb{R}^N$  is such that  $T_{\psi} = T$   $\mu$ -a.e.:*

1. *If  $\{h_k\}_{k=1}^{\infty}, \{\epsilon_k\}_{k=1}^{\infty} \subset \mathbb{R}_{>0}$ ,  $\{\psi_k\}_{k=1}^{\infty}, \psi_k \in \mathcal{K}^{\epsilon_k}$ , are sequences such that  $w_{h_k, \epsilon_k}(\psi_k) \rightarrow w$ ,  $h_k \searrow 0$ ,  $\epsilon_k \searrow 0$  as  $k \rightarrow \infty$ , and  $\mathcal{L}(\text{Lag}_i(\psi)) > 0$ , then*

$$\lim_{k \rightarrow 0} d_{\mathcal{H}}(\text{Lag}_i(\psi_k), \text{Lag}_i(\psi)) = 0.$$

2. *If  $q > 1$ ,  $\psi_{h, \epsilon} \in \mathcal{K}^{\epsilon}$ , there are universal constants  $C_1, C_2 > 0$  such that*

$$d_{\mathcal{H}}(\text{Lag}_i(\psi_{h, \epsilon}), \text{Lag}_i(\psi))^n \leq \frac{C_1 C_{pw} N^5 q (N\epsilon + \|w_{h, \epsilon}(\psi_{h, \epsilon}) - w\|_1 + 2N\sqrt{2C_L h})}{\epsilon^{1/q} (q-1) (\arccos(1 - C_2 \mathcal{L}(\text{Lag}_i(\psi))^2))^{n-1}},$$

as long as

$$(2.8) \quad \frac{N^5 C_{\Delta} C_{\nabla} C_{pw} q (N\epsilon + \|w_{h, \epsilon}(\psi_{h, \epsilon}) - w\|_1 + 2N\sqrt{2C_L h})}{\epsilon^{1/q} (q-1)} < \mathcal{L}(\text{Lag}_i(\psi)),$$

where  $C_{\Delta}$  and  $C_L$  are the universal constants defined in [BK20, Lemma 5.5] and Lemma A.1, respectively.

*Remark 2.15.* Another possible numerical approach could be to take  $F = F_{w, h, \epsilon}$  for some fixed  $h$  and  $\epsilon$  in the dual problem (2.4) (which would yield a strictly concave function in  $\psi$ ) and then apply a Newton method to its gradient in order to find the maximizer. The main reason we have elected to take a different approach is to be able to obtain Theorems 2.11 and 2.14 above: again it is crucial to know how much error the regularization process itself introduces. Suppose one were to take the above route and obtain a sequence of dual variables  $\psi_k$  along the iteration, which in turn induce maps  $T_{\psi_k}$  as in Remark 2.4. The sequence of mass vectors  $G(\psi_k)$  of each induced target measure  $(T_{\psi_k})_{\#} \mu$  will converge to the optimal mass of the particular regularization chosen, but it is unclear how close this is to the *unregularized* problem with  $F = F_w$ ; this error is crucial in understanding how close the associated Laguerre cells over the course of the iteration are to the true cells for the unregularized problem. With our Algorithm 1, we are able to control this error through the estimate (2.6).

**2.2. Outline of the paper.** In section 3, we give some useful properties of the mapping  $w_{h,\epsilon}$ . In section 4, we prove Theorem 2.6 on the convergence rate of our Algorithm 1. We also give a crude estimate on the number of iterations necessary to get within a desired error in terms of the parameters  $h$ ,  $\epsilon$ , and  $N$ . In section 5, we prove Theorems 2.11 and 2.14 on the convergence of the Laguerre cells. In section 6, we present some numerical examples. These examples will include a comparison of performance with the algorithm from [KMT19] and cases which are outside of the scope of this previous work. Appendix A contains a short result on strong convexity of the transport cost as a function of the dual variables  $\psi$ , needed for Theorem 2.14.

**3. Properties of the mapping  $w_{h,\epsilon}$ .** In this section, we gather some properties and estimates on the mapping  $w_{h,\epsilon}$  which will be crucial in the proofs of all of our main theorems. For the remainder of the paper, we assume that  $c$  satisfies (Reg) and (Twist) and that  $\mu$  is absolutely continuous. In this section and the following, we also assume  $c$  satisfies (QC),  $\mu = \rho dx$  for some density  $\rho \in C^{0,\alpha}(X)$ , for some  $\alpha \in (0, 1]$ , and  $X$  is a bounded set,  $c$ -convex with respect to  $Y$  such that  $\text{spt } \mu \subset X$ .

**3.1. Solutions of the approximating problem with  $F_{w,h,\epsilon}$ .** We will begin by justifying the remarks following Algorithm 1.

**DEFINITION 3.1.** *The subdifferential of a convex function  $F : \mathbb{R}^N \rightarrow \mathbb{R} \cup \{+\infty\}$  at any point  $x$  is defined by the set*

$$\partial F(x) := \{p \in \mathbb{R}^N \mid F(y) \geq F(x) + \langle p, y - x \rangle \ \forall y \in \mathbb{R}^N\}.$$

**PROPOSITION 3.2.** *Fix  $h, \epsilon > 0$ , and  $w \in \mathbb{R}^N$  with  $w^i \geq 0$ ,  $\sum_{i=1}^N w^i \geq 1$ . Then if  $\psi \in \mathbb{R}^N$  is such that  $w_{h,\epsilon}(\psi) = w$ , the pair  $(T_\psi, G(\psi))$  is the unique solution to the minimization problem (1.1) with the storage fee function given by  $F_{w,h,\epsilon}$  (with  $T_\psi$  defined as in Remark 2.4).*

*Proof.* We first calculate that for any  $t_0 \geq 0$  and  $t \in (\epsilon, t_0 + \epsilon)$ ,  $\frac{d}{dt} \sigma_{t_0,h}(t - \epsilon) = h \frac{2(t - \epsilon) - t_0}{2\sqrt{(t - \epsilon)(t_0 - t + \epsilon)}}$ . Thus, for any  $t$  and  $t_1 \geq 0$ , if we take the choice

$$t_0 = 2(t - \epsilon) \left( 1 + \left( \frac{t_1}{h} \right)^2 - \frac{t_1}{h} \sqrt{1 + \left( \frac{t_1}{h} \right)^2} \right) = (t - \epsilon)g\left(\frac{t_1}{h}\right),$$

we obtain

$$\begin{aligned} \frac{d}{dt} \sigma_{t_0,h}(t - \epsilon) &= h \frac{2(t - \epsilon) - (2(t - \epsilon)(1 + (\frac{t_1}{h})^2) - \frac{t_1}{h} \sqrt{1 + (\frac{t_1}{h})^2})}{2\sqrt{(t - \epsilon)((2(t - \epsilon)(1 + (\frac{t_1}{h})^2) - \frac{t_1}{h} \sqrt{1 + (\frac{t_1}{h})^2}) - (t - \epsilon))}} \\ &= t_1 \frac{\sqrt{1 + (\frac{t_1}{h})^2} - \frac{t_1}{h}}{\sqrt{\left(\sqrt{1 + (\frac{t_1}{h})^2} - \frac{t_1}{h}\right)^2}} = t_1. \end{aligned}$$

Thus, taking  $t = G(\psi)$  and  $t_1 = \psi^i$ ,  $t_0 = (w_{h,\epsilon}(\psi))^i$  for each  $i$  in the calculation above, we see that if  $w_{h,\epsilon}(\psi) = w$ , we will have  $\psi \in \partial F_{w,h,\epsilon}(G(\psi))$ . Since  $F_{w,h,\epsilon}$  is a proper, convex function that is  $+\infty$  outside the set  $\Lambda$ , by [BK19, Theorem 4.7] we obtain that the pair  $(T_\psi, G(\psi))$  is the unique minimizing pair in the problem (1.1) with storage fee function  $F_{w,h,\epsilon}$ .  $\square$

**3.2. Estimates on  $w_{h,\epsilon}$ .** Next we will obtain invertibility of  $Dw_{h,\epsilon}$  on the set  $\Sigma_{w,h,\epsilon}$ . This normalization will be critical in obtaining the necessary estimates to justify convergence of our Newton algorithm; since the masses  $G(\psi)$  are invariant under the addition of multiples of  $\mathbf{1}$ , the normalization  $\psi \in \Sigma_{w,h,\epsilon}$  is not guaranteed for an optimizer and must be enforced. For the remainder of this section and the following section 4, we will not be as explicit in terms of the dependence of various quantities on  $N$ . Related to this, for any vector valued map  $\Phi : \Omega \rightarrow \mathbb{R}^N$  on any domain  $\Omega \subset \mathbb{R}^N$ , we will write associated  $\alpha$ -Hölder seminorms as

$$[\Phi]_{C^{0,\alpha}(\bar{\Omega})} := \sup_{x \neq y \in \Omega} \frac{\|\Phi(x) - \Phi(y)\|}{\|x - y\|^\alpha} \leq \sqrt{N} \max_{1 \leq i \leq N} \sup_{x \neq y \in \Omega} \frac{|\Phi^i(x) - \Phi^i(y)|}{\|x - y\|^\alpha},$$

$$[D\Phi]_{C^{0,\alpha}(\bar{\Omega})} := \sup_{x \neq y \in \Omega} \frac{\|D\Phi(x) - D\Phi(y)\|}{\|x - y\|^\alpha} \leq N \max_{1 \leq i, j \leq N} \sup_{x \neq y \in \Omega} \frac{|D_j \Phi^i(x) - D_j \Phi^i(y)|}{\|x - y\|^\alpha},$$

and

$$\|\Phi\|_{C^1(\Omega)} := \sup_{x \in \Omega} \|\Phi(x)\| + \sup_{x \in \Omega} \|D\Phi(x)\|, \quad \|\Phi\|_{C^{1,\alpha}(\bar{\Omega})} := \|\Phi\|_{C^1(\Omega)} + [D\Phi]_{C^{0,\alpha}(\bar{\Omega})},$$

where  $\|D\Phi(x)\|$  is the operator norm. In particular, for universal constants  $C > 0$  (that only depend on  $N$ ) we obtain  $\|\Phi(\psi_1) - \Phi(\psi_2)\| \leq C[\Phi]_{C^{0,\alpha}(\bar{\Omega})} \|\psi_1 - \psi_2\|^\alpha$ , and similarly for  $D\Phi$ .

**PROPOSITION 3.3.** *Fix  $h > 0$ ,  $\epsilon \in (0, \frac{1}{2N})$ ,  $\epsilon_0 > 0$ , and  $w \in \mathbb{R}^N$  with  $\sum_{i=1}^N w^i \geq 1$ ,  $w^i \geq 0$ , and suppose  $c$ ,  $X$ , and  $\mu$  satisfy the same conditions as Theorem 2.6. Then the following hold:*

1.  $\Sigma_{w,h,\epsilon}$  is bounded and nonempty.
2.  $w_{h,\epsilon}$  is differentiable on  $\mathcal{K}^\epsilon$ .
3.  $Dw_{h,\epsilon}(\psi)$  is invertible whenever  $\psi \in \Sigma_{w,h,\epsilon} \cap \mathcal{W}^{\epsilon_0}$ .

Moreover, if  $h \leq 1$ , there exists a universal constant  $C > 0$  such that

$$(3.1) \quad \text{diam}(\Sigma_{w,h,\epsilon}) \leq C\epsilon^{-\frac{1}{2}},$$

$$(3.2) \quad \|w_{h,\epsilon}\|_{C^{1,\alpha}(\bar{\Sigma}_{w,h,\epsilon})} =: L \leq C \max\left(h^{-2}\epsilon^{-2}, h^{-3}\epsilon^{-\frac{1}{2}}\right),$$

$$(3.3) \quad \sup_{\psi \in \Sigma_{w,h,\epsilon} \cap \mathcal{W}^{\epsilon_0}} \|Dw_{h,\epsilon}(\psi)^{-1}\| =: \kappa^{-1} \leq C\epsilon_0^{-1}h^{-6}\epsilon^{-\frac{3}{2}}.$$

*Proof of Proposition 3.3.* Throughout the proof,  $C > 0$  will denote a universal constant whose value may change from line to line.

We first calculate

$$\begin{aligned} g'(t) &= 2\left(2t - \sqrt{1+t^2} - \frac{t^2}{\sqrt{1+t^2}}\right) \\ &= \frac{2(2t\sqrt{1+t^2} - 1 - t^2 - t^2)}{\sqrt{1+t^2}} = -\frac{2(t - \sqrt{1+t^2})^2}{\sqrt{1+t^2}} < 0. \end{aligned}$$

In particular,  $g$  is continuous and strictly decreasing on  $\mathbb{R}$ , and it is easily seen that  $\lim_{t \rightarrow -\infty} g = +\infty$  and  $\lim_{t \rightarrow +\infty} g = 1$ . Now notice there exists at least one vector  $\psi \in \mathcal{K}^\epsilon$ ; for such a  $\psi$ ,  $G^i(\psi) - \epsilon > 0$  for all  $i$ . Since adding a multiple of  $\mathbf{1}$  to  $\psi$  does not change the value of  $G(\psi)$  and  $\sum_{i=1}^N (G^i(\psi) - \epsilon) < 1 \leq \sum_{i=1}^N w^i$ , we can see that there exists some  $r \in \mathbb{R}$  such that  $\sum_{i=1}^N w_{h,\epsilon}^i(\psi + r\mathbf{1}) = \sum_{i=1}^N (G^i(\psi + r\mathbf{1}) - \epsilon)g(\frac{\psi^i + r}{h}) = \sum_{i=1}^N w^i$ , i.e.,  $\Sigma_{w,h,\epsilon}$  is nonempty.

Next we show the boundedness of  $\Sigma_{w,h,\epsilon}$ . If  $\psi \in \Sigma_{w,h,\epsilon}$ , we calculate

$$\sum_{i=1}^N w^i = \sum_{i=1}^N (G^i(\psi) - \epsilon) g\left(\frac{\psi^i}{h}\right) \leq \sum_{i=1}^N (G^i(\psi) - \epsilon) \max_j g\left(\frac{\psi^j}{h}\right) = \max_j g\left(\frac{\psi^j}{h}\right) (1 - N\epsilon).$$

Hence  $\max_j g\left(\frac{\psi^j}{h}\right) \geq \frac{\sum_{i=1}^N w^i}{1 - N\epsilon} \geq \frac{1}{1 - N\epsilon} > 1$ . In particular, we must have an upper bound on some component  $\psi^k$ , i.e.,  $\psi^k \leq \tilde{M}_1$ , where  $\tilde{M}_1 := hg^{-1}(\frac{1}{1 - N\epsilon}) < +\infty$ . Now since  $X$  is compact, there exist constants  $M_1$  and  $m_1$  such that  $m_1 < c(\cdot, y_i) < M_1$  for all  $i \in \{1, \dots, N\}$ . If, for any  $i$ ,  $\psi^i > \tilde{M}_1 + M_1 - m_1$ , then we would have  $\text{Lag}_i(\psi) = \emptyset$ , contradicting  $\psi \in \mathcal{K}^\epsilon$ .

A similar calculation yields the bound  $\min_j g\left(\frac{\psi^j}{h}\right) \leq \frac{\sum_{i=1}^N w^i}{1 - N\epsilon} \leq \frac{N}{1 - N\epsilon} \leq 2N$ , and thus by an analogous argument we obtain the uniform bounds

$$\begin{aligned} \tilde{m} &\leq \psi^i \leq \tilde{M} \quad \forall \psi \in \Sigma_{w,h,\epsilon}, \quad i \in \{1, \dots, N\}, \\ \tilde{M} &:= \tilde{M}_1 + M_1 - m_1 = hg^{-1}\left(\frac{1}{1 - N\epsilon}\right) + M_1 - m_1 > 0, \\ (3.4) \quad \tilde{m} &:= \tilde{M}_2 - M_1 + m_1 := hg^{-1}(2N) - M_1 + m_1 < 0. \end{aligned}$$

We now calculate bounds on  $\tilde{M}$  and  $\tilde{m}$  in terms of  $N$  and  $\epsilon$ . If  $g(t) = a$  for some value  $a > 1$ , we find

$$\frac{a}{2} = 1 + t^2 - t\sqrt{1 + t^2} = 1 + t(t - \sqrt{1 + t^2}) = 1 + t\left(\frac{-1}{t + \sqrt{1 + t^2}}\right) = \frac{\sqrt{1 + t^2}}{t + \sqrt{1 + t^2}},$$

and hence

$$\begin{aligned} (3.5) \quad \left(1 - \frac{a}{2}\right)\sqrt{1 + t^2} &= \frac{at}{2} \implies \left(1 - \frac{a}{2}\right)^2 = t^2\left(\frac{a^2}{4} - \left(1 - \frac{a}{2}\right)^2\right) \implies t^2 = \frac{(2 - a)^2}{4a - 4}. \end{aligned}$$

Now if  $a = \frac{1}{1 - N\epsilon} < 2$ , we have  $t = g^{-1}(a) > 0$ , and hence by (3.5),

$$(3.6) \quad 0 < \tilde{M} \leq C \left(1 + h \frac{2 - \frac{1}{1 - N\epsilon}}{2\sqrt{\frac{1}{1 - N\epsilon} - 1}}\right) \leq C \left(1 + h \frac{1}{2\sqrt{N\epsilon(1 - N\epsilon)}}\right) \leq \frac{C}{\sqrt{2N\epsilon}},$$

where we have used that  $\epsilon < \frac{1}{2N}$ . Similarly, for  $a = 2N > 2$ ,  $t = g^{-1}(a) < 0$ , and hence using (3.5) again yields

$$(3.7) \quad 0 > \tilde{m} = -C \left(1 + h \frac{2N - 2}{2\sqrt{2N - 1}}\right) \geq -C \left(1 + \frac{hN}{\sqrt{N}}\right) \geq -C\sqrt{N}.$$

Combining this with (3.6) immediately gives (3.1).

We will also have use for some estimates on  $g$  and  $g'$ . We calculate

$$\begin{aligned}
g'\left(\frac{\tilde{M}}{h}\right) &= -\frac{2\left(\frac{\tilde{M}}{h} - \sqrt{1 + \left(\frac{\tilde{M}}{h}\right)^2}\right)^2}{\sqrt{1 + \left(\frac{\tilde{M}}{h}\right)^2}} = -\frac{2(\tilde{M} - \sqrt{h^2 + \tilde{M}^2})^2}{h\sqrt{h^2 + \tilde{M}^2}} \\
&= -\frac{2h^3}{\sqrt{h^2 + \tilde{M}^2}(\tilde{M} + \sqrt{h^2 + \tilde{M}^2})^2} \leq -\frac{h^3}{2(h^2 + \tilde{M}^2)^{3/2}} \\
&\leq -\frac{h^3}{2(\frac{2N\epsilon h^2 + C}{2N\epsilon})^{3/2}} \leq -Ch^3 N^{\frac{3}{2}} \epsilon^{\frac{3}{2}},
\end{aligned}$$

where we have used (3.6) in the last line. At the same time,

$$g'\left(\frac{\tilde{m}}{h}\right) = -\frac{2(\tilde{m} - \sqrt{h^2 + \tilde{m}^2})^2}{h\sqrt{h^2 + \tilde{m}^2}} \geq -\frac{CN}{h^2}.$$

Since  $g'$  is monotone and negative, we have for any  $\psi \in \Sigma_{w,h,\epsilon}$  and index  $i$  the estimates

$$(3.8) \quad Ch^3 N^{\frac{3}{2}} \epsilon^{\frac{3}{2}} \leq \left| g'\left(\frac{\psi^i}{h}\right) \right| \leq \frac{CN}{h^2}.$$

Additionally using (3.7) and that  $h \leq 1$ , for any  $\psi \in \Sigma_{w,h,\epsilon}$  and index  $i$  we have (recall  $\tilde{m}$  could be negative here)

$$\begin{aligned}
1 &\leq g\left(\frac{\psi^i}{h}\right) \leq g\left(\frac{\tilde{m}}{h}\right) = 2 \left(1 + \left(\frac{\tilde{m}}{h}\right)^2 - \frac{\tilde{m}}{h} \sqrt{1 + \left(\frac{\tilde{m}}{h}\right)^2}\right) \\
(3.9) \quad &= \frac{2\sqrt{h^2 + \tilde{m}^2}}{h^2} \left(\sqrt{h^2 + \tilde{m}^2} - \tilde{m}\right) \leq \frac{C\tilde{m}^2}{h^2} \leq \frac{CN}{h^2}.
\end{aligned}$$

Under the current assumptions, we see by [KMT19, Theorem 4.1] that  $G$  is uniformly  $C^{1,\alpha}$  on  $\Sigma_{w,h,\epsilon} \subset \mathcal{K}^\epsilon$ . We then calculate the derivative of  $w_{h,\epsilon}$  as

$$\begin{aligned}
Dw_{h,\epsilon}(\psi) &= \text{diag}\left(g\left(\frac{\psi^i}{h}\right)\right) DG(\psi) + \frac{1}{h} \text{diag}\left(\left(G^i(\psi) - \epsilon\right) g'\left(\frac{\psi^i}{h}\right)\right) \\
(3.10) \quad &= \text{diag}\left(g\left(\frac{\psi^i}{h}\right)\right) \left(\frac{1}{h} \text{diag}\left(\frac{(G^i(\psi) - \epsilon) g'\left(\frac{\psi^i}{h}\right)}{g\left(\frac{\psi^i}{h}\right)}\right) + DG(\psi)\right),
\end{aligned}$$

where  $\text{diag}$  of a vector in  $\mathbb{R}^N$  is the  $N \times N$  diagonal matrix with the entries of the vector on the diagonal. Since  $g \geq 1$  on  $\mathbb{R}$ , we see that  $\text{diag}(g(\frac{\psi^i}{h}))$  is invertible with all eigenvalues larger than 1. For any unit vector  $V \in \mathbb{R}^N$  we have

$$\begin{aligned}
&\left\langle \frac{1}{h} \text{diag}\left(\frac{(G^i(\psi) - \epsilon) g'\left(\frac{\psi^i}{h}\right)}{g\left(\frac{\psi^i}{h}\right)}\right) V, V \right\rangle + \langle DG(\psi)V, V \rangle \\
&= \frac{1}{h} \sum_{i=1}^N \frac{(G^i(\psi) - \epsilon) g'\left(\frac{\psi^i}{h}\right)}{g\left(\frac{\psi^i}{h}\right)} (V^i)^2 + \langle DG(\psi)V, V \rangle =: A + B.
\end{aligned}$$

By [KMT19, Theorems 1.1 and 1.3],  $DG$  is symmetric, every off diagonal entry is nonnegative, and each row sums to zero, and hence  $B \leq 0$ . We also calculate

$$\begin{aligned}
A &\leq \frac{1}{h} \max_j \frac{(G^j(\psi) - \epsilon)g'(\frac{\psi^j}{h})}{g(\frac{\psi^j}{h})} \sum_{i=1}^N (V^i)^2 = \frac{1}{h} \max_j \frac{(G^j(\psi) - \epsilon)g'(\frac{\psi^j}{h})}{g(\frac{\psi^j}{h})} \\
&= \frac{1}{h} \max_j \frac{w_{h,\epsilon}^j(\psi)g'(\frac{\psi^j}{h})}{g(\frac{\psi^j}{h})^2} \leq -C\epsilon_0 h^6 N^{-\frac{1}{2}} \epsilon^{\frac{3}{2}},
\end{aligned}$$

where we use (3.9) and that  $\psi \in \mathcal{W}^{\epsilon_0}$ , and hence  $Dw_{h,\epsilon}(\psi)$  is invertible and we obtain (3.3).

Finally, since  $\Sigma_{w,h,\epsilon}$  is bounded by above and  $g'$  is clearly a  $C^1$  function on  $\mathbb{R}$ , we can again use [KMT19, Theorem 4.1] to conclude that  $w_{h,\epsilon}$  is actually  $C^{1,\alpha}$  on  $\Sigma_{w,h,\epsilon}$ . The only thing left is to verify the dependencies of  $L > 0$  from (3.2). Since  $g$  is decreasing on  $\mathbb{R}$ , by (3.9) we immediately see that  $\|w_{h,\epsilon}\|_{L^\infty(\Sigma_{w,h,\epsilon})} \leq \frac{CN}{h^2}$ . Also calculating using (3.8), (3.10), (3.9), and that  $\|G\|_{C^1(\overline{\mathcal{K}^\epsilon})} \leq CN$  from [KMT19, Theorem 1.3], we see that  $\|w_{h,\epsilon}\|_{C^1(\Sigma_{w,h,\epsilon})} \leq C(N^2 h^{-2} + Nh^{-2}) \leq \frac{CN^2}{h^2}$ .

For the remainder of the proof, we will not keep explicit track of the dependencies on  $N$ . Finally, note that

$$\begin{aligned}
[Dw_{h,\epsilon}]_{C^{0,\alpha}} &\leq C \left( \|g(\frac{\cdot}{h})\|_{L^\infty} [DG]_{C^{0,\alpha}} + [g(\frac{\cdot}{h})]_{C^{0,\alpha}} \|DG\|_{L^\infty} \right. \\
&\quad \left. + \frac{1}{h} ([G - \epsilon \mathbf{1}]_{C^{0,\alpha}} \|g'(\frac{\cdot}{h})\|_{L^\infty} + \|G - \epsilon \mathbf{1}\|_{L^\infty} [g'(\frac{\cdot}{h})]_{C^{0,\alpha}}) \right) \\
&\leq C \left( \|g(\frac{\cdot}{h})\|_{L^\infty} [DG]_{C^{0,\alpha}} + \text{diam}(\Sigma_{w,h,\epsilon}) \|g'(\frac{\cdot}{h})\|_{L^\infty} \|DG\|_{L^\infty} \right. \\
&\quad \left. + \frac{\text{diam}(\Sigma_{w,h,\epsilon})}{h} (\|DG\|_{L^\infty} \|g'(\frac{\cdot}{h})\|_{L^\infty} + \|G - \epsilon \mathbf{1}\|_{L^\infty} [g'(\frac{\cdot}{h})]_{C^{0,1}}) \right), \tag{3.11}
\end{aligned}$$

where all norms and seminorms of  $g$  and  $g'$  are over  $[\tilde{m}, \tilde{M}]$  and the remainder over  $\Sigma_{w,h,\epsilon}$ .

Fixing an index  $i$ , for any  $\psi_1 \neq \psi_2 \in \Sigma_{w,h,\epsilon}$  we have

$$\left| g'\left(\frac{\psi_1^i}{h}\right) - g'\left(\frac{\psi_2^i}{h}\right) \right| \leq \sup_{t \in [\tilde{m}, \tilde{M}]} \left| g''\left(\frac{t}{h}\right) \right| \left| \frac{\psi_1^i}{h} - \frac{\psi_2^i}{h} \right| \leq \frac{C \|\psi_1 - \psi_2\|}{h}, \tag{3.12}$$

since by direct computation we see that

$$g''(t) = \frac{-4t^3 + 4(1+t^2)^{3/2} - 6t}{(1+t^2)^{3/2}} = 4 - 2 \frac{2t^3 + 3t}{(1+t^2)^{3/2}} = 4 - 4 \frac{t}{(1+t^2)^{1/2}} - 2 \frac{t}{(1+t^2)^{3/2}},$$

and so

$$|g''(t)| \leq 4 + 4 \left| \frac{t}{(1+t^2)^{1/2}} \right| + 2 \left| \frac{t}{(1+t^2)^{3/2}} \right| \leq 4 + 4 + 2 \min(|t|, |t|^{-2}) \leq 10.$$

At the same time using (3.8),

$$\left| g\left(\frac{\psi_1^i}{h}\right) - g\left(\frac{\psi_2^i}{h}\right) \right| \leq \sup_{t \in [\tilde{m}, \tilde{M}]} \left| g'\left(\frac{t}{h}\right) \right|^2 \left| \frac{\psi_1^i}{h} - \frac{\psi_2^i}{h} \right| \leq \frac{C}{h^5} \|\psi_1 - \psi_2\|. \tag{3.13}$$

Finally, carefully tracing through the proofs leading to [KMT19, Theorem 4.1] yields that

$$[DG]_{C^{0,\alpha}(\overline{\mathcal{K}^\epsilon})} \leq \frac{C}{\epsilon^2}. \tag{3.14}$$

Combining with (3.8), (3.9), (3.13), (3.12), and that  $\|G\|_{C^1(\overline{\mathcal{K}^\epsilon})} \leq CN$  in (3.11), we obtain

$$[Dw_{h,\epsilon}]_{C^{0,\alpha}(\Sigma_{w,h,\epsilon})} \leq C \max\left(h^{-2}\epsilon^{-2}, h^{-3}\epsilon^{-\frac{1}{2}}\right). \quad \square$$

**4. Convergence of Algorithm 1.** Here we provide the proof of our first main theorem on global linear and locally superlinear convergence of Algorithm 1. We remark that the proof below also shows that  $\Sigma_{w,h,\epsilon}$  is locally a  $C^1$  manifold of codimension 1 in  $\mathbb{R}^n$ . Again, we will not track explicit dependencies on  $N$ .

**PROPOSITION 4.1.** *There is a function  $r \in C^{1,\alpha}(\overline{\mathcal{K}^\epsilon})$  such that for any  $\psi \in \mathbb{R}^N$ ,  $r(\psi)$  is the unique number such that  $\pi(\psi) := \psi - r(\psi)\mathbf{1} \in \Sigma_{w,h,\epsilon}$ . Moreover, for some universal  $C > 0$ ,*

$$\|D\pi\|_{C^{0,\alpha}(\overline{\mathcal{K}^\epsilon}; \mathbb{R}^N)} \leq \frac{C}{h^{18}\epsilon^9}.$$

*Proof.* First we carry out some preliminary analysis. Again,  $C > 0$  will denote a suitable universal constant throughout the proof. Define  $\mathbb{R}^N \times \mathbb{R} \ni (\psi, r) \rightarrow \Phi(\psi, r) \in \mathbb{R}$  by

$$\begin{aligned} \Phi(\psi, r) &= \sum_{i=1}^N w_{h,\epsilon}^i(\psi - r\mathbf{1}) - w^i = \sum_{i=1}^N (G^i(\psi - r\mathbf{1}) - \epsilon)g\left(\frac{\psi^i - r}{h}\right) - \sum_{i=1}^N w^i \\ &= \sum_{i=1}^N (G^i(\psi) - \epsilon)g\left(\frac{\psi^i - r}{h}\right) - \sum_{i=1}^N w^i. \end{aligned}$$

Note that for any  $\psi \in \mathbb{R}^N$  such that  $w_{h,\epsilon}^i(\psi) \geq 0$  for all  $i \in \{1, \dots, N\}$ , we must have  $G^i(\psi) \geq \epsilon$ , and hence  $\psi \in \mathcal{K}^\epsilon$  for such  $\psi$ . A quick calculation yields that if  $(\psi, r)$  are such that  $\psi \in \mathcal{K}^\epsilon$  and  $\psi - r\mathbf{1} \in \Sigma_{w,h,\epsilon}$ , we have, using the calculation immediately preceding (3.8),

$$\frac{\partial}{\partial r} \Phi(\psi, r) = -\frac{1}{h} \sum_{i=1}^N (G^i(\psi) - \epsilon)g'\left(\frac{\psi^i - r}{h}\right) \geq Ch^3 N^{\frac{3}{2}} \epsilon^{\frac{3}{2}} (1 - N\epsilon) > 0.$$

Now the strict monotonicity of  $g$  along with the fact that  $\sum_{i=1}^N w^i \geq 1 > \sum_{i=1}^N (G^i(\psi) - \epsilon)$  and  $g(\mathbb{R}) = (1, \infty)$  implies that for any  $\psi \in \mathbb{R}^N$ , there exists a unique  $r(\psi) \in \mathbb{R}$  such that  $\Phi(\psi, r(\psi)) = 0$ , and thus the function  $\psi \mapsto r(\psi)$  is well-defined. By the above calculation and the implicit function theorem, we have that this function  $r$  is differentiable near any  $\psi \in \mathcal{K}^\epsilon$ . Differentiating the expression  $\Phi(\psi, r(\psi)) = 0$  with respect to  $\psi^j$  at such a  $\psi$ , we find that

$$\begin{aligned}
0 &= \sum_{i=1}^N \left( D_j G^i(\psi) g\left(\frac{\psi^i - r(\psi)}{h}\right) + (G^i(\psi) - \epsilon) g'\left(\frac{\psi^i - r(\psi)}{h}\right) \frac{\delta_j^i - D_j r(\psi)}{h} \right) \\
\implies D_j r(\psi) &= \frac{\sum_{i=1}^N h D_j G^i(\psi) g\left(\frac{\psi^i - r(\psi)}{h}\right) + \delta_j^i (G^i(\psi) - \epsilon) g'\left(\frac{\psi^i - r(\psi)}{h}\right)}{\sum_{i=1}^N (G^i(\psi) - \epsilon) g'\left(\frac{\psi^i - r(\psi)}{h}\right)} \\
(4.1) \quad &= \frac{(G^j(\psi) - \epsilon) g'\left(\frac{\psi^j - r(\psi)}{h}\right) + h \sum_{i=1}^N D_j G^i(\psi) g\left(\frac{\psi^i - r(\psi)}{h}\right)}{\sum_{i=1}^N (G^i(\psi) - \epsilon) g'\left(\frac{\psi^i - r(\psi)}{h}\right)}.
\end{aligned}$$

We can see that  $\|Dr\|$  is uniformly bounded on  $\mathcal{K}^\epsilon$ : we calculate

$$\begin{aligned}
\|D_j r\|_{L^\infty(\mathcal{K}^\epsilon)} &\leq 1 + \frac{\left| \sum_{i=1}^N D_j G^i(\psi) g\left(\frac{\psi^i - r(\psi)}{h}\right) \right|}{\left| \frac{1}{h} \sum_{i=1}^N (G^i(\psi) - \epsilon) g'\left(\frac{\psi^i - r(\psi)}{h}\right) \right|} \\
(4.2) \quad &\leq 1 + \frac{g\left(\frac{m}{h}\right) \sum_{i=1}^N |D_j G^i(\psi)|}{\frac{h^3 \epsilon^{3/2}}{h} (1 - N\epsilon)} \leq 1 + \frac{C\left(\frac{1}{h^2}\right)}{h^2 \epsilon^{3/2} (1 - N\epsilon)} \leq \frac{C}{h^4 \epsilon^{3/2}},
\end{aligned}$$

where we have used  $\|G\|_{C^1(\overline{\mathcal{K}^\epsilon})} \leq C$  from [KMT19, Theorem 1.3], (3.8), (3.9), and that  $\epsilon < \frac{1}{2N}$ .

Since  $\mathcal{K}^\epsilon = \bigcap_{i=1}^N (G^i)^{-1}((\epsilon, \infty))$ , the implicit function theorem combined with [KMT19, Theorem 5.1] along with the fact that  $\partial X$  is locally Lipschitz shows that  $\partial \mathcal{K}^\epsilon$  is locally Lipschitz. Thus  $W^{1,\infty}(\mathcal{K}^\epsilon) = C^{0,1}(\overline{\mathcal{K}^\epsilon})$ , and hence  $r$  is uniformly Lipschitz continuous on  $\mathcal{K}^\epsilon$ .

We will now show a Hölder bound on  $Dr$ . Note that for each  $j$ , we can write  $D_j r = \frac{H_1}{H_2}$ , where  $H_1(\psi) := \frac{1}{h} (G^j(\psi) - \epsilon) g'\left(\frac{\psi^j - r(\psi)}{h}\right) + \sum_{i=1}^N D_j G^i(\psi) g\left(\frac{\psi^i - r(\psi)}{h}\right)$  belongs to  $C^{0,\alpha}(\overline{\mathcal{K}^\epsilon})$  (using [KMT19, Theorem 4.1]) and  $H_2(\psi) := \frac{1}{h} \sum_{i=1}^N (G^i(\psi) - \epsilon) g'\left(\frac{\psi^i - r(\psi)}{h}\right)$  belongs to  $C^{0,1}(\overline{\mathcal{K}^\epsilon})$ , with  $H_2 \leq -\frac{Ch^3 N^{3/2}}{h} (1 - N\epsilon) < 0$  uniformly. Note that

$$\begin{aligned}
H_2(\pi(\psi)) &= \frac{1}{h} \sum_{i=1}^N (G^i(\psi - r(\psi)\mathbf{1}) - \epsilon) g'\left(\frac{(\psi - r(\psi)\mathbf{1})^i - r(\psi - r(\psi)\mathbf{1})}{h}\right) \\
&= \frac{1}{h} \sum_{i=1}^N (G^i(\psi) - \epsilon) g'\left(\frac{(\psi - r(\psi)\mathbf{1})^i}{h}\right) = H_2(\psi).
\end{aligned}$$

Thus for  $\psi_1 \neq \psi_2 \in \mathcal{K}^\epsilon$ , using (3.8),

$$\begin{aligned}
|D_j r(\psi_1) - D_j r(\psi_2)| &= \left| \frac{H_1(\psi_1)}{H_2(\psi_1)} - \frac{H_1(\psi_2)}{H_2(\psi_2)} \right| \\
&\leq \left| \frac{H_1(\psi_1) - H_1(\psi_2)}{H_2(\psi_1)} \right| + \left| \frac{H_1(\psi_2)(H_2(\psi_2) - H_2(\psi_1))}{H_2(\psi_1)H_2(\psi_2)} \right| \\
&= \left| \frac{H_1(\psi_1) - H_1(\psi_2)}{H_2(\psi_1)} \right| + \left| \frac{H_1(\psi_2)(H_2(\pi(\psi_2)) - H_2(\pi(\psi_1)))}{H_2(\psi_1)H_2(\psi_2)} \right| \\
&\leq \frac{[H_1]_{C^{0,\alpha}(\overline{\mathcal{K}^\epsilon})} \|\psi_1 - \psi_2\|^\alpha}{\frac{Ch^3 N^{3/2}}{h} (1 - N\epsilon)} + \frac{\|H_1\|_{L^\infty(\mathcal{K}^\epsilon)} [H_2]_{C^{0,1}(\overline{\mathcal{K}^\epsilon})} \|\pi(\psi_2) - \pi(\psi_1)\|}{(\frac{Ch^3 N^{3/2}}{h} (1 - N\epsilon))^2} \\
&\leq C \left( \frac{[H_1]_{C^{0,\alpha}(\overline{\mathcal{K}^\epsilon})}}{h^2 N^{3/2} (1 - N\epsilon)} \right. \\
(4.3) \quad &\quad \left. + \frac{\|H_1\|_{L^\infty(\mathcal{K}^\epsilon)} [H_2]_{C^{0,1}(\overline{\mathcal{K}^\epsilon})} \|\pi(\psi_2) - \pi(\psi_1)\|^{1-\alpha} [\pi]_{C^{0,1}(\overline{\mathcal{K}^\epsilon})}^\alpha}{(h^2 N^{3/2} (1 - N\epsilon))^2} \right) \|\psi_1 - \psi_2\|^\alpha,
\end{aligned}$$

and hence  $D_j r$  is uniformly  $C^{0,\alpha}$  on  $\mathcal{K}^\epsilon$ . Our next task will be to estimate  $[Dr]_{C^{0,\alpha}(\overline{\mathcal{K}^\epsilon})}$ . In order to do this, we estimate each of the terms in the above expression.

A quick calculation yields

$$(4.4) \quad \|H_1\|_{L^\infty(\mathcal{K}^\epsilon)} \leq C \left( \frac{1}{h^3} + \frac{1}{h^2} \right) \leq \frac{C}{h^3},$$

and since  $\pi(\psi) \in \Sigma_{w,h,\epsilon}$ , by (3.1) we have

$$(4.5) \quad \|\pi(\psi_2) - \pi(\psi_1)\| \leq \text{diam}(\Sigma_{w,h,\epsilon}) \leq \frac{C}{\epsilon^{\frac{1}{2}}}.$$

To estimate  $[H_2]_{C^{0,1}(\overline{\mathcal{K}^\epsilon})}$ , let  $H_{3,i}(\psi) := (G^i(\psi) - \epsilon)g'(\frac{\psi^i}{h})$  so that

$$H_2(\psi) = \frac{1}{h} \sum_i H_{3,i}(\pi(\psi)).$$

Just as we estimated the final two terms in (3.11), we see that  $[H_{3,i}]_{C^{0,1}(\Sigma_{w,h,\epsilon})} \leq \frac{C}{h^2}$  by using the bound  $\|G\|_{C^1(\overline{\mathcal{K}^\epsilon})} \leq C$  with (3.8) and (3.12). Furthermore, since  $\pi(\psi) = \psi - r(\psi)\mathbf{1}$ ,

$$(4.6) \quad [\pi]_{C^{0,1}(\overline{\mathcal{K}^\epsilon})} \leq 1 + N^{1/2} [r]_{C^{0,1}(\overline{\mathcal{K}^\epsilon})} \leq \frac{C}{h^4 \epsilon^{3/2}}$$

by (4.2). Hence

$$(4.7) \quad [H_2]_{C^{0,1}(\overline{\mathcal{K}^\epsilon})} \leq \frac{1}{h} \sum_{i=1}^N [H_{3,i} \circ \pi]_{C^{0,1}(\overline{\mathcal{K}^\epsilon})} \leq \frac{1}{h} \sum_{i=1}^N [H_{3,i}]_{C^{0,1}(\Sigma_{w,h,\epsilon})} [\pi]_{C^{0,1}(\overline{\mathcal{K}^\epsilon})} \leq \frac{C}{h^7 \epsilon^{\frac{3}{2}}}.$$

Finally, we bound  $[H_1]_{C^{0,\alpha}(\overline{\mathcal{K}^\epsilon})}$ . Let  $H_{4,i}(\psi) := D_j G^i(\psi)g(\frac{\psi^i}{h})$  so that  $H_1(\psi) = (G^j(\psi) - \epsilon)g'(\frac{\psi^j - r(\psi)}{h}) + \sum_i H_{4,i}(\pi(\psi))$ . For  $\psi_1, \psi_2 \in \overline{\mathcal{K}^\epsilon}$ , we have

$$\begin{aligned} & |H_{4,i}(\pi(\psi_1)) - H_{4,i}(\pi(\psi_2))| \\ &= \left| (D_j G^i(\psi_1) - D_j G^i(\psi_2))g\left(\frac{\pi(\psi_1)^i}{h}\right) - D_j G^i(\psi_2) \left( g\left(\frac{\pi(\psi_1)^i}{h}\right) - g\left(\frac{\pi(\psi_2)^i}{h}\right) \right) \right| \\ &\leq [DG]_{C^{0,\alpha}(\overline{\mathcal{K}^\epsilon})} g\left(\frac{\tilde{m}}{h}\right) \|\psi_1 - \psi_2\|^\alpha + \|G\|_{C^1(\overline{\mathcal{K}^\epsilon})} \sup_{s \in [\tilde{m}, \tilde{M}]} \left| g'\left(\frac{s}{h}\right) \right| \frac{\|\pi(\psi_1) - \pi(\psi_2)\|}{h} \\ &\leq \left( [DG]_{C^{0,\alpha}(\overline{\mathcal{K}^\epsilon})} g\left(\frac{\tilde{m}}{h}\right) + \frac{C}{h^3} \|\pi(\psi_1) - \pi(\psi_2)\|^{1-\alpha} [\pi]_{C^{0,1}(\overline{\mathcal{K}^\epsilon})}^\alpha \right) \|\psi_1 - \psi_2\|^\alpha \\ &\leq C \left( \frac{1}{h^2 \epsilon^2} + \frac{1}{h^{3+4\alpha} \epsilon^{\frac{1}{2}+\alpha}} \right) \|\psi_1 - \psi_2\|^\alpha \leq \frac{C}{h^7 \epsilon^2} \|\psi_1 - \psi_2\|^\alpha, \end{aligned}$$

where we have used (3.8) to estimate  $g'$ , (3.9) to estimate  $g(\frac{\tilde{m}}{h})$ , [KMT19, Theorem 1.3] to estimate  $\|G\|_{C^1(\overline{\mathcal{K}^\epsilon})}$ , (3.14) for  $[DG]_{C^{0,\alpha}(\overline{\mathcal{K}^\epsilon})} \leq \frac{C}{\epsilon^2}$ , and (4.5). Hence we see, using (4.6), that

$$\begin{aligned}
& [H_1]_{C^{0,\alpha}(\bar{\mathcal{K}}^\epsilon)} \\
& \leq C \left( \text{diam}(\Sigma_{w,h,\epsilon}) [G^j]_{C^{0,1}(\Sigma_{w,h,\epsilon})} \|g'(\frac{\cdot}{h})\|_{L^\infty([\tilde{m},\tilde{M}])} \right. \\
& \quad \left. + (\tilde{M} - \tilde{m}) \|G^j\|_{L^\infty(\bar{\mathcal{K}}^\epsilon)} [g'(\frac{\cdot}{h})]_{C^{0,1}([\tilde{m},\tilde{M}])} \right. \\
& \quad \left. + \sum_{i=1}^N [H_{4,i}]_{C^{0,\alpha}(\Sigma_{w,h,\epsilon})} \right) [\pi]_{C^{0,1}(\bar{\mathcal{K}}^\epsilon)} \\
& \leq C \left( \frac{1}{h^2 \epsilon^{\frac{1}{2}}} + \frac{1}{h \epsilon^{\frac{1}{2}}} + \frac{1}{h^7 \epsilon^2} \right) \frac{1}{h^4 \epsilon^{\frac{3}{2}}} \leq \frac{C}{h^{11} \epsilon^{\frac{7}{2}}}.
\end{aligned}$$

Putting the above together with (4.3), (4.4), (4.5), and (4.7), we get

$$\begin{aligned}
[Dr]_{C^{0,\alpha}(\bar{\mathcal{K}}^\epsilon)} & \leq C \left( \frac{[H_1]_{C^{0,\alpha}(\bar{\mathcal{K}}^\epsilon)}}{h^2 N^{\frac{3}{2}} (1 - N\epsilon)} + \frac{\|H_1\|_{L^\infty(\mathcal{K}^\epsilon)} [H_2]_{C^{0,1}(\bar{\mathcal{K}}^\epsilon)} \|\pi(\psi_2) - \pi(\psi_1)\|^{1-\alpha} [\pi]_{C^{0,1}(\bar{\mathcal{K}}^\epsilon)}^\alpha}{(h^2 N^{\frac{3}{2}} (1 - N\epsilon))^2} \right) \\
& \leq C \left( \frac{\frac{1}{h^{11} \epsilon^{\frac{7}{2}}}}{h^2 \epsilon^{\frac{3}{2}}} + \frac{\frac{1}{h^3} \cdot \frac{1}{h^7 \epsilon^{\frac{3}{2}}} \cdot \frac{1}{\epsilon^{\frac{1}{2}(1-\alpha)}} \cdot \frac{1}{h^{4\alpha} \epsilon^{\frac{3\alpha}{2}}}}{h^4 \epsilon^3} \right) \\
& = C \left( \frac{1}{h^{13} \epsilon^5} + \frac{1}{h^{14+4\alpha} \epsilon^{5+4\alpha}} \right) \leq \frac{C}{h^{18} \epsilon^9}.
\end{aligned}$$

Finally,

$$\|D\pi\|_{C^{0,\alpha}(\bar{\mathcal{K}}^\epsilon; \mathbb{R}^N)} \leq C(1 + \|Dr\|_{L^\infty(\mathcal{K}^\epsilon)} + [Dr]_{C^{0,\alpha}(\bar{\mathcal{K}}^\epsilon)}) \leq \frac{C}{h^{18} \epsilon^9}$$

by the calculation above combined with (4.2).  $\square$

With the above estimate, we can now prove linear convergence and locally super-linear convergence of our algorithm. This is done essentially as in [KMT19].

*Proof of Theorem 2.6.* Let  $\bar{\psi} := \psi_k$  be the vector chosen at the  $k$ th step of Algorithm 1,  $\bar{v} := (Dw_{h,\epsilon}(\bar{\psi}))^{-1}(w_{h,\epsilon}(\bar{\psi}) - w)$ , and define the curve  $\bar{\psi}(t) := \pi(\bar{\psi} - t\bar{v})$  (where  $\pi$  is defined in Proposition 4.1). We also take  $\tilde{L} := \max(1, \|D\pi\|_{C^{0,\alpha}(\bar{\mathcal{K}}^\epsilon; \mathbb{R}^N)})$ , which has the bound claimed in the statement of the theorem by Proposition 4.1. As noted above,  $\bar{\psi} \in \mathcal{K}^\epsilon \cap \mathcal{W}^{\epsilon_0}$ , and hence by Proposition 3.3 we have the estimates (3.2) and (3.3). Let  $\tau_1 := \inf\{t \geq 0 \mid \bar{\psi}(t) \notin \mathcal{W}^{\frac{\epsilon_0}{2}}\}$ ; then  $w_{h,\epsilon}^j(\bar{\psi}(\tau_1)) = \frac{\epsilon_0}{2}$  for some  $1 \leq j \leq N$ , and thus (using that  $\bar{\psi} \in \Sigma_{w,h,\epsilon}$  so  $\pi(\bar{\psi}) = \bar{\psi}$  and  $\|\bar{v}\| \leq \frac{\|w_{h,\epsilon}(\bar{\psi}) - w\|}{\kappa}$ ) we calculate

$$\begin{aligned}
\frac{\epsilon_0}{2} & \leq \|w_{h,\epsilon}(\bar{\psi}(\tau_1)) - w_{h,\epsilon}(\bar{\psi})\| \leq L\|\bar{\psi}(\tau_1) - \bar{\psi}\| \\
& = L\|\pi(\bar{\psi} - \tau_1\bar{v}) - \pi(\bar{\psi})\| \leq L\tilde{L}\tau_1\|\bar{v}\| \leq \frac{L\tilde{L}\tau_1\|w_{h,\epsilon}(\bar{\psi}) - w\|}{\kappa}.
\end{aligned}$$

The above gives a lower bound of  $\frac{\kappa\epsilon_0}{2L\tilde{L}\|w_{h,\epsilon}(\bar{\psi}) - w\|}$  on the first exit time  $\tau_1$ , and  $w_{h,\epsilon}$  is uniformly  $C^{1,\alpha}$  on the image  $\bar{\psi}([0, \tau_1])$  while  $\pi$  remains uniformly  $C^{1,\alpha}$  on the segment  $[\bar{\psi}, \bar{\psi} - \tau_1\bar{v}]$ . We will now Taylor expand in  $t$ . Note that

$$\begin{aligned}
\frac{d}{dt} \Big|_{t=0} w_{h,\epsilon}(\bar{\psi}(t)) & = -Dw_{h,\epsilon}(\bar{\psi}(t))\bar{v} + \langle Dr(\bar{\psi}(t)), \bar{v} \rangle Dw_{h,\epsilon}(\bar{\psi}(t))\mathbf{1} \Big|_{t=0} \\
& = -(w_{h,\epsilon}(\bar{\psi}) - w) + \langle Dr(\bar{\psi}), \bar{v} \rangle Dw_{h,\epsilon}(\bar{\psi})\mathbf{1}.
\end{aligned}$$

Using (4.1) and that  $\bar{\psi} \in \Sigma_{w,h,\epsilon}$ , we obtain

$$\begin{aligned}\langle Dr(\bar{\psi}), \bar{v} \rangle &= \frac{\langle Dw_{h,\epsilon}(\bar{\psi})^T \mathbf{1}, Dw_{h,\epsilon}(\bar{\psi})^{-1}(w_{h,\epsilon}(\bar{\psi}) - w) \rangle}{\langle Dw_{h,\epsilon}(\bar{\psi}) \mathbf{1}, \mathbf{1} \rangle} \\ &= \frac{\langle \mathbf{1}, w_{h,\epsilon}(\bar{\psi}) - w \rangle}{\langle Dw_{h,\epsilon}(\bar{\psi}) \mathbf{1}, \mathbf{1} \rangle} = 0.\end{aligned}$$

Now Taylor expanding we obtain

$$\begin{aligned}w_{h,\epsilon}(\bar{\psi}(t)) &= w_{h,\epsilon}(\bar{\psi}(0)) + \left( \frac{d}{du} \Big|_{u=0} w_{h,\epsilon}(\bar{\psi}(u)) \right) t \\ &\quad + \int_0^t \left( \frac{d}{du} \Big|_{u=s} w_{h,\epsilon}(\bar{\psi}(u)) - \frac{d}{du} \Big|_{u=0} w_{h,\epsilon}(\bar{\psi}(u)) \right) ds \\ (4.8) \quad &=: (1-t)w_{h,\epsilon}(\bar{\psi}) + tw + R(t).\end{aligned}$$

We see that

$$\begin{aligned}R^i(t) &= \int_0^t \left( \langle \nabla w_{h,\epsilon}^i(\bar{\psi}(s)), \dot{\bar{\psi}}(s) \rangle - \langle \nabla w_{h,\epsilon}^i(\bar{\psi}(0)), \dot{\bar{\psi}}(0) \rangle \right) ds \\ &= \int_0^t \left( \langle \nabla w_{h,\epsilon}^i(\bar{\psi}(s)) - \nabla w_{h,\epsilon}^i(\bar{\psi}(0)), \dot{\bar{\psi}}(s) \rangle + \langle \nabla w_{h,\epsilon}^i(\bar{\psi}(0)), \dot{\bar{\psi}}(s) - \dot{\bar{\psi}}(0) \rangle \right) ds.\end{aligned}$$

We will examine the two inner products separately. For  $t \in [0, \tau_1]$ , we have

$$\begin{aligned}&\left| \int_0^t \langle \nabla w_{h,\epsilon}^i(\bar{\psi}(s)) - \nabla w_{h,\epsilon}^i(\bar{\psi}(0)), \dot{\bar{\psi}}(s) \rangle ds \right| \leq \int_0^t \|\nabla w_{h,\epsilon}^i(\bar{\psi}(s)) - \nabla w_{h,\epsilon}^i(\bar{\psi}(0))\| \|\dot{\bar{\psi}}(s)\| ds \\ &\leq \int_0^t ([Dw_{h,\epsilon}]_{C^{0,\alpha}(\Sigma_{w,h,\epsilon})} \|\bar{\psi}(s) - \bar{\psi}(0)\|^\alpha) (\|D\pi(\bar{\psi} - s\bar{v})\| \|\bar{v}\|) ds \\ &\leq \int_0^t ([Dw_{h,\epsilon}]_{C^{0,\alpha}(\Sigma_{w,h,\epsilon})} \|D\pi\|_{C^{0,\alpha}(\bar{K}^\epsilon)}^\alpha \|s\bar{v}\|^{\alpha^2}) (\|D\pi(\bar{\psi} - s\bar{v})\| \|\bar{v}\|) ds \\ &\leq \frac{L\tilde{L}^{1+\alpha} \|\bar{v}\|^{\alpha^2+1}}{\alpha^2+1} t^{\alpha^2+1}\end{aligned}$$

and

$$\begin{aligned}&\left| \int_0^t \langle \nabla w_{h,\epsilon}^i(\bar{\psi}(0)), \dot{\bar{\psi}}(s) - \dot{\bar{\psi}}(0) \rangle ds \right| \leq \int_0^t \|\nabla w_{h,\epsilon}^i(\bar{\psi}(0))\| \|\dot{\bar{\psi}}(s) - \dot{\bar{\psi}}(0)\| ds \\ &\leq \int_0^t \|Dw_{h,\epsilon}(\bar{\psi}(0))\| \| (D\pi(\bar{\psi}) - D\pi(\bar{\psi} - s\bar{v})) \bar{v} \| ds \\ &\leq \int_0^t \|Dw_{h,\epsilon}(\bar{\psi}(0))\| \|D\pi\|_{C^{0,\alpha}(\bar{K}^\epsilon)} \|s\bar{v}\|^\alpha \|\bar{v}\| ds \\ &= \frac{L\tilde{L} \|\bar{v}\|^{1+\alpha}}{\alpha+1} t^{\alpha+1} \leq \frac{L\tilde{L}^{1+\alpha} \|\bar{v}\|^{1+\alpha}}{\alpha^2+1} t^{\alpha^2+1},\end{aligned}$$

where we have used  $\dot{\bar{\psi}}(s) = -(D\pi(\bar{\psi} - s\bar{v}))(\bar{v})$ . Note that since  $\sum_{i=1}^N w_{h,\epsilon}(\bar{\psi})^i = \sum_{i=1}^N w^i$ , we have the bound

$$\|w_{h,\epsilon}(\bar{\psi}) - w\| \leq 2 \sum_{i=1}^N w^i \leq 2N.$$

Hence for  $t \in [0, \tau_1]$  we obtain the bound on the remainder term  $R$  above as

$$\begin{aligned}\|R(t)\| &\leq \frac{(1 + \|\bar{v}\|^{\alpha-\alpha^2})L\tilde{L}^{1+\alpha}\sqrt{N}\|\bar{v}\|^{1+\alpha^2}}{\alpha^2+1}t^{\alpha^2+1} \\ &\leq \frac{(1 + (\frac{2N}{\kappa})^{\alpha-\alpha^2})L\tilde{L}^{1+\alpha}\sqrt{N}\|w_{h,\epsilon}(\bar{\psi}) - w\|^{1+\alpha^2}}{\kappa^{1+\alpha^2}}t^{\alpha^2+1} \\ &\leq \frac{3NL\tilde{L}^{1+\alpha}\sqrt{N}\|w_{h,\epsilon}(\bar{\psi}) - w\|^{1+\alpha^2}}{\kappa^{1+\alpha}}t^{\alpha^2+1}.\end{aligned}$$

At this point, the remainder of the proof proceeds exactly as that of [KMT19, Proposition 6.1], following equation (6.3) there, with  $w_{h,\epsilon}$  replacing the map  $G$  and  $\alpha^2$  instead of  $\alpha$ . For the convenience of the reader, we give the analogous expressions for  $\tau_i$ , which are

$$\begin{aligned}\tau_1 &\geq \frac{\kappa\epsilon_0}{2L\tilde{L}\|w_{h,\epsilon}(\bar{\psi}) - w\|}, \\ \tau_2 &= \min\left(\tau_1, \frac{\kappa^{\frac{1+\alpha}{\alpha^2}}\epsilon_0^{\frac{1}{\alpha^2}}}{(3N^{3/2}L\tilde{L}^{1+\alpha})^{\frac{1}{\alpha^2}}\|w_{h,\epsilon}(\bar{\psi}) - w\|^{1+\frac{1}{\alpha^2}}}\right), \\ \tau_3 &= \min\left(\tau_2, \frac{\kappa^{\frac{1+\alpha}{\alpha^2}}}{(6N^{3/2}L\tilde{L}^{1+\alpha})^{\frac{1}{\alpha^2}}\|w_{h,\epsilon}(\bar{\psi}) - w\|}, 1\right).\end{aligned}$$

With these expressions, we can calculate

$$\bar{\tau}_k \leq \tau_3.$$

Then global linear and local superlinear convergence follow as in [KMT19, Proposition 6.1].  $\square$

We conclude by using the above estimate Proposition 4.1 to give a crude estimate on the number of iterations necessary to obtain an approximation of a solution to within an error of  $\zeta$ . Note that Corollary 4.2 is far from tight, as it does not take into account that our rate derived in Proposition 4.1 goes to zero or that we have locally  $1 + \alpha^2$ -superlinear convergence, but still serves as a starting point.

**COROLLARY 4.2.** *There exists a universal constant  $C > 0$  so that for every  $\zeta > 0$ , and  $\epsilon_0, h, \epsilon$  sufficiently small depending on universal quantities, Algorithm 1 terminates in at most  $\frac{\log \frac{\zeta}{N}}{\log(1-\eta)}$  steps, where  $\eta = C\epsilon_0^{\frac{2+\alpha}{\alpha^2}}h^{\frac{24}{\alpha}+\frac{27}{\alpha^2}}\epsilon^{\frac{21}{2\alpha}+\frac{25}{2\alpha^2}}$ .*

*Proof.* If  $\bar{\tau}_k \neq 1$ , we have

$$\begin{aligned}\bar{\tau}_k &= \frac{\epsilon_0^{\frac{1}{\alpha^2}}\kappa^{\frac{1+\alpha}{\alpha^2}}}{(6N^{3/2}L\tilde{L}^{1+\alpha})^{\frac{1}{\alpha^2}}\|w_{h,\epsilon}(\bar{\psi}_k) - w\|N^{\frac{1}{\alpha^2}}} \\ &\geq C \frac{\epsilon_0^{\frac{1}{\alpha^2}}(\epsilon_0 h^6 \epsilon^{\frac{3}{2}})^{\frac{1+\alpha}{\alpha^2}}}{((h^{-18}\epsilon^{-9})^{1+\alpha} \max(h^{-2}\epsilon^{-2}, h^{-3}\epsilon^{-\frac{1}{2}}))^{\frac{1}{\alpha^2}}} \\ &\geq C \frac{\epsilon_0^{\frac{1}{\alpha^2}}(\epsilon_0 h^6 \epsilon^{\frac{3}{2}})^{\frac{1+\alpha}{\alpha^2}}}{((h^{-18}\epsilon^{-9})^{1+\alpha}(h^{-3}\epsilon^{-2}))^{\frac{1}{\alpha^2}}} = C\epsilon_0^{\frac{2+\alpha}{\alpha^2}}h^{\frac{24}{\alpha}+\frac{27}{\alpha^2}}\epsilon^{\frac{21}{2\alpha}+\frac{25}{2\alpha^2}},\end{aligned}$$

and we may assume  $h, \epsilon_0, \epsilon$  are sufficiently small so that  $1 - \frac{C\epsilon_0^{\frac{2+\alpha}{\alpha^2}} h^{\frac{24}{\alpha} + \frac{27}{\alpha^2}} \epsilon^{\frac{21}{2\alpha} + \frac{25}{2\alpha^2}}}{2} \geq \frac{1}{2}$ . Hence regardless of which value  $\bar{\tau}_k$  takes at each iteration, after  $\ell$  iterations we have

$$\|w(\psi_\ell) - w\| \leq (1 - \eta)^\ell \|w(\psi_0) - w\| \leq 2N(1 - \eta)^\ell,$$

where  $\eta = C\epsilon_0^{\frac{2+\alpha}{\alpha^2}} h^{\frac{24}{\alpha} + \frac{27}{\alpha^2}} \epsilon^{\frac{21}{2\alpha} + \frac{25}{2\alpha^2}}$ . Solving  $(1 - \eta)^\ell \|w(\psi_0) - w\| \leq 2N(1 - \eta)^\ell \leq \zeta$  for  $\ell$ , we see that it suffices to take  $\ell \geq \frac{\log \frac{\zeta}{2N}}{\log(1 - \eta)}$ .  $\square$

**5. Stability of Laguerre cells.** In this section, we prove that the convergence in our algorithm can be seen in terms of the Laguerre cells themselves instead of just in terms of the  $w(\psi_k)$ .

**5.1. Proof of Theorem 2.11.** We first prove  $\mu$ -symmetric convergence of Laguerre cells. For use in this proof, we define

$$(5.1) \quad \mathcal{C}(\tilde{\lambda}) = \min_{S_\# \mu = \nu_{\tilde{\lambda}}} \int c(x, S(x)) d\mu = \sup_{\psi \in \mathbb{R}^N} \left( - \int \psi^{c^*} d\mu - \langle \psi, \tilde{\lambda} \rangle \right).$$

*Proof of Theorem 2.11.* Let  $w \in \mathbb{R}^N$  with  $\sum_{i=1}^N w^i \geq 1$ ,  $w^i \geq 0$ , and  $\psi_{h,\epsilon} \in \mathcal{K}^\epsilon$ , and let  $(T, \lambda)$  be a pair minimizing (1.1) with the storage fee function  $F_w$ . Then if we define  $\lambda_{h,\epsilon} := G(\psi_{h,\epsilon})$  and  $\bar{w} := w_{h,\epsilon}(\psi_{h,\epsilon})$ , by Proposition 3.2, the pair  $(T_{\psi_{h,\epsilon}}, \lambda_{h,\epsilon})$  minimizes (1.1) with a storage fee equal to  $F_{\bar{w},h,\epsilon}$ . By [BK19, Theorem 4.7], there also exists a pair  $(T_{\bar{w},\epsilon}, \lambda_{\bar{w},\epsilon})$  which minimizes (1.1) with storage fee  $F_{\bar{w},0,\epsilon}$ . Since  $\mathcal{C}(\lambda_{h,\epsilon}) + F_{\bar{w},h,\epsilon}(\lambda_{h,\epsilon}) = \min_{\tilde{\lambda} \in \Lambda} (\mathcal{C}(\tilde{\lambda}) + F_{\bar{w},h,\epsilon}(\tilde{\lambda})) \leq \mathcal{C}(\lambda_{\bar{w},\epsilon}) + F_{\bar{w},h,\epsilon}(\lambda_{\bar{w},\epsilon})$ , we have

$$\mathcal{C}(\lambda_{h,\epsilon}) - \mathcal{C}(\lambda_{\bar{w},\epsilon}) \leq F_{\bar{w},h,\epsilon}(\lambda_{\bar{w},\epsilon}) - F_{\bar{w},h,\epsilon}(\lambda_{h,\epsilon}) \leq -F_{\bar{w},h,\epsilon}(\lambda_{h,\epsilon}) \leq h.$$

Next by Corollary A.2 from Appendix A, we have  $\frac{1}{32C_L N} \|\lambda_{h,\epsilon} - \lambda_{\bar{w},\epsilon}\|^2 \leq \mathcal{C}(\lambda_{h,\epsilon}) - \mathcal{C}(\lambda_{\bar{w},\epsilon}) \leq h$ , as  $\lambda_{\bar{w},\epsilon}$  is the minimizer of  $\mathcal{C}$  on the convex set  $\prod_{i=1}^N [\epsilon, \bar{w}^i + \epsilon]$ , which can be seen from  $F_{\bar{w},0,\epsilon} = \delta(\cdot \mid \prod_{i=1}^N [\epsilon, \bar{w}^i + \epsilon])$ .

Since the  $l^1$  and  $l^2$  norms on  $\mathbb{R}^N$  are comparable,

$$\|\lambda_{h,\epsilon} - \lambda_{\bar{w},\epsilon}\|_1 \leq \sqrt{N} \|\lambda_{h,\epsilon} - \lambda_{\bar{w},\epsilon}\| \leq 4N\sqrt{2C_L h}.$$

Since  $(T, \lambda)$  minimizes (1.1) with storage fee  $\delta(\cdot \mid \prod_{i=1}^N [0, w^i])$ , by [BK20, Theorem 2.6], we obtain  $\|\lambda_{\bar{w},\epsilon} - \lambda\|_1 \leq 2N\epsilon + 2\|\bar{w} - w\|_1$ . By the triangle inequality,

$$\|G(\psi_{h,\epsilon}) - \lambda\|_1 = \|\lambda_{h,\epsilon} - \lambda\|_1 \leq 2(N\epsilon + \|\bar{w} - w\|_1 + 2N\sqrt{2C_L h}),$$

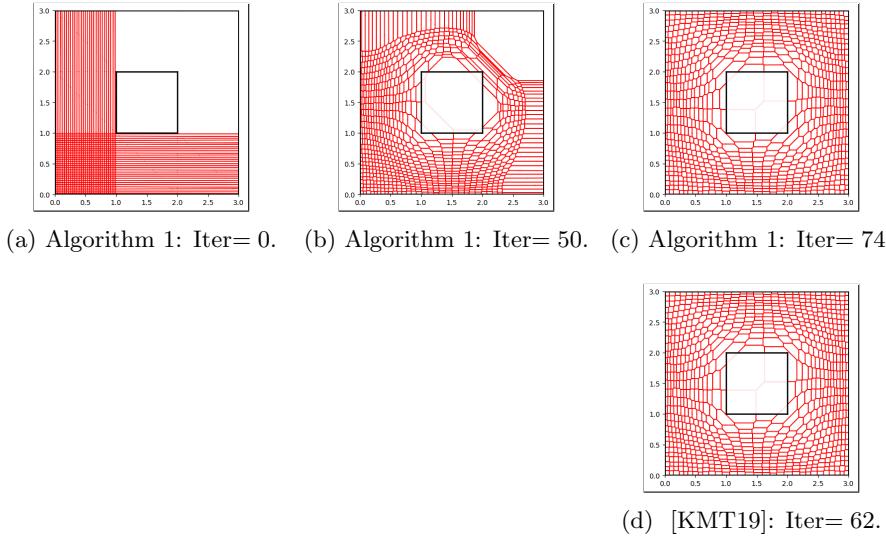
proving (2.6), and then [BK20, Corollary 2.8] gives

$$\sum_{i=1}^N \Delta_\mu(\text{Lag}_i(\psi_{h,\epsilon}), T^{-1}(\{y_i\})) \leq 8N(N\epsilon + \|\bar{w} - w\|_1 + 2N\sqrt{2C_L h}),$$

proving (2.7).  $\square$

**5.2. Proof of Theorem 2.14.** Next we prove convergence in terms of Hausdorff distance.

*Proof of Theorem 2.14.* We begin with statement (1). By [BK19, Proposition 3.5, Proposition 4.4, Corollary 4.5], there exists some  $\psi \in \mathbb{R}^N$  such that  $T = T_\psi$   $\mu$ -a.e.

FIG. 1. *Laguerre cells of Example 6.1.*

and  $\lambda = G(\psi)$ . Under the hypotheses of (1), by (2.6) in Theorem 2.11, we see that  $\|G(\psi_k) - \lambda\| \rightarrow 0$  as  $k \rightarrow \infty$ . Then since minimizers of (1.1) are minimizers of a classical optimal transport problem once the weight  $\lambda$  is known, we can apply [BK20, Corollary 1.11], which gives the claim in (1). Claim (2) also follows from [BK20, section 5], since we know  $\|G(\psi_{h,\epsilon}) - \lambda\|_1 \leq 2(N\epsilon + \|\bar{w} - w\|_1 + 2N\sqrt{2C_Lh})$  by (2.6) in Theorem 2.11.  $\square$

**6. Numerical examples.** In this section, we present some numerical examples produced by an implementation of Algorithm 1. In each example, the source measure  $\mu$  is supported on the 2D square  $[0, 3]^2$ , and the finite set  $Y$  is a  $30 \times 30$  uniform grid of points with a random perturbation added, contained in the square  $[0, 1]^2$ . Each example was calculated to an error of  $10^{-10}$ , with parameters  $h = \frac{1}{2}$  and  $\epsilon = 10^{-6}$ ; each figure below shows the boundaries of the associated Laguerre cells after various numbers of iterations. The code is based on a modification of the PyMongeAmpere interface developed by Quentin Mérigot.<sup>1</sup>

*Example 6.1.* In this example, the source measure  $\mu$  has density identically zero on the square  $[1, 2]^2$ , identically equals a positive constant on the boundary of  $[0, 3]^2$ , and is linearly interpolated over a triangulation of  $[0, 3]^2$  using 18 triangles (see the figure in [KMT19, section 6.3] for the triangulation; this measure is the same as what appears in that section) and then normalized to unit mass. By a small modification of [KMT19, Appendix A], this  $\mu$  satisfies a Poincaré–Wirtinger inequality. The weights  $w$  are randomly generated, and taken to sum to one, so this example is a classical optimal transport problem.

Algorithm 1 reaches the specified error in 74 iterations, while the algorithm of [KMT19] takes 62 iterations, and hence the two have comparable performance for classical optimal transport with source satisfying a Poincaré–Wirtinger inequality. The final diagram of Laguerre cells for both algorithms is presented in Figure 1 (seeded

<sup>1</sup>Mérigot's original code is available online from <https://github.com/mrgt/PyMongeAmpere>.

with the same random values).

*Example 6.2.* In this example, the source measure  $\mu$  is the same as in Example 6.1, and the vector  $w$  associated to the storage fee is randomly generated. Since  $\sum_{i=1}^N w^i > 1$ , this is *not* a classical optimal transport problem but is an optimal transport problem with storage fees.

Algorithm 1 reaches the specified error tolerance in 57 iterations. Attempting to run the algorithm from [KMT19] with a target measure given by the weights  $w$  fails to reduce the error beyond  $2 \cdot 10^{-2}$  and produces dual vectors leading to clearly incorrect Laguerre cells. This is to be expected, as this example is not a classical optimal transport problem. The final Laguerre cells for Algorithm 1 are given in Figure 2.

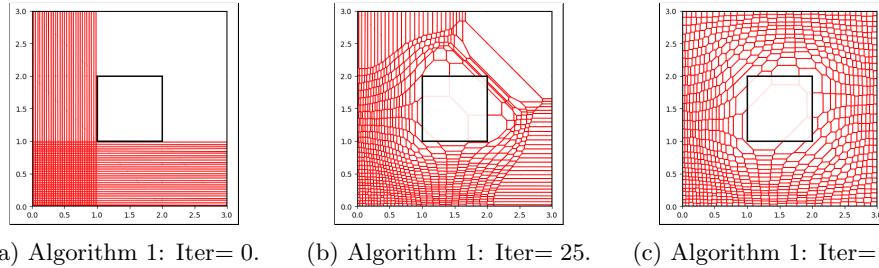


FIG. 2. *Laguerre cells of Example 6.2.*

*Example 6.3.* In this final example, the source measure  $\mu$  is taken to have density identically zero on the strip  $[1, 2] \times [0, 3]$ , equal to a positive constant on the edges  $\{0, 1\} \times [0, 3]$ , and then is linearly interpolated over the same triangulation as in Example 6.1 (and again normalized to unit mass). In particular, as  $\text{spt } \mu$  is not connected, this measure does *not* satisfy a  $(q, 1)$ -Poincaré–Wirtinger inequality for any  $q \geq 1$ . The weights  $w$  are taken with random weights summing to one, and hence this corresponds to a classical optimal transport problem.

Algorithm 1 reaches the error tolerance in 123 iterations, while the algorithm from [KMT19] fails to produce any reduction of error from the initial state. This is due to the lack of a Poincaré–Wirtinger inequality for  $\mu$ . The final Laguerre cells for Algorithm 1 are given in Figure 3.

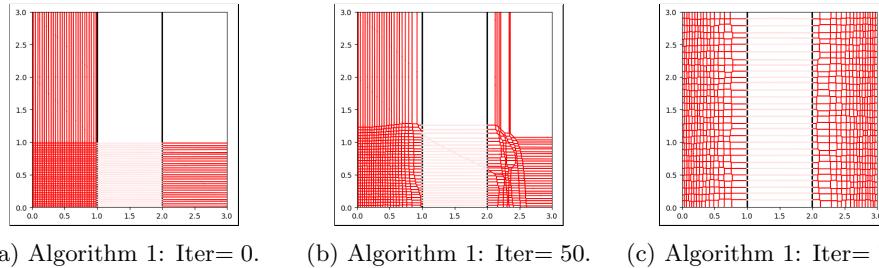


FIG. 3. *Laguerre cells of Example 6.3.*

## Appendix A. Strong convexity of $\mathcal{C}$ .

LEMMA A.1.  $\mathcal{C}$  as defined by (5.1) is strongly convex. In particular,

$$t\mathcal{C}(x) + (1-t)\mathcal{C}(y) \geq \mathcal{C}(tx + (1-t)y) + \frac{1}{8C_L N} t(1-t)\|y-x\|^2,$$

where  $[G]_{C^{0,1}(\mathbb{R}^N)} \leq C_L N$ , and  $C_L > 0$  is universal.

*Proof.* Let  $B(\psi) = \int \psi^c d\mu$ . We see that  $\mathcal{C}(\lambda) = B^*(-\lambda)$ ; also by [AG17],  $B$  is  $C^{1,1}$ ,  $\nabla B = -G$ , and  $B$  is convex (see [KMT19, Theorem 1.1], which does not require  $\mu$  to satisfy a Poincaré–Wirtinger inequality). By [AG17, Theorem 5.1], we see that the Lipschitz constant of  $G$  is bounded from above by  $C_L N$ , where  $C_L > 0$  is some universal constant. Now

$$\begin{aligned} 0 &\leq tB(x) + (1-t)B(y) - B(tx + (1-t)y) \\ &= tB(x) + (1-t) \left( B(x) + \langle y-x, \nabla B(x) \rangle \right. \\ &\quad \left. + \int_0^1 \langle \nabla B((1-s)x + sy) - \nabla B(x), y-x \rangle ds \right) \\ &\quad - \left( B(x) + \langle tx + (1-t)y - x, \nabla B(x) \rangle \right. \\ &\quad \left. + (1-t) \int_0^1 \langle \nabla B((1-s(1-t))x + s(1-t)y) - \nabla B(x), y-x \rangle ds \right) \\ &\leq (1-t) \int_0^1 \|\nabla B((1-s)x + sy) - \nabla B(x)\| \|y-x\| ds \\ &\quad + (1-t) \int_0^1 \|\nabla B((1-s(1-t))x + s(1-t)y) - \nabla B(x)\| \|y-x\| ds \\ &\leq C_L N (1-t) \left( \int_0^1 s \|y-x\|^2 ds + (1-t) \int_0^1 s \|y-x\|^2 ds \right) \\ &\leq (1-t) C_L N \|y-x\|^2. \end{aligned}$$

By repeating a similar argument, we get  $tB(x) + (1-t)B(y) - B(tx + (1-t)y) \leq tC_L N \|y-x\|^2$ . Hence  $tB(x) + (1-t)B(y) - B(tx + (1-t)y) \leq 2C_L N t(1-t) \|y-x\|^2$ .

In the terminology of [AP95, Definition 1], we have shown that  $B$  is  $\sigma$ -smooth, where  $\sigma(x) := 2C_L N x^2$ . Since it is well known that  $\sigma^*(z) = \frac{1}{8C_L N} z^2$ , by [AP95, Proposition 2.6] we see that  $\mathcal{C}$  is  $\sigma^*$ -convex, i.e.,  $t\mathcal{C}(x) + (1-t)\mathcal{C}(y) \geq \mathcal{C}(tx + (1-t)y) + \frac{1}{8C_L N} t(1-t) \|y-x\|^2$ , finishing the proof.  $\square$

COROLLARY A.2. Let  $K$  be a convex subset of the domain of  $\mathcal{C}$ . Let  $\lambda_{\min}$  be the minimizer of  $\mathcal{C}$  on  $K$ , and let  $\lambda \in K$  be arbitrary. Then  $\mathcal{C}(\lambda) - \mathcal{C}(\lambda_{\min}) \geq \frac{1}{32C_L N} \|\lambda - \lambda_{\min}\|^2$ .

*Proof.* By choice of  $\lambda_{\min}$ , we have  $\frac{1}{2}\mathcal{C}(\lambda) \geq \frac{1}{2}\mathcal{C}(\lambda_{\min})$  and  $-\mathcal{C}(\lambda_{\min}) \geq -\mathcal{C}(\frac{1}{2}(\lambda + \lambda_{\min}))$ . Hence by the above lemma we have  $\mathcal{C}(\lambda) - \mathcal{C}(\lambda_{\min}) \geq \frac{1}{2}(\mathcal{C}(\lambda) + \mathcal{C}(\lambda_{\min})) - \mathcal{C}(\frac{1}{2}(\lambda + \lambda_{\min})) \geq \frac{1}{32C_L N} \|\lambda - \lambda_{\min}\|^2$ .  $\square$

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