Convergence of Constrained Anderson Acceleration *

Mathieu Barré[†], Adrien Taylor[†], and Alexandre d'Aspremont [‡]

Abstract. Anderson Acceleration (AA) is a popular technique for speeding up convergence of iterative processes towards their limit points. AA proceeds by extrapolating a better approximation of the limit using a weighted combinations of previous iterates. Whereas AA was originally developed for accelerating convergence of iterative methods for solving linear systems, simple additional *stabilization strategies* allow it to extrapolate the solution of nonlinear systems as well. In this work, we study a *constrained* version of AA for solving nonlinear systems arising in optimization problems, where the stabilization strategy consists in bounding the magnitude of the extrapolation weights. We provide explicit convergence bounds for constrained AA, and as a byproduct, upper bounds on a constrained version of the Chebyshev problem on polynomials.

Key words. optimization, extrapolation methods, numerical analysis, Chebyshev polynomials

AMS subject classifications. 65K05, 90C25, 26C05

1. Introduction.

Let $F : \mathbb{R}^n \to \mathbb{R}^n$ be an operator and consider the problem of finding its fixed point, i.e. a solution $x_* \in \mathbb{R}^n$ to

$$x_* = F(x_*). \tag{1.1}$$

When F is a contraction, one can find such a point by running fixed point iterations

$$x_{k+1} = F(x_k)$$

starting from an initial guess $x_0 \in \mathbb{R}^n$. Obtaining faster convergence rates has been a key concern in numerical analysis. Anderson acceleration methods extrapolate a new point hopefully closer to the solution using a linear combination of fixed point iterates x_k. This idea was first applied to univariate sequences, fitting a linear model on the iterates and using the fixed point of this model as the extrapolated point [1, 37, 6, 8]. Extrapolation techniques were then extended to linearly converging vector valued sequences [2, 31, 39, 40] with convergence guarantees in the linear case, i.e. when F is an affine operator.

In the nonlinear case (i.e. when F is not an affine operator), convergence results can also be derived using a perturbation argument. However, the weights used to construct extrapolated points are typically obtained by solving ill conditioned quadratic programs, resulting in stability issues. The magnitudes of these weights typically blow up, breaking convergence

*July 2, 2021

Funding: MB acknowledges support from an AMX fellowship. AT acknowledges support from the European Research Council (grant SEQUOIA 724063). AA acknowledges support from the French government under management of Agence Nationale de la Recherche as part of the "Investissements d'avenir" program, reference ANR-19-P3IA-0001 (PRAIRIE 3IA Institute), the ML & Optimisation joint research initiative with the fonds AXA pour la recherche and Kamet Ventures, as well as a Google focused award.

[†]INRIA, D.I. École Normale Supérieure, Paris, France. (mathieu.barre@inria.fr,adrien.taylor@inria.fr).

[‡]CNRS, D.I. École Normale Supérieure, Paris, France. (aspremon@ens.fr)

properties of the acceleration procedure (see examples in e.g. [35, Figure 4]). Therefore, convergence guarantees in the nonlinear case mostly rely on additional mechanisms for controlling magnitudes of extrapolation weights.

1.1. Preliminaries.

Notations. Depending on the context $\|\cdot\|$ either denotes the classical Euclidean norm (when applied to a vector in $\mathbb{R}^n$), or the operator norm (when applied to a matrix in $\mathbb{R}^{n\times n}$). For $B\subset\mathbb{R}^n$, $\operatorname{diam}(B)=\max_{x,y\in B}\|x-y\|$. We denote by $\mathbf{S}_n^+$ the cone of symmetric positive semidefinite matrices of dimension n and by $Sp(A)\in\mathbb{C}$ the set of eigenvalues of a matrix A. For $k\in\mathbb{N}$, $\mathbb{R}_k[X]$ is the vector space of polynomials of degree smaller than k, and real coefficients. We denote by $\|\cdot\|_1$ either the sum of the absolute values of the components of a vector (standard ℓ_1 norm when applied on $\mathbb{R}^n$) or, when applied to a polynomial, the sum of the absolute values of its coefficients. Finally, I denotes the identity operator.

We study the linear convergence of a constrained Anderson acceleration scheme on an operator $F:\mathbb{R}^n\to\mathbb{R}^n$. In recent applications of Anderson extrapolation in optimization, F is typically a gradient step with constant step size (e.g.,[35, 22]). We use two types of assumptions on F throughout.

Assumption 1.1. *F is ρ-Lipschitz with $\rho<1$, and can be decomposed as*

$$F=G+\xi$$

for a linear $G\in\mathbf{S}_n^+$ with $G\preccurlyeq\rho I$ and a nonlinear $\xi:\mathbb{R}^n\to\mathbb{R}^n$ α-Lipschitz with $\alpha\geq 0$.

Assumption 1.2. *F is ρ-Lipschitz with $\rho<1$ and is continuously differentiable with positive semidefinite and η-Lipschitz Jacobian F' where $\eta\geq 0$.*

The ρ-Lipschitzness assumption implies that F has a unique fixed point x_* and the iterates of the fixed point iterations $x_{k+1}=F(x_k)$ satisfy $\|x_{k+1}-x_k\|\leq\rho\|x_k-x_{k-1}\|$ and $x_k\to x_*$. The second assumption implies that for $x_0\in\mathbb{R}^n$ and a compact set $B\subset\mathbb{R}^n$ containing x_0, one can decompose F as $F=G+\xi$ with $G=F'(x_0)$ and $\xi=F-F'(x_0)$. Moreover ξ is locally Lipschitz over B with Lispchitz constant roughly equal to $\eta\operatorname{diam}(B)$, decreasing with the diameter of B. Note that Assumption 1.2 does not enforce Assumption 1.1 to hold as it implies local Lipschitzness.

Remark 1.3. We illustrate these assumptions in the optimization setting.

- When $f:\mathbb{R}^n\to\mathbb{R}$ is a quadratic function with $\mu I\preceq\nabla^2 f\preceq LI$ and $0<\mu\leq L$, the gradient step operator $F=I-\frac{1}{L}\nabla f$ is affine and satisfies Assumption 1.1 with $\rho=\left(1-\frac{\mu}{L}\right)$ and $\xi=0$.
- When $f:\mathbb{R}^n\to\mathbb{R}$ is a $\mathcal{C}^2$, μ-strongly convex function with L-Lipschitz gradient for $0<\mu\leq L$, and η-Lipschitz Hessian, the gradient step operator $F=I-\frac{1}{L}\nabla f$ is nonlinear and satisfies Assumption 1.2 with $\rho=\left(1-\frac{\mu}{L}\right)$ (see e.g., [33]).

We focus on a fixed depth version of Anderson acceleration. For a predetermined constant $k\in\mathbb{N}$, this simple method consists in performing $k+1$ fixed point iterations with F and use these $k+1$ iterates to get an extrapolated point. We can then restart the method at the extrapolated point. The extrapolated solution is obtained by solving a quadratic program with a bound on the ℓ_1 norm of extrapolation weights. This choice of norm is motivated by

Algorithm 1.1 Constrained Anderson Acceleration

Input:

- $x_0 \in \mathbb{R}^n$, initial guess.
- Contractive operator F.
- $C \geq 1$, bound on the extrapolation weights.
- $k \in \mathbb{N}^*$, a constant controlling the number of iterates used in extrapolation.

for $i = 0, \ldots, k$ **do**

  $x_{i+1} = F(x_i)$

end for

Form $R = \begin{bmatrix} x_0 - x_1 & \cdots & x_k - x_{k+1} \end{bmatrix}$ and compute

$$\tilde{c} = \underset{\mathbf{1}^T c = 1,\ \|c\|_1 \leq C}{\operatorname{argmin}} \|Rc\| \tag{1.2}$$

Output: Extrapolated point $x_e = \sum_{i=0}^{k} \tilde{c}_i x_i$.

a tightness result derived in Theorem 3.9, but any norm would lead to similar developments. The procedure is described in Algorithm 1.1.

In practice, k is set to a small constant (e.g. 5 or 10) and Algorithm 1.1 is restarted by plugging the extrapolated output as input (see e.g., [36]) for a new run of the method. The linearly constrained quadratic subproblem in (1.2) for computing the extrapolation weights is low dimensional and can be easily solved by e.g., interior-point methods.

We look at convergence bounds of the form $\|F(x_e) - x_e\| \leq \tilde{\rho}\|F(x_0) - x_0\|$, where x_e is the output of Algorithm 1.1 started at x_0 and the quantity $\|F(x) - x\|$ controls how far x is from being a fixed point of F. This choice allows to chain together the convergence guarantees for consecutive run of Algorithm 1.1. When F satisfies Assumption 1.1 we always have that $\|F(x_k) - x_k\| \leq \rho^k \|F(x_0) - x_0\|$ hence we consider that extrapolation provides convergence acceleration as soon as $\tilde{\rho} < \rho^k$

1.2. Related work. Several recent results have been focused on improving convergence guarantees for acceleration methods. In [35], the authors apply a regularized formulation of Anderson extrapolation in an optimization setting. Regularization yields accelerated linear convergence rates in some asymptotic regimes, without any additional hypothesis on the independence of the residuals. [7] also proposes a stabilized version guaranteeing local linear acceleration without any linear independence hypothesis but with an assumption on the conditioning of the Jacobian.

Acceleration mechanisms, and Anderson acceleration in particular, have a strong link with quasi-Newton methods [12, 32]. A variant of Anderson acceleration called the DIIS procedure has been studied in [32] and yields accelerated local linear convergence under a linear independence hypothesis on differences of consecutive residuals and an hypothesis on the conditioning of the Jacobian of $I - F$ at a fixed point x_*. The idea of imposing a sufficient linear independence condition on the difference of the residuals is also present in [29]. It has also been shown in [41] that when the extrapolation weights are bounded, AA is locally linearly convergent. However, none of these conditions guarantee *a priori* improved linear convergence rates, as they are impossible to check without actually running the method.

A globally convergent modification of the DIIS procedure is proposed in [10] consisting in using only positive weights in the extrapolation. However, using only positive weights amounts to forming convex combination of previous iterates which severely limits acceleration. An adaptive regularization scheme in [27] provides acceleration guarantees under boundedness hypothesis on the extrapolation weights, extending the work of [41]. A globally converging Anderson acceleration type algorithm is also presented in [42]; however, due to the very general assumptions made in the paper, no convergence rate is provided. In [11], an adaptive restart strategy yields local superlinear convergence without any assumption on conditioning, but the region around the optimum where superlinear convergence occurs is dependent on the ambient dimension d and its size goes to 0 when d tends to infinity.

Finally, these extrapolation methods were widely extended in the optimization community: to the stochastic setting [34], to composite optimization problems in [24, 22], to splitting methods [30, 15], to coordinate descent [4] and to accelerate momentum based methods in [5].

1.3. Contributions.

The setting of this paper is essentially that of [35], which is more restrictive than those of [29, 27, 7, 11] (in particular because of the symmetry assumption on G). This setup allows proving explicit, dimension independent, worst-case local linear convergence rates, a priori, without additional assumption on the iterates themselves, or on the optimum.

We study a constrained Anderson acceleration (CAA) algorithm that imposes hard bounds on the extrapolation weights as suggested in [41, Section 2.2] and [36], and provide a simple worst-case analysis in a nonlinear setting. We do so by extending the Chebyshev arguments of [35] to the constrained case. Overall, our contribution is threefold.

(i) We provide an explicit upper bound for the optimal value of a constrained Chebychev problem on polynomials. We show this bound is tight on a range of parameters and show numerically that it is close to the optimal value elsewhere.
(ii) We use this bound to construct an explicit, dimension free, worst-case local linear convergence rate for CAA applied to nonlinear operators, and quantify this local acceleration rate.
(iii) We describe an adaptive strategy to adjust the constraints on extrapolation weights, when CAA is applied to a gradient step operator.

2. Constrained Anderson Acceleration.

We first recall some standard results on Anderson acceleration on linear operators when $\alpha = 0$ in Assumption 1.1 (or $\eta = 0$ in Assumption 1.2). We then introduce constraints on the extrapolation coefficients for stabilizing the extrapolation procedure, and deal with nonlinearities through the introduction of perturbation parameters $\alpha > 0$ in Assumption 1.1 (or $\eta > 0$ in Assumption 1.2).

2.1. Anderson Acceleration on Linear Problems.

Let us consider the case $\alpha = 0$ (i.e., F is affine), where Algorithm 1.1 can be used with $C = \infty$. We recall the well-known convergence result on Anderson acceleration in the linear case.

Proposition 2.1. *Let F be satisfying Assumption 1.1 with $\alpha = 0$, $x_e \in \mathbb{R}^n$ be the output of Algorithm 1.1 initiated at some $x_0 \in \mathbb{R}^n$ such that $F(x_0) \neq x_0$, and let $C = \infty$ and $k > 0$.*

We have that

$$\frac{\|F(x_e)-x_e\|}{\|F(x_0)-x_0\|} \le \min_{\substack{p\in\mathbb{R}_k[X]\\ p(1)=1}} \max_{x\in[0,\rho]} |p(x)| = \rho_* := \tfrac{2\beta^k}{1+\beta^{2k}},$$

with $\beta = \frac{1-\sqrt{1-\rho}}{1+\sqrt{1-\rho}}$. *In addition* $\rho_* < \rho^k$.

Proof. Reformulation of [35, Proposition 2.1]. ■

In the following, α or η may be nonzero and the previous proposition does not apply.

2.2. Constrained Anderson Acceleration on Nonlinear Problems. When applying the extrapolation step (1.2) to a nonlinear operator F, the conditioning of the matrix $R^TR \in \mathbf{S}^+_{k+1}$ becomes an important issue. This matrix might be singular in some particular situations (see below), but more importantly becomes very close to singular in typical situations. For instance, when F is a gradient step operator of a smooth convex function, consecutive gradients tend to get aligned (in particular, this can be easily formalized when F is the gradient step operator of a convex quadratic function), leading to a very ill-conditioned R^TR in that case. Furthermore, if F is the gradient of a convex quadratic function with Hessian $H \succeq 0$, and x_0 is an eigenvector of H, the matrix R^TR will be singular. This means the solution vector $\tilde{c}$ can have coefficients with very large magnitude. When $\alpha > 0$, those coefficients are multiplied with the nonlinear part of F and can make the iterates of the algorithm diverge (see [35] for an example of such divergence). A solution to fix this issue is to check the conditioning of the matrix (or some related quantity) and adjust iterations depending on it (e.g. restart [11] or discard iterates [7]). A more direct method consists in controlling the magnitude of these coefficients, by e.g. regularizing (1.2), as in [35] (with $C=\infty$), or by imposing hard constraints on $\tilde{c}$, as we do here. Whereas regularization renders computations easier in practice, imposing constraints makes the analysis simpler.

Proposition 2.2. *Let F be an operator satisfying Assumption 1.1, $\alpha \ge 0$ and $x_e \in \mathbb{R}^n$ be the output of Algorithm 1.1 initiated at $x_0 \in \mathbb{R}^n$ with $C \ge 1$ and $k \ge 1$. We have*

$$\|F(x_e)-x_e\| \le \left(\max_{x\in[0,\rho]} |p^C_*(x)| + 3C\alpha k\right)\|F(x_0)-x_0\|, \tag{2.1}$$

where

$$p^C_* \in \operatorname*{argmin}_{\substack{p\in\mathbb{R}_k[X]\\ p(1)=1\\ \|p\|_1\le C}} \max_{x\in[0,\rho]} |p(x)|,$$

and $\|p\|_1$ is the ℓ_1 norm of the vector of coefficients of p. In addition, under Assumption 1.2, the bound in (2.1) holds with $\alpha = kC\eta\|F(x_0)-x_0\|$.

Proof. The proof mostly relies on reformulations and triangle inequalities. It is deferred to Appendix A. ■

The following corollary simply states that one can allow a small relative error in the computation of (1.2) in Algorithm 1.1 while keeping linear convergence.

Corollary 2.3. *Let F be an operator satisfying Assumption 1.1, $\alpha \geq 0$ and $x_e \in \mathbb{R}^n$ be the output of Algorithm 1.1 initiated at $x_0 \in \mathbb{R}^n$ with $C \geq 1$ and $k \geq 1$. If (1.2) is solved with relative precision $\varepsilon\|F(x_0) - x_0\|$ on its optimality gap for some $\varepsilon > 0$, that is*

$$\|Rc\| - \|R\tilde{c}\| \leq \varepsilon\|F(x_0) - x_0\|,$$

then

$$\|(F - I)x_e\| \leq \left(\max_{x\in[0,\rho]} |p_*^C(x)| + 3C\alpha k + \varepsilon\right) \|(F - I)x_0\|.$$

Under Assumption 1.2, this bound holds with $\alpha = kC\eta\|F(x_0) - x_0\|$.

The result of Proposition 2.2 is independent of the dimension of the ambient space. Moreover, we can also get dimension dependent local superlinear convergence.

Remark 2.4. Let $\rho \in]0, 1[$ and F be satisfying Assumption 1.2. Let $x_e \in \mathbb{R}^n$ be the output of Algorithm 1.1 initiated at $x_0 \in \mathbb{R}^n$ with $C \geq 1$ and $k \geq 1$. A slight modification in the proof of Proposition 2.2 yields

$$\|F(x_e) - x_e\| \leq \left(\min_{\substack{p\in\mathbb{R}_k[X] \\ p(1)=1, \|p\|_1\leq C}} \|p(G)\| + 3C^2\eta k^2\|F(x_0) - x_0\|\right) \|F(x_0) - x_0\|.$$

Let $\lambda_1, \ldots, \lambda_n \in [0, \rho[$ be the eigenvalues of G, when $C \geq \frac{(1+\rho)^n}{(1-\rho)^n}$ the polynomial $\chi(X) = \frac{\prod_{i=1}^n(X-\lambda_i)}{\prod_{i=1}^n(1-\lambda_i)}$ satisfies $\chi(G) = 0$, $\chi(1) = 1$ and $\|\chi\|_1 \leq C$, thus for $k = n$

$$\|F(x_e) - x_e\| \leq 3C^2\eta n^2\|F(x_0) - x_0\|^2,$$

which gives local superlinear convergence. Setting $k = n$ is of course somewhat impractical when the ambient dimension of the problem gets large.

In the rest of the paper, we focus on convergence rates that are dimension independent. Proposition 2.2 highlights a trade-off between (i) allowing coefficients to have larger magnitudes, i.e., via a large C, leading to a smaller $\max_{x\in[0,\rho]} |p_*^C(x)|$ that gets closer to the optimal rate ρ_*, and (ii) diminishing C to better control the nonlinear part of F but getting a slower rate $\max_{x\in[0,\rho]} |p_*^C(x)|$, closer to ρ^k. In the next section, we bound $\max_{x\in[0,\rho]} |p_*^C(x)|$ as a function of C, to make this trade-off explicit.

3. Constrained Chebychev Problem.

The Chebyshev problem, defined in the following theorem, is central to many results of numerical analysis. For instance, it is used to provide convergence rates for several algorithms such as Lanczos' method for eigenvalue computations [16], conjugate gradients [38], Anderson acceleration, or Chebyshev iterations [17, 25, 26].

We first introduce rescaled Chebyshev polynomials, that will be used throughout the rest of this section.

Definition 3.1. *Let $a < b < 1 \in \mathbb{R}$ and $k > 0$, we call rescaled Chebyshev polynomial of the first kind, of degree k, on $[a, b]$ the polynomial*

$$R_k^{[a,b]}(X) := \frac{T_k(\frac{2(X-a)}{b-a} - 1)}{|T_k(\frac{2(1-a)}{b-a} - 1)|},$$

where T_k is the Chebyshev polynomial of the first kind, of degree k.

We recall a fundamental result on rescaled Chebyshev polynomials from [17, Section 3].

Theorem 3.2 ([17]). *Let $\rho \in]0,1[$ and $k > 0$, we call Chebyshev problem of degree k on $[0,\rho]$ the following optimization problem on polynomials*

$$\text{(Cheb)} \qquad \rho_* := \min_{\substack{p\in\mathbb{R}_k[X]\\ p(1)=1}} \max_{x\in[0,\rho]} |p(x)|,$$

whose solution is $p_*(X) = R_k^{[0,\rho]}(X)$, and $\rho_* = \frac{2\beta^k}{1+\beta^{2k}}$ with $\beta = \frac{1-\sqrt{1-\rho}}{1+\sqrt{1-\rho}}$.

Proof. For completeness, a proof of this result is provided in Appendix B.2. ■

The following corollary extends the result of Theorem 3.2 and will be useful at the end of this section.

Corollary 3.3. *Let $\rho \in]0,1[$, $k > 0$ and $\varepsilon \geq 0$. It holds that*

$$\rho_\varepsilon := \min_{\substack{p\in\mathbb{R}_k[X]\\ p(1)=1}} \max_{x\in[-\varepsilon,\rho]} |p(x)|, \tag{3.1}$$

whose solution is the rescaled Chebyshev polynomial $R_k^{[-\varepsilon,\rho]}(X)$, and $\rho_\varepsilon = \frac{2\beta_\varepsilon^k}{1+\beta_\varepsilon^{2k}}$ with $\beta_\varepsilon = 1 - \sqrt{1-\frac{\rho+\varepsilon}{1+\varepsilon}} \Big/ 1 + \sqrt{1-\frac{\rho+\varepsilon}{1+\varepsilon}}$.

Proof. The proof follows the same line as that of Theorem 3.2. ■

We have seen in Proposition 2.2 that we need to control the optimal value of a slightly modified version of (Cheb) with an additional constraint on the ℓ_1 norm of the vector of coefficients of the polynomial. Adding this constraint breaks the explicit result of Theorem 3.2 and no closed form solution for this constrained Chebyshev problem is known for arbitrary choices of C. In this section we seek upper bounds on the optimal value to this problem.

Let $k > 0$ and $\rho \in]0,1[$, we are interested in the following constrained Chebyshev problem

$$\text{(Cstr-Cheb)} \qquad \tilde{\rho}(C) := \min_{\substack{p\in\mathbb{R}_k[X]\\ p(1)=1\\ \|p\|_1\leq C}} \max_{x\in[0,\rho]} |p(x)|.$$

Before detailing explicit upper bounds on this problem, we first explain how to compute this $\tilde{\rho}(C)$ numerically for $C \geq 1$. Note that the feasible set is trivially empty when $C < 1$.

3.1. Numerical Solutions. When $C \geq 1$, the problem (Cstr-Cheb) has a non empty feasible set, and this feasible set is convex (intersection of an affine space with an ℓ_1 ball). The objective function is a norm on $\mathbb{R}_k[X]$, hence is convex. The problem (Cstr-Cheb) is equivalent to

$$\begin{aligned} \tilde{\rho}(C) = \quad & \min \quad t \\ & p \in \mathbb{R}_k[X],\ t \in \mathbb{R}, \\ & p(1) = 1,\ \|p\|_1 \leq C, \\ & -t \leq p(x) \leq t,\ \forall x \in [0,\rho]. \end{aligned} \tag{3.2}$$

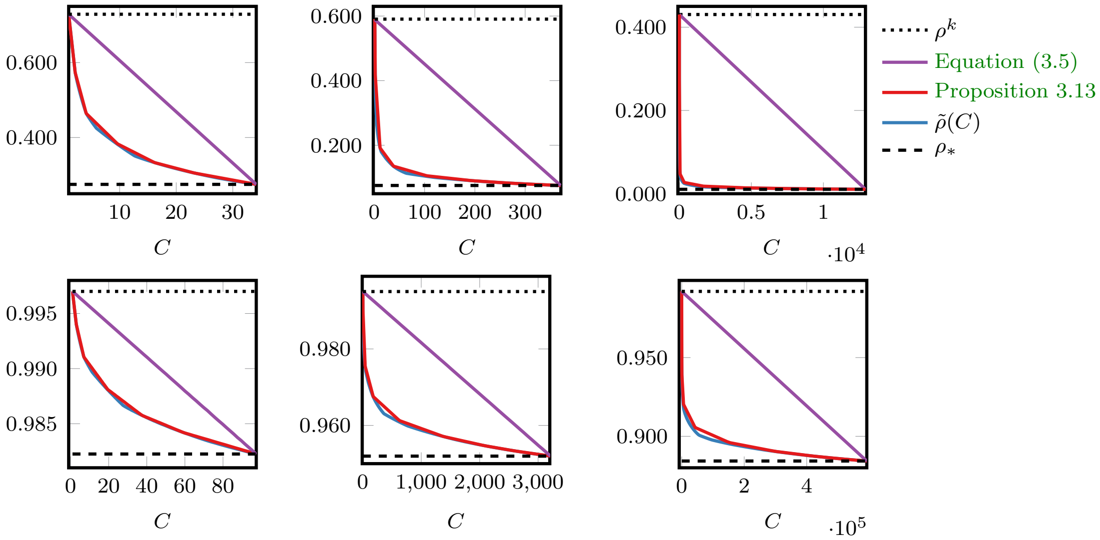

Figure 1. *Dotted curves correspond to the fixed point iterations rate ρ^k, purple ones are bounds on $\tilde\rho(C)$ from (3.5) using convexity. Red curves correspond to the bound on $\tilde\rho(C)$ presented in Proposition 3.13 with $M = k$, blue ones correspond to numerical solutions to (3.3) (i.e., numerical value of $\tilde\rho(C)$) and the dashed ones to accelerated rate ρ_* defined in (Cheb). On x-axis C goes from 1 to C_* defined in (3.4). Top : $\rho = 0.9$. Bottom: $\rho = 0.999$. Left: $k = 3$. Middle: $k = 5$. Right: $k = 8$.*

This problem involves polynomial positivity constraints on a bounded interval. A classical argument to transform this local positivity into positivity on $\mathbb{R}$ uses the following change of variable.

$$p(x) \geq 0 \;\forall x \in [0, \rho] \iff (1+x^2)^k p\left(\rho \frac{x^2}{1+x^2}\right) \geq 0 \;\forall x \in \mathbb{R}.$$

Positivity constraints for univariate polynomials can be expressed using a sum of squares (SOS) formulation [28, 19] (see e.g., [21, Theorem 1] for a short proof). Standard packages can be used to solve the following reformulation of (3.2) with SOS constraints.

$$\begin{aligned} \tilde\rho(C) = \quad & \min \quad t \\ & p \in \mathbb{R}_k[X],\; t \in \mathbb{R}, \\ & p(1) = 1,\; \|p\|_1 \leq C, \\ & (1+x^2)^k p(\rho \tfrac{x^2}{1+x^2}) + (1+x^2)^k t \geq 0 \;\forall x \in \mathbb{R}, \\ & (1+x^2)^k t - (1+x^2)^k p(\rho \tfrac{x^2}{1+x^2}) \geq 0 \;\forall x \in \mathbb{R}. \end{aligned} \tag{3.3}$$

We used YALMIP [20] and MOSEK [3] and numerical solutions to (3.3) are detailed in Figure 1 (in blue) for a few values of ρ and k.

3.2. Exact and Upper Bounds. The main goal of this section is to provide an explicit upper bound for the function $\tilde\rho(C)$ defined in (Cstr-Cheb), which we later combine with the result of Proposition 2.2.

3.2.1. Naive Upper Bound and Base Properties. We start by presenting a property of the function $\tilde\rho$ that will be very useful to stitch together several upper bounds that will be derived on $\tilde\rho$ in what follows.

Proposition 3.4. *The function* $\tilde{\rho}$ *defined in* (Cstr-Cheb) *is convex on* $[1,+\infty[$.

Proof. Let $C_0, C_1 \in [1,+\infty[$ and $t \in [0,1]$, when p_0 and p_1 are feasible points for problem (Cstr-Cheb) with C equal to C_0 and C_1, then $(1-t)p_0+tp_1$ is feasible for problem (Cstr-Cheb) with $C = (1-t)C_0 + tC_1$. Thus, by convexity of the objective function we have that $\tilde{\rho}((1-t)C_0 + tC_1) \leq (1-t)\tilde{\rho}(C_0) + t\tilde{\rho}(C_1)$. ■

We write C_* the ℓ_1-norm of the rescaled Chebyshev polynomial $p_* = R_k^{[-0,\rho]}$ of Theorem 3.2, i.e.

$$C_* = \|R_k^{[-0,\rho]}\|_1, \text{ where } R_k^{[-0,\rho]} \text{ solves (Cheb)}. \tag{3.4}$$

We start with a few observations on the behaviour of $\tilde{\rho}$ at the boundaries of its domain.

Remark 3.5. From Theorem 3.2, when C is larger than C_*, problem (Cstr-Cheb) becomes unconstrained and $\tilde{\rho}(C)$ is constant equal to ρ_*.

Remark 3.6. When $C = 1$, the feasible set of (Cstr-Cheb) consists only of convex combinations of monomials of degree smaller than k. Among them, X^k has the minimal absolute value on $[0,\rho]$ and $\tilde{\rho}(1) = \rho^k$.

Based on the two previous remarks and Proposition 3.4 we obtain a first natural upper bound on $\tilde{\rho}$ written

$$\tilde{\rho}(C) \leq \tfrac{C_*-C}{C_*-1}\rho^k + \tfrac{C-1}{C_*-1}\rho_*, \qquad \text{for } C \in [1, C_*]. \tag{3.5}$$

This is a very coarse upper bound since $C_* >> 1$. Indeed we can observe in Figure 1 that there is an important gap between $\tilde{\rho}$ and the coarse upper bound from (3.5) that is displayed in purple. Bellow, we show that using a refined set of sample points in $[1, C_*]$ along with convexity of $\tilde{\rho}$ allows obtaining more precise upper bounds.

3.2.2. Behaviour for C Close to 1. It turns out that when C is close to 1, the behaviour of $\tilde{\rho}(C)$ can be explicitly characterized. Indeed, in the next lemma we provide an explicit expression for $\tilde{\rho}(C)$ when C is in an explicit neighbourhood of 1.

Lemma 3.7. *Let* $C_1 = \frac{2+\rho^k}{2-\rho^k}$*, for* $C \in [1, C_1]$ *we have the following expression for* $\tilde{\rho}$

$$\tilde{\rho}(C) = \tfrac{C+1}{2}\rho^k - \tfrac{C-1}{2}.$$

Proof. Let us show that $p(X) = \frac{C+1}{2}X^k - \frac{C-1}{2}$ solves of (Cstr-Cheb). First notice that p is feasible as $\|p\|_1 = C$ and $p(1) = 1$. In addition, since p is increasing on $[0,\rho]$, $|p|$ reach its maximum on the boundary and $\max_{x\in[0,\rho]} |p(x)| = \max(|p(\rho)|, |p(0)|) = p(\rho) = \frac{C+1}{2}\rho^k - \frac{C-1}{2}$ using that $C \in [1, \frac{2+\rho^k}{2-\rho^k}]$.

Let q be another feasible polynomial such that $q = \sum_{i=0}^k q_i X^i$, $\sum_{i=0}^k q_i = 1$ and $\sum_{i=0}^k |q_i| \leq C$. We show that $|q(\rho)| \geq |p(\rho)|$. First we have that

$$q(\rho) = \sum_{q_i \geq 0} q_i\rho^i + \sum_{q_i \leq 0} q_i\rho^i \geq \sum_{q_i \geq 0} q_i\rho^k + \sum_{q_i \leq 0} q_i = \sum_{q_i \geq 0} q_i\rho^k + \left(1 - \sum_{q_i \geq 0} q_i\right).$$

In addition, one notices that $\sum_{q_i\geq 0} q_i - \sum_{q_i\leq 0} q_i = \sum_{i=0}^{k} |q_i| \leq C$ thus using that $\sum_{q_i\leq 0} q_i = 1 - \sum_{q_i\geq 0} q_i$, we obtain $\sum_{q_i\geq 0} q_i \leq \frac{C+1}{2}$, and

$$q(\rho) \geq \tfrac{C+1}{2}(\rho^k - 1) + 1 = p(\rho) > 0.$$

Thus $|q(\rho)| = q(\rho) \geq p(\rho) = \max_{x\in[0,\rho]} |p(x)|$. Then $\max_{x\in[0,\rho]} |q(x)| \geq \max_{x\in[0,\rho]} |p(x)|$ so p is an optimal solution of (Cstr-Cheb). ■

Using Remark 3.5 and Lemma 3.7, we can obtain exact expression for $\tilde{\rho}$ when $k = 1$.

Remark 3.8. For $k = 1$, we have $C_* = \frac{2+\rho}{2-\rho} = C_1$ and

$$\tilde{\rho}(C) = \begin{cases} \frac{C+1}{2}\rho^k - \frac{C-1}{2} & \text{for } C \in [1, C_1] \\ \frac{2}{2-\rho} & \text{for } C \geq C_1 \end{cases}.$$

We can also give an explicit form for solutions of (Cstr-Cheb) in a neighborhood of C_* as detailed below.

3.2.3. Behaviour for C Around C_*. In this section, we show that solutions to the Chebyshev problem with light constraints (C close to C_*) are also rescaled Chebyshev polynomials (see Definition 3.1) on a segment $[-\varepsilon, \rho]$ instead of $[0, \rho]$, with $\varepsilon \geq 0$.

Theorem 3.9. *Let $\rho \in]0, 1[$, $k > 0$ and*

$$\tilde{\varepsilon} = \rho \frac{1+\cos(\frac{2k-1}{2k}\pi)}{1-\cos(\frac{2k-1}{2k}\pi)}.$$

For any $\varepsilon \in [0, \tilde{\varepsilon}]$ we have

$$R_k^{[-\varepsilon,\rho]} \in \underset{\substack{p\in\mathbb{R}_k[X],\, p(1)=1 \\ \|p\|_1 \leq \left\|R_k^{[-\varepsilon,\rho]}\right\|_1}}{\operatorname{argmin}} \max_{x\in[0,\rho]} |p(x)|,$$

which implies

$$\tilde{\rho}\left(\left\|R_k^{[-\varepsilon,\rho]}\right\|_1\right) = \max_{x\in[-\varepsilon,\rho]} \left|R_k^{[-\varepsilon,\rho]}(x)\right|.$$

Proof. We present a proof sketch, and refer to Appendix C for a complete argument. Assume that $R_k^{[-\varepsilon,\rho]}$ is not a global minimum of the convex problem in (Cstr-Cheb), $R_k^{[-\varepsilon,\rho]}$ is not a local solution either, hence we can find $h \in \mathbb{R}_k[X] \neq 0$ with small enough norm such that

(i) $\|R_k^{[-\varepsilon,\rho]} + h\|_1 \leq \|R_k^{[-\varepsilon,\rho]}\|_1$ and $h(1) = 0$ (i.e. $R_k^{[-\varepsilon,\rho]} + h$ feasible),

(ii) $\max_{x\in[0,\rho]} |R_k^{[-\varepsilon,\rho]}(x) + h(x)| < \max_{x\in[0,\rho]} |R_k^{[-\varepsilon,\rho]}(x)|$ (i.e. $R_k^{[-\varepsilon,\rho]} + h$ has a smaller objective value).

Due to the particular form of $R_k^{[-\varepsilon,\rho]}$ (i.e. equioscillation of Chebyshev Polynomials recalled in Lemma B.3), conditions (i) and (ii) on h imply that it has k roots in $]0, 1]$. Thus h keeps the same sign on $]-\infty, 0]$ (which is $(-1)^k$), so $(-1)^k h(-1) > 0$.

We then choose $\tilde{\varepsilon}$ such that for all $\varepsilon \in [0, \tilde{\varepsilon}]$, the roots of $R_k^{[-\varepsilon,\rho]}$ are nonnegative, and show that this forces the coefficients $(c_i)_i$ of $R_k^{[-\varepsilon,\rho]}$ to alternate signs (in particular c_i the coefficient of degree i has sign $(-1)^{k+i}$).

For $h(x) = \sum_{i=0}^k h_i x^i$ with norm small enough we can write $\|R_k^{[-\varepsilon,\rho]} + h\|_1 = \|R_k^{[-\varepsilon,\rho]}\|_1 + \sum_{i=0}^k \operatorname{sign}(c_i) h_i = \|R_k^{[-\varepsilon,\rho]}\|_1 + \sum_{i=0}^k (-1)^{k+i} h_i = \|R_k^{[-\varepsilon,\rho]}\|_1 + (-1)^k h(-1)$ and (ii) leads to $(-1)^k h(-1) \leq 0$, providing a contradiction. Therefore, $R_k^{[-\varepsilon,\rho]}$ has to be a global minimum. ■

As mentioned in this proof, the coefficients of $R_k^{[-\varepsilon,\rho]}$ for $\varepsilon \in [0, \tilde{\varepsilon}]$ have alternating signs, so $\left\|R_k^{[-\varepsilon,\rho]}\right\|_1$ is in fact $|R_k^{[-\varepsilon,\rho]}(-1)|$. This relation is key in the proof of the previous theorem, and is the main motivation behind the choice of the ℓ_1 norm on coefficients (versus e.g. ℓ_2). Furthermore, this yields a somewhat simple expression for $\left\|R_k^{[-\varepsilon,\rho]}\right\|_1$, as follows.

Lemma 3.10. *Let $\rho \in]0,1[$, and $k > 0$. For any $\varepsilon \in [0, \tilde{\varepsilon}]$ with*

$$\tilde{\varepsilon} = \rho \frac{1+\cos(\frac{2k-1}{2k}\pi)}{1-\cos(\frac{2k-1}{2k}\pi)},$$

we have

$$\|R_k^{[-\varepsilon,\rho]}\|_1 = \frac{\left(1+\frac{\rho-\varepsilon}{2}-\sqrt{(1+\rho)(1-\varepsilon)}\right)^k+\left(1+\frac{\rho-\varepsilon}{2}+\sqrt{(1+\rho)(1-\varepsilon)}\right)^k}{\left(1+\frac{\rho-\varepsilon}{2}-\sqrt{(1-\rho)(1+\varepsilon)}\right)^k+\left(1+\frac{\rho-\varepsilon}{2}+\sqrt{(1-\rho)(1+\varepsilon)}\right)^k}.$$

Furthermore, the function $\varepsilon \to \left\|R_k^{[-\varepsilon,\rho]}\right\|_1$ is continuous and decreasing on $[0, \tilde{\varepsilon}]$.

Proof. Using $\|R_k^{[-\varepsilon,\rho]}\|_1 = |R_k^{[-\varepsilon,\rho]}(-1)|$, we apply the classical expression for $T_k(x)$ with $|x| \geq 1$ (see e.g [23, Eq 1.49]) $T_k(x) = \frac{1}{2}\left((x - \sqrt{x^2-1})^k + (x + \sqrt{x^2-1})^k\right)$. Using this formula, we arrive to (after a bit of work)

$$\left\|R_k^{[-\varepsilon,\rho]}\right\|_1 = \frac{\left|T_k(\frac{-2-\rho+\varepsilon}{\rho+\varepsilon})\right|}{\left|T_k(\frac{2-\rho+\varepsilon}{\rho+\varepsilon})\right|} = \frac{\left(1+\frac{\rho-\varepsilon}{2}-\sqrt{(1+\rho)(1-\varepsilon)}\right)^k+\left(1+\frac{\rho-\varepsilon}{2}+\sqrt{(1+\rho)(1-\varepsilon)}\right)^k}{\left(1-\frac{\rho-\varepsilon}{2}-\sqrt{(1-\rho)(1+\varepsilon)}\right)^k+\left(1-\frac{\rho-\varepsilon}{2}+\sqrt{(1-\rho)(1+\varepsilon)}\right)^k}.$$

A base study of variations reveals that the numerator is decreasing and the denominator increasing on $[0, \tilde{\varepsilon}]$. ■

Remark 3.11. In particular, one can express the value of C_* using Lemma 3.10 applied to the unconstrained Chebyshev problem (Cheb) ($\varepsilon = 0$), yielding

$$C_* = \frac{\left(2+\rho-2\sqrt{1+\rho}\right)^k + \left(2+\rho+2\sqrt{1+\rho}\right)^k}{\left(2-\rho-2\sqrt{1-\rho}\right)^k + \left(2-\rho+2\sqrt{1-\rho}\right)^k}.$$

Remark 3.12. Theorem 3.9 and Lemma 3.10 do not provide explicit expressions of $\tilde{\rho}(C)$ for $C \in [\tilde{C}, C_*]$ with $\tilde{C} = \|R_k^{[-\tilde{\varepsilon},\rho]}\|_1$. Indeed, we cannot explicitly invert the relation $\varepsilon \to \|R_k^{[-\varepsilon,\rho]}\|_1$. However one can get arbitrarily tight upper bounds by sampling $(\varepsilon_i)_{i\in[1,M]} \in$

$[0, \tilde{\varepsilon}]$. Then, one can compute $C_i = \|R_k^{[-\varepsilon_i,\rho]}\|_1$ explicitly using Lemma 3.10. Note that since $\varepsilon \to \left\|R_k^{[-\varepsilon,\rho]}\right\|_1$ is continuous and decreasing on $[0, \tilde{\varepsilon}]$, we can obtain an arbitrarily good covering of $[\tilde{C}, C_*]$ using the C_i. Finally, using convexity from Proposition 3.4 to interpolate linearly between the C_i and $\tilde{\rho}(C_i)$, provides a piecewise linear upper bound on $[\tilde{C}, C_*]$ which can be made arbitrarily close to $\tilde{\rho}$ by increasing M.

Note however that the interval $[\tilde{C}, C_*]$ is actually quite narrow compared with $[1, C_*]$. We describe the construction of upper bounds for all $C \geq 1$ in the next section.

3.2.4. Construction of Upper Bounds for all Values of C . To construct an upper bounds on $\tilde{\rho}(C)$ for all $C \in [1, C_*]$, we use the idea presented above, based on bounding $\tilde{\rho}$ at a finite number of points, then using convexity to interpolate upper bounds between these points. Given $M \in \mathbb{N}^*$ accounting for the number of intermediate breaking points, the upper bound is built as follows.

(i) Select $M+2$ constraint parameters $C_i \in [1, C_*]$ for $i = 0, \ldots, M+1$ with $C_0 = 1$, $C_1 = \frac{2+\rho^k}{2-\rho^k}$ (from Lemma 3.7) and $C_{M+1} = C_*$.

(ii) Using feasible polynomials of (Cstr-Cheb), obtain ρ_i such that $\tilde{\rho}(C_i) \leq \rho_i$ for $i = 0, \ldots, M+1$, with $\rho_0 = \rho^k$, $\rho_1 = \tilde{\rho}(C_1) = \frac{\rho^k}{2-\rho^k}$ (from Lemma 3.7) and $\rho_{M+1} = \rho_*$.

(iii) Use the lower convex hull of the (C_i, ρ_i) as an upper bound on $\tilde{\rho}$ on $[1, C_*]$.

Note that we only focus on $[1, C_*]$ since we know that $\tilde{\rho}(C) = \rho_*$ when $C \geq C_*$ (see Remark 3.11).

Proposition 3.13. *Let $k > 2$, $\rho \in]0, 1[$ and $M \geq 2$, $(\varepsilon_i)_{i\in[2,M]} = \left(\frac{\rho}{2^{i-2}}\right)_{i\in[2,M]}$. Let*

$$(C_i)_{i\in[2,M]} = \left(\min \left\|R_k^{[-\varepsilon_i,\rho]}\right\|_1, C_*\right)_{i\in[2,M]}, \quad C_0 = 1, \quad C_1 = \frac{2+\rho^k}{2-\rho^k}, \quad \text{and } C_{M+1} = C_*.$$

We denote by $(\rho_i)_{i\in[2,M]} = \left(\frac{2\beta_i^k}{1+\beta_i^{2k}}\right)_{i\in[2,M]}$, with $\beta_i = 1 - \sqrt{1 - \frac{\rho+\varepsilon_i}{1+\varepsilon_i}} \Big/ 1 + \sqrt{1 - \frac{\rho+\varepsilon_i}{1+\varepsilon_i}}$, $\rho_0 = \rho^k$, $\rho_1 = \frac{\rho^k}{2-\rho^k}$ and $\rho_{M+1} = \rho_*$. Then, we index $C_{[i]}$ such that $1 = C_0 = C_{[0]} \leq C_{[1]} \leq \ldots \leq C_{[M+1]} = C_{M+1} = C_*$, and define $\tilde{\rho}_b$ on $[1, +\infty]$ as

$$\tilde{\rho}_b(C) = \begin{cases} \min\limits_{\substack{j,l \\ C_{[j]} \leq C_{[i]} \\ C_{[l]} \geq C_{[i+1]}}} \frac{C - C_{[j]}}{C_{[l]} - C_{[j]}}\rho_{[l]} + \frac{C_{[l]} - C}{C_{[l]} - C_{[j]}}\rho_{[j]} & \text{for } C \in [C_{[i]}, C_{[i+1]}] \\ \rho_*, & \text{for } C \geq C_* \end{cases},$$

which is an upper bound on $\tilde{\rho}$.

Proof. The values $C_i = \left\|R_k^{[-\varepsilon_i,\rho]}\right\|_1$ can computed explicitly using e.g. [23, Equation 2.18] to obtain the coefficients of T_k. If $C > C_*$ we saw that $\tilde{\rho}(C) = \rho_*$. Otherwise C is between a $C_{[i]}$ and a $C_{[i+1]}$ and the result follows from the convexity of $\tilde{\rho}$. ∎

To select the C_i in step (i), we rely on the intuition provided by Theorem 3.9 and on numerical observations. Indeed we noticed that for a large range of ε (more precisely for

$\varepsilon \in [0,\rho]$), $\max_{[0,\rho]} \left|R_k^{[-\varepsilon,\rho]}(x)\right|$ is a good upper bound for $\tilde{\rho}\left(\left\|R_k^{[-\varepsilon,\rho]}\right\|_1\right)$. Therefore, we sample $M-1$ values $\varepsilon_i \in [0,\rho]$ and use $C_i = \left\|R_k^{[-\varepsilon_i,\rho]}\right\|_1$ in step (i). Then, we set $\rho_i = \max_{[0,\rho]} \left|R_k^{[-\varepsilon_i,\rho]}(x)\right|$ ($= \rho_{\varepsilon_i}$ from Corollary 3.3) in step (ii) and finally apply step (iii) to get the upper bound. As shown in Figure 1, Proposition 3.13 provides upper bounds, represented in red on the figure, that are close to $\tilde{\rho}(C)$.

Setting $\varepsilon_2 = \rho$ in the previous proposition is motivated by two observations, (i) numerically $\rho_\varepsilon = \max_{x\in[0,\rho]} |R_k^{[-\varepsilon,\rho]}(x)|$ is close to $\rho\left(\left\|R_k^{[-\varepsilon,\rho]}\right\|_1\right)$ for $\varepsilon \in [0,\rho]$ and diverges from it for larger ε, (ii) we can study $R_k^{[-\rho,\rho]}$ and get a relatively simple expression for $\|R_k^{[-\rho,\rho]}\|_1$ as described below.

Lemma 3.14. *Let $\rho \in]0,1[$ and $k \geq 1$,*

$$C_2 := \left\|R_k^{[-\rho,\rho]}\right\|_1 = \frac{(1-\sqrt{1+\rho^2})^k + (1+\sqrt{1+\rho^2})^k}{(1-\sqrt{1-\rho^2})^k + (1+\sqrt{1-\rho^2})^k}. \tag{3.6}$$

Proof. From Definition 3.1 we have $R_k^{[-\rho,\rho]}(X) = \frac{T_k(\frac{X}{\rho})}{T_k(\frac{1}{\rho})}$. Then, noticing that $\|R_k^{[-\rho,\rho]}\|_1 = \frac{\left|T_k(\frac{i}{\rho})\right|}{T_k(\frac{1}{\rho})}$ (with i the unit imaginary number) allows to use the nice formulation for the value of Chebyshev polynomials (see e.g., [23, Eq 1.49])

$$\|R_k^{[-\rho,\rho]}\|_1 = \frac{\left|\left(i-(i^2-\rho)^{1/2}\right)^k + \left(i-(i^2-\rho)^{1/2}\right)^k)\right|}{(1-\sqrt{1-\rho^2})^k + (1+\sqrt{1-\rho^2})^k} = C_2.$$

■

In order to get more insights on how this upper bound behaves at C_2, we study the regime $\rho \sim 1$.

Remark 3.15. We have

$$\rho_2 := \max_{x\in[0,\rho]} |R_k^{[-\rho,\rho]}(x)| = \frac{2\rho^k}{(1+\sqrt{1-\rho^2})^k + (1-\sqrt{1-\rho^2})^k} \leq \rho^k.$$

When $\rho \to 1$ we can show

$$1-\rho^k \sim k(1-\rho),\ 1-\rho_* \sim k^2(1-\rho) \text{ and } 1-\rho_2 \sim \tfrac{k}{2k-1}k^2(1-\rho).$$

In addition,

$$C_2 \sim \frac{(1+\sqrt{2})^k + (1-\sqrt{2})^k}{(1+\sqrt{2})^{2k} + (1-\sqrt{2})^{2k}} C_* \leq \frac{1}{2^k} C_*.$$

In the bad conditioned regime where $\rho \sim 1$, decreasing the constraint C by a factor 2^k, only deteriorates the convergence rate by a factor $\frac{k}{2k-1}$.

We now, present a simpler and more practical upper bound, which corresponds to a scenario where the C_i's are ordered.

Remark 3.16. Following the notations of Proposition 3.13, a simpler upper bound when the C_i's are ordered is

$$\tilde{\rho}_{bo}(C) := \begin{cases} \frac{C-C_i}{C_{i+1}-C_i}\rho_{i+1} + \frac{C_{i+1}-C}{C_{i+1}-C_i}\rho_i & \text{for } C \in [C_i, C_{i+1}] \text{ and } 0 \leq i \leq M \\ \rho_* & \text{for } C \geq C_* \end{cases}. \tag{3.7}$$

Numerically $\left\|R_k^{[-\varepsilon,\rho]}\right\|_1$ appears to be decreasing with ε, as the intuition suggests. Indeed, when ε gets larger, the graph of $R_k^{[-\varepsilon,\rho]}$ exhibits wider oscillations, which would imply a decrease in the magnitude of its coefficients. For now, this remains a conjecture as we could not prove it formally. Note however that for $M = 2$, we can show (see Appendix D) that $C_0 < C_1 < C_2 < C_3$ and thus, (3.7) defines a simplified upper bound.

In the next section we use this simplified bound on the constrained Chebyshev problem to provide explicit bounds on constrained Anderson acceleration for gradient step operators.

4. Convergence of CAA on Gradient Steps. As discussed above, combining Proposition 3.13 and Proposition 2.2 gives an explicit linear rate of convergence for one pass of Algorithm 1.1. In what follows, we focus on applications of these results to the optimization setting where F is an operator representing an optimization method.

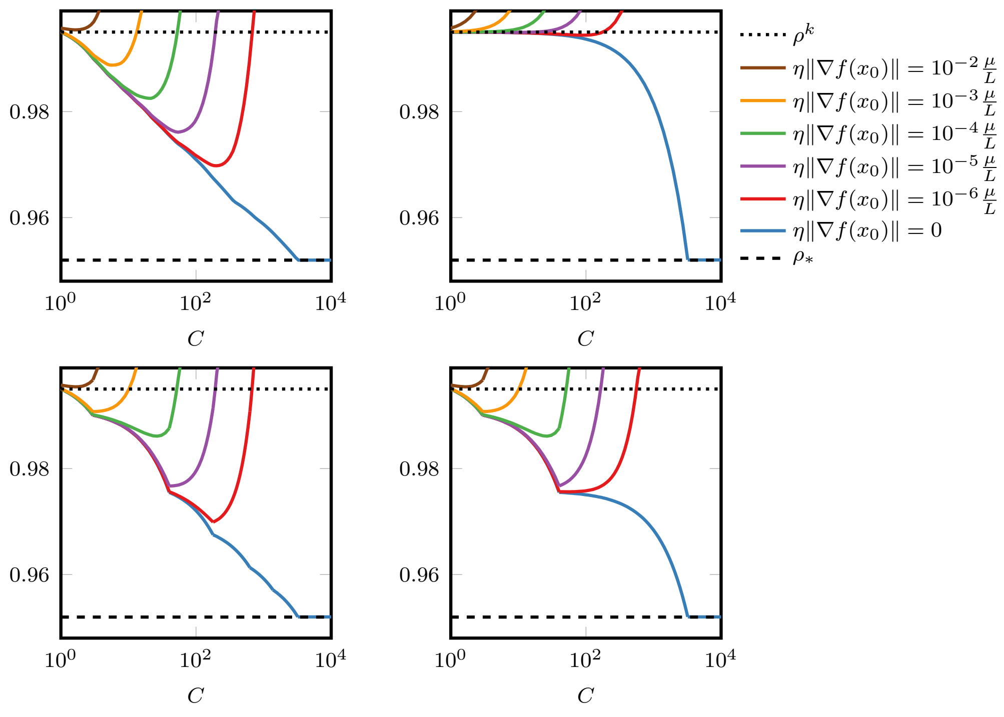

Figure 2. *Bounds on the convergence rate of Algorithm 1.1 with $k = 5$, $\mu = 10^{-3}$ and $L = 1$. Top Left: bound from (4.1), Top Right: bound from (3.5), Bottom Left: bound from (4.2) with $M = k+1$. Bottom Right: bound from (4.2) with $M = 2$. Note that the apparent nonconvexity of the bounds is due to the x-axis being represented in logarithmic scale.*

4.1. Convergence Bounds. In this section, we come back to the problem of accelerating convergence of a first-order method, and consider that F is specifically encoding a gradient step of a function f (see e.g., [35]). It is well known (see for instance [33]) that when f is μ-strongly convex with L-Lipschitz gradient for $0 < \mu < L$, $F = (I - \frac{1}{L}\nabla f)$ is a $\rho = \big(1 - \frac{\mu}{L}\big)$-Lipschitz operator. In addition, we assume that $\nabla^2 f$, the Hessian of f, is η-Lipschitz for $\eta > 0$, which implies that F satisfies Assumption 1.2.

Given $x_0 \in \mathbb{R}^n$, Proposition 2.2 shows that the output x_e of Algorithm 1.1 with $k \geq 1$ and $C \geq 1$ satisfies

$$\|\nabla f(x_e)\| \leq \big(\tilde{\rho}(C) + 3\tfrac{\eta}{L}k^2C^2\|\nabla f(x_0)\|\big)\,\|\nabla f(x_0)\|, \tag{4.1}$$

where $\tilde{\rho}$ is defined in (Cstr-Cheb). When C is fixed, there are two ways of for improving the convergence rate of CAA : (i) having a Hessian with a small Lipschitz constant η, which means being globally close to a quadratic, or (ii) being sufficiently close to the optimum (i.e., $\|\nabla f(x_0)\|$ small).

To make our bounds more concrete, we now combine (4.1) with the upper bound from Proposition 3.13. For clarity, we only consider the simple upper bound from Remark 3.16. The next proposition provides a range of values of C, depending on the perturbation parameter $\frac{\eta}{L^2}\|\nabla f(x_0)\|$ (which measures deviation from quadratic case), for which acceleration is guaranteed with Algorithm 1.1 compared to the baseline convergence rate ρ^k after k iterations of the fixed step gradient method.

Proposition 4.1. *Let $f : \mathbb{R}^n \to \mathbb{R}$ be a μ-strongly convex function with L-Lipschitz gradient and η-Lipschitz Hessian. Let x_e be the output of Algorithm 1.1 with $x_0 \in \mathbb{R}^n$, $k > 2$ and $C \geq 1$.*

$$\|\nabla f(x_e)\| \leq \big(\tilde{\rho}_{bo}(C) + 3\tfrac{\eta}{L^2}k^2C^2\|\nabla f(x_0)\|\big)\,\|\nabla f(x_0)\|. \tag{4.2}$$

where $\tilde{\rho}_{bo}$ is defined in (3.7) with $M \geq 2$ and $\rho = 1 - \frac{\mu}{L}$. In addition,

(i) If $\frac{\eta}{L^2}\|\nabla f(x_0)\| < \frac{\rho^k(1-\rho^k)(2-\rho^k)}{3k^2(2+\rho^k)^2}$ then

$$\exists\,\delta > 0 \text{ s.t. } \|\nabla f(x_e)\| < \rho^k\,\|\nabla f(x_0)\| \text{ for } C \in [\tfrac{2+\rho^k}{2-\rho^k} - \delta, \tfrac{2+\rho^k}{2-\rho^k} + \delta].$$

(ii) If $\frac{\eta}{L^2}\|\nabla f(x_0)\| < \min(\frac{\rho^k(1-\rho^k)(2-\rho^k)}{3k^2(2+\rho^k)^2}, \frac{\rho^k-\rho_2}{3k^2C_2^2})$ then

$$\|\nabla f(x_e)\| < \rho^k\,\|\nabla f(x_0)\| \text{ for } C \in [\tfrac{2+\rho^k}{2-\rho^k}, C_2].$$

(iii) If $\frac{\eta}{L^2}\|\nabla f(x_0)\| < \min(\frac{\rho^k(1-\rho^k)(2-\rho^k)}{3k^2(2+\rho^k)^2}, \frac{\rho^k-\rho_*}{3k^2C_*^2})$ then

$$\|\nabla f(x_e)\| < \rho^k\,\|\nabla f(x_0)\| \text{ for } C \in [\tfrac{2+\rho^k}{2-\rho^k}, C_*].$$

Proof. Using Proposition 2.2, the result follows from upper bounding

$$\hat{\rho}(C) := \tilde{\rho}(C) + 3\tfrac{\eta}{L^2}k^2C^2\,\|\nabla f(x_0)\|\,,$$

by ρ^k. In addition, since $\tilde{\rho}$ is convex in C (see Proposition 3.4) so is $\hat{\rho}$.

The case (i) follows directly from the fact that $\tilde{\rho}(C_1) = \rho_1 = \frac{\rho^k}{2-\rho^k}$ (see Lemma 3.7). For (ii) (resp. (iii)), we have $\tilde{\rho}(C_2) \leq \tilde{\rho}_{bo}(C_2) = \rho_2$ (resp. $\tilde{\rho}(C_*) = \rho_*$), thus taking $\frac{\eta}{L^2}\|\nabla f(x_0)\| < \min(\frac{\rho^k(1-\rho^k)(2-\rho^k)}{3k^2(2+\rho^k)^2}, \frac{\rho^k-\rho_2}{3k^2C_2^2})$ (resp. $\frac{\eta}{L^2}\|\nabla f(x_0)\| < \min(\frac{\rho^k(1-\rho^k)(2-\rho^k)}{3k^2(2+\rho^k)^2}, \frac{\rho^k-\rho_*}{3k^2C_*^2})$) implies $\hat{\rho}(C_1) < \rho^k$ and $\hat{\rho}(C_2) < \rho^k$ (resp. $\hat{\rho}(C_*) < \rho^k$), which gives the result using convexity of $\hat{\rho}$. ■

Figure 2 displays the values of bounds from (4.2) with fixed k, μ and L for various values of the perturbation parameter $\eta\|\nabla f(x_0)\|$. We observe that we do not loose much by using the simple upper bound with $M = 2$ compared with the numerical value of $\tilde{\rho}(C)$ obtained by solving (3.3). In the next section we study a version of Algorithm 1.1 with restarts.

4.2. Guarded and Adaptive Methods. Due to the particular form of the perturbation parameter α, proportional to $\eta\|\nabla f(x_0)\|$ in the case of the gradient step operator, we see that as soon as $\eta\|\nabla f(x_0)\|$ is small enough to get $\tilde{\rho}(C) + 3\frac{\eta}{L^2}k^2C^2\|\nabla f(x_0)\| < 1$, one can restart Algorithm 1.1 to get a decreasing sequence of perturbation parameters, leading to faster convergence guarantees. Adding a *guarded step* to this scheme produces Algorithm 4.1. The guarded step consists in using the extrapolated point x_e only if the gradient norm at this point is smaller than those of previous iterates, yielding global convergence guarantees.

Algorithm 4.1 Guarded Constrained Anderson Acceleration

Input:
- $x_0 \in \mathbb{R}^n$, initial guess.
- f strongly convex function with L-Lipschitz gradient.
- $k \in \mathbb{N}^*$, a constant controlling the number of gradient steps used in extrapolation.
- N number of outer iterations.

for $i = 0 \dots N-1$ **do**
  $x_i^0 = x_i$
  for $j = 0 \dots k$ **do**
    $x_i^{j+1} = x_i^j - \frac{1}{L}\nabla f(x_i^j)$
  end for
  $R = \begin{bmatrix} x_i^0 - x_i^1 & \cdots & x_i^k - x_i^{k+1} \end{bmatrix}$
  Choose $C_{(i)} \geq 1$
  Compute $\tilde{c} = \underset{\mathbf{1}^T c=1,\ \|c\|_1 \leq C_{(i)}}{\operatorname{argmin}} \|Rc\|$
  $x_i^e = \sum_{j=0}^k \tilde{c}_j x_i^j$
  $x_{i+1} = \underset{x \in \{x_i^e, x_i^k\}}{\operatorname{argmin}} \|\nabla f(x)\|$ *(guarded step)*
end for
Output: x_N

Proposition 4.2. *Let f be a μ-strongly convex function, with L-Lipschitz gradient and η-Lispchitz Hessian. Let $(x_i)_i \in \mathbb{R}^n$ be the sequence of iterates of Algorithm 4.1 on f, initiated* *at* $x_0 \in \mathbb{R}^n$ *with* $k > 2$*,* $N \geq 1$ *and with parameters* $(C_{(i)})_i$ *such that* $C_{(i)} \geq 1$*. It holds that*

$$\|\nabla f(x_N)\| \leq \prod_{i=1}^{N} \hat{\rho}_i(C_{(i-1)})\|\nabla f(x_0)\|,$$

where

$$\hat{\rho}_i(C) = \min\left(\rho^k, \tilde{\rho}_{bo}(C) + 3\tfrac{\eta}{L^2}\|\nabla f(x_{i-1})\|k^2C^2\right), \tag{4.3}$$

with $\tilde{\rho}_{bo}$ *defined in* (3.7) *with* $\rho = 1 - \frac{\mu}{L}$*.*

Proof. This is a direct consequence of Proposition 4.1. ■

Using the explicit expression (4.2), one can for instance get a (conservative) lower bound on the number of iterations of Algorithm 4.1 for acceleration to occur (i.e. escape the guarded regime, which does nothing more than just iterating F).

Corollary 4.3. *Let* f *be a* μ*-strongly convex function, with* L*-Lipschitz gradient and* η*-Lispchitz Hessian. Let* $(x_i)_i \in \mathbb{R}^n$ *be the sequence of iterates of Algorithm 4.1 on* f*, initiated at* $x_0 \in \mathbb{R}^n$ *with* $k > 2$*,* $N \geq 1$ *and with parameters* $(C_{(i)})_i$ *such that* $C_{(i)} \in [3, C_*]$*. It holds that*

$$N \geq \frac{\log\left(\frac{\eta}{L^2}\frac{3k^2(2+\rho^k)^2\|\nabla f(x_0)\|}{\rho^k(1-\rho^k)(2-\rho^k)}\right)}{k\log\frac{1}{\rho}} \implies \prod_{i=1}^{N}\hat{\rho}_i(C_{(i-1)}) < \rho^{kN},$$

with $\hat{\rho}_i(C_{(i-1)})$ *defined in* (4.3)*.*

Proof. We use (iii) from Proposition 4.1 along with $\frac{2+\rho^k}{2-\rho^k} \leq 3$. ■

We notice that choosing $(C_{(i)})_i$ such that $\|\nabla f(x_{i-1})\|C^2_{(i-1)}$ tends to 0 with i makes the perturbation terms $3\frac{\eta}{L^2}\|\nabla f(x_{i-1})\|k^2C^2_{(i-1)}$ in the convergence rate of Proposition 4.1 vanish with iterations. In addition, when the sequence $(C_{(i)})_i$ is unbounded above, there exists a rank i_0 such that $\tilde{\rho}_{bo}(C_{(i)}) = \rho_* \ \forall i \geq i_0$. Satisfying these two properties simultaneously would guarantee that $\hat{\rho}_i\left(C_{(i-1)}\right) \underset{i\to+\infty}{\longrightarrow} \rho_*$ (with $\hat{\rho}_i$ defined in (4.3)). We propose such an adaptive choice of $(C_{(i)})_i$ in the next corollary.

Corollary 4.4. *Under the conditions and notations of Proposition 4.2, with* $(C_{(i)})_i$ *satisfying*

$$C_{(i)} = i\left(\frac{L}{\|\nabla f(x_i)\|}\right)^{\delta} \quad \textit{for } i \in \mathbb{N}, \tag{Adapt-Ctr}$$

with $0 < \delta < \frac{1}{2}$*, we have that*

$$\hat{\rho}_N(C_{(N-1)}) \underset{N\to+\infty}{\longrightarrow} \rho_*,$$

meaning that asymptotically we reach the convergence rate of unconstrained Anderson acceleration on quadratics.

Proof. With this choice of $C_{(i)}$ we have

$$\hat{\rho}_i(C_{(i-1)}) = \min\left(\rho^k, \tilde{\rho}_{bo}(C_{(i-1)}) + 3\tfrac{\eta}{L^{2(1-\delta)}}\|\nabla f(x_{i-1})\|^{1-2\delta}k^2\right).$$

We have $\|\nabla f(x_{i-1})\|$ that goes to 0 when i grows, which implies that $C_{(i-1)}$ tends to $+\infty$ and thus $\tilde{\rho}_{bo}((C_{(i-1)})) = \rho_*$ for i large enough. The choice $0 < \delta < \frac{1}{2}$ finally leads to the desired conclusion. ■

The next section is dedicated to numerical testing of Algorithm 4.1 with the choice of constraints parameters (Adapt-Ctr).

4.3. Numerical Experiments. For solving (1.2), we consider the following reformulation

$$\min_{\substack{\mathbf{1}^T c=1\\ \|c\|_1\leq C}} \frac{1}{2}\|Rc\|^2, \tag{4.4}$$

which we solve using a Frank-Wolfe method [14, 18]. Indeed, as the constraint set is the convex hull of the set of points $\{\frac{C+1}{2}e_i + \frac{1-C}{2}e_j, i,j = 1,\ldots,k+1,\, i \neq j\}$ where e_i is the unit vector of $\mathbb{R}^{k+1}$ with a one at the i-th position and zeros elsewhere. Frank-Wolfe methods have the advantage to offer simple access to an upper bound of the primal gap which is the stopping criterion we are interested in (see Corollary 2.3).

Figure 3 contains experiments performed on ℓ_2 regularized logisitc regression. Blue curves correspond to gradient descent with step size $\frac{1}{L}$ where L is the Lipschitz constant of the objective function. Red curves are obtained with Algorithm 4.1 using $C_i = +\infty$ (i.e. Anderson acceleration) and in that case (1.2) only involves solving a linear system. Finally, green curves correspond to Algorithm 4.1 using constraint parameters (Adapt-Ctr) with $\delta = 0.49$ (CAA).

Using an unconstrained or unregularized version of Anderson acceleration is often the best practical choice, although it is not generically guaranteed to even converge in all situations beyond quadratic minimization. We observe on Figure 3 that our constrained version (CAA) which provably guarantees acceleration exhibits similar good practical performances.

Code. The implementation of CAA that we used for numerical experiments of Subsection 4.3 is available at

https://github.com/mathbarre/ConstrainedAndersonAcceleration

Conclusion. In this work, we proposed upper bounds on the optimal value of a constrained Chebyshev problem, and used them to produce explicit, dimension independent, local convergence bounds on constrained Anderson acceleration applied to nonlinear operators with a particular emphasis on gradient step operators. In this setting, we proposed a guarded method with an adaptive choice of constraint parameter. Our convergence bounds are somewhat conservative as they rely on treating the nonlinear part of the operator as a perturbation of the linear setting. Some open questions remain. Can we remove the symmetry requirements in Assumptions 1.1 and 1.2 and still use a constrained Chebyshev arguments? Can we prove better convergence bounds on Anderson acceleration without decoupling linear and nonlinear parts of the operator? This last part would however require very different proof techniques.

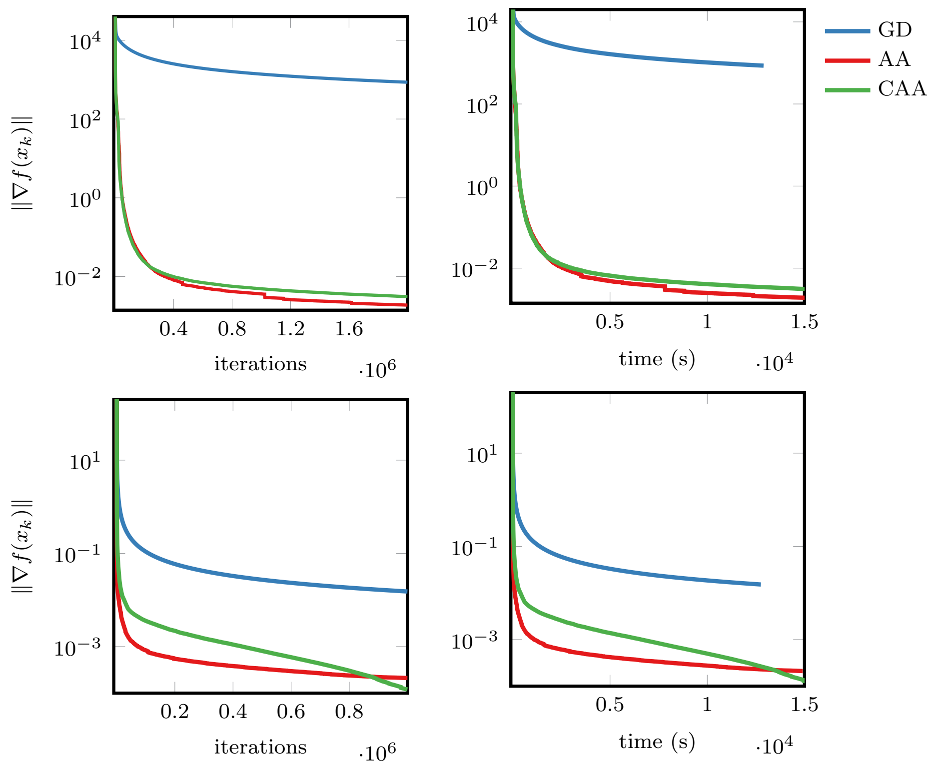

Figure 3. *Comparison of Gradient descent (GD), vanilla Anderson acceleration (AA) and constrained Anderson acceleration with adaptive constraints parameters (CAA) on Logistic regression with ℓ_2 regularization fixed to $10^{-8}L$ where L is the Lipschitz constant of the logisitc regression. Top: Madelon dataset. Bottom: RCV1 dataset. Datasets are taken from the LIBSVM library [9].*

References.

[1] A. C. Aitken, *On Bernoulli's numerical solution of algebraic equations*, Proceedings of the Royal Society of Edinburgh, 46 (1927), pp. 289–305.

[2] D. G. Anderson, *Iterative procedures for nonlinear integral equations*, Journal of the ACM (JACM), 12 (1965), pp. 547–560.

[3] M. ApS, *The MOSEK optimization toolbox for MATLAB manual. Version 9.0.*, 2019, http://docs.mosek.com/9.0/toolbox/index.html.

[4] Q. Bertrand and M. Massias, *Anderson acceleration of coordinate descent*, in International Conference on Artificial Intelligence and Statistics, PMLR, 2021, pp. 1288–1296.

[5] R. Bollapragada, D. Scieur, and A. d'Aspremont, *Nonlinear acceleration of momentum and primal-dual algorithms*, arXiv preprint arXiv:1810.04539, (2018).

[6] C. Brezinski, *Accélération de la convergence en analyse numérique*, vol. 584, Springer, 2006.

[7] C. Brezinski, S. Cipolla, M. Redivo-Zaglia, and Y. Saad, *Shanks and anderson-type acceleration techniques for systems of nonlinear equations*, arXiv preprint arXiv:2007.05716, (2020).

[8] C. Brezinski and M. Redivo-Zaglia, *The genesis and early developments of aitken's process, shanks' transformation, the ε–algorithm, and related fixed point methods*, Numerical Algorithms, 80 (2019), pp. 11–133.

[9] C.-C. Chang and C.-J. Lin, *LIBSVM: A library for support vector machines*, ACM Transactions on Intelligent Systems and Technology, 2 (2011), pp. 27:1–27:27. Software available at http://www.csie.ntu.edu.tw/~cjlin/libsvm.

[10] X. Chen and C. Kelley, *Convergence of the ediis algorithm for nonlinear equations*, SIAM Journal on Scientific Computing, 41 (2019), pp. A365–A379.

[11] M. Chupin, M.-S. Dupuy, G. Legendre, and É. Séré, *Convergence analysis of adaptive diis algorithms with application to electronic ground state calculations*, arXiv preprint arXiv:2002.12850, (2020).

[12] H.-R. Fang and Y. Saad, *Two classes of multisecant methods for nonlinear acceleration*, Numerical Linear Algebra with Applications, 16 (2009), pp. 197–221.

[13] D. A. Flanders and G. Shortley, *Numerical determination of fundamental modes*, Journal of Applied Physics, 21 (1950), pp. 1326–1332.

[14] M. Frank and P. Wolfe, *An algorithm for quadratic programming*, Naval research logistics quarterly, 3 (1956), pp. 95–110.

[15] A. Fu, J. Zhang, and S. Boyd, *Anderson accelerated douglas-rachford splitting*, arXiv preprint arXiv:1908.11482, (2019).

[16] G. Golub and C. Van Loan, *Matrix computation*, North Oxford Academic, (1990).

[17] G. Golub and R. Varga, *Chebyshev semi-iterative methods, successive overrelaxation iterative methods, and second order richardson iterative methods*, Numerische Mathematik, 3 (1961), pp. 157–168.

[18] M. Jaggi, *Revisiting frank-wolfe: Projection-free sparse convex optimization.*, in Proceedings of the 30th international conference on machine learning, no. CONF, 2013, pp. 427–435.

[19] J.-B. Lasserre, *Global optimization with polynomials and the problem of moments*, SIAM Journal on optimization, 11 (2001), pp. 796–817.

[20] J. Löfberg, *Yalmip : A toolbox for modeling and optimization in matlab*, in In Proceedings of the CACSD Conference, Taipei, Taiwan, 2004.
[21] V. Magron, M. S. El Din, and M. Schweighofer, *Algorithms for weighted sum of squares decomposition of non-negative univariate polynomials*, Journal of Symbolic Computation, 93 (2019), pp. 200–220.
[22] V. Mai and M. Johansson, *Anderson acceleration of proximal gradient methods*, in International Conference on Machine Learning, PMLR, 2020, pp. 6620–6629.
[23] J. C. Mason and D. C. Handscomb, *Chebyshev polynomials*, CRC press, 2002.
[24] M. Massias, A. Gramfort, and J. Salmon, *Celer: a fast solver for the lasso with dual extrapolation*, in International Conference on Machine Learning, 2018, pp. 3315–3324.
[25] A. S. Nemirovskiy and B. T. Polyak, *Iterative methods for solving linear ill-posed problems under precise information.*, ENG. CYBER., (1984), pp. 50–56.
[26] A. S. Nemirovsky, *Information-based complexity of linear operator equations*, Journal of Complexity, 8 (1992), pp. 153–175.
[27] W. Ouyang, J. Tao, A. Milzarek, and B. Deng, *Nonmonotone globalization for anderson acceleration using adaptive regularization*, arXiv preprint arXiv:2006.02559, (2020).
[28] P. A. Parrilo, *Structured semidefinite programs and semialgebraic geometry methods in robustness and optimization*, PhD thesis, California Institute of Technology, 2000.
[29] S. Pollock and L. Rebholz, *Anderson acceleration for contractive and noncontractive operators*, arXiv preprint arXiv:1909.04638, (2019).
[30] C. Poon and J. Liang, *Trajectory of alternating direction method of multipliers and adaptive acceleration*, in Advances in Neural Information Processing Systems, 2019, pp. 7355–7363.
[31] P. Pulay, *Convergence acceleration of iterative sequences. the case of scf iteration*, Chemical Physics Letters, 73 (1980), pp. 393–398.
[32] T. Rohwedder and R. Schneider, *An analysis for the diis acceleration method used in quantum chemistry calculations*, Journal of mathematical chemistry, 49 (2011), p. 1889.
[33] E. K. Ryu and S. Boyd, *Primer on monotone operator methods*, Appl. Comput. Math, 15 (2016), pp. 3–43.
[34] D. Scieur, F. Bach, and A. d'Aspremont, *Nonlinear acceleration of stochastic algorithms*, in Advances in Neural Information Processing Systems, 2017, pp. 3982–3991.
[35] D. Scieur, A. d'Aspremont, and F. Bach, *Regularized nonlinear acceleration*, in Advances In Neural Information Processing Systems, 2016, pp. 712–720.
[36] D. Scieur, E. Oyallon, A. d'Aspremont, and F. Bach, *Online regularized nonlinear acceleration*, arXiv preprint arXiv:1805.09639, (2018).
[37] D. Shanks, *Non-linear transformations of divergent and slowly convergent sequences*, Journal of Mathematics and Physics, 34 (1955), pp. 1–42.
[38] J. R. Shewchuk, *An introduction to the conjugate gradient method without the agonizing pain*, 1994.
[39] A. Sidi, W. F. Ford, and D. A. Smith, *Acceleration of convergence of vector sequences*, SIAM Journal on Numerical Analysis, 23 (1986), pp. 178–196.
[40] D. A. Smith, W. F. Ford, and A. Sidi, *Extrapolation methods for vector sequences*, SIAM review, 29 (1987), pp. 199–233.

[41] A. Toth and C. Kelley, *Convergence analysis for anderson acceleration*, SIAM Journal on Numerical Analysis, 53 (2015), pp. 805–819.
[42] J. Zhang, B. O'Donoghue, and S. Boyd, *Globally convergent type-i anderson acceleration for nonsmooth fixed-point iterations*, SIAM Journal on Optimization, 30 (2020), pp. 3170–3197.

Appendix A. Proof Proposition 2.2. We consider fixed point iterations of F, of the form

$$x_{i+1} = G(x_i) + \xi(x_i).$$

Equivalently, such iterations can be described as

$$x_{i+1} - x_* = G(x_i - x_*) + \xi(x_i) - \xi(x_*),$$

with $x_* = F(x_*)$. Expanding previous expression, one can rewrite the iterative process as

$$x_{i+1} - x_* = G^{i+1}(x_0 - x_*) + \sum_{j=0}^{k} G^{i-j}(\xi(x_j) - \xi(x_*)),$$

or in terms of the fixed point residual $F(x_i) - x_i = x_{i+1} - x_i$,

$$x_{i+1} - x_i = (G-I)G^i(x_0 - x_*) + (G-I)\sum_{j=0}^{i-1} G^{i-j-1}\left(\xi(x_j) - \xi(x_*)\right) + \xi(x_i) - \xi(x_*).$$

Let us use those expressions, along with a triangle inequality, to work out the fixed-point residual after extrapolation

$$\begin{aligned}
&\|(F-I)(x_e)\| \\
&= \|(G-I)(x_e - x_*) + \xi(x_e) - \xi(x_*)\| \\
&= \left\| \sum_{i=0}^{k} \tilde{c}_i (G-I)(x_i - x_*) + \xi(x_e) - \xi(x_*) \right\| \\
&= \left\| \sum_{i=0}^{k} \tilde{c}_i G^i (G-I)(x_0 - x_*) + (G-I)\sum_{i=0}^{k} \tilde{c}_i \sum_{j=0}^{i-1} G^{i-1-j}(\xi(x_j) - \xi(x_*)) + \xi(x_e) - \xi(x_*) \right\| \\
&= \left\| \sum_{i=0}^{k} \tilde{c}_i (x_{i+1} - x_i) - \sum_{i=0}^{k} \tilde{c}_i \xi(x_i) + \xi(x_e) \right\|,
\end{aligned}$$

where we used $\sum_{i=0}^{k} \tilde{c}_i = 1$ in the last step. We finally arrive to

$$\|(F-I)(x_e)\| \le \left\| \sum_{i=0}^{k} \tilde{c}_i (x_{i+1} - x_i) \right\| + \left\| \xi(x_e) - \sum_{i=0}^{k} \tilde{c}_i \xi(x_i) \right\|, \tag{A.1}$$

where the first term on the right hand side is exactly the quantity that is minimized in Algorithm 1.1. We then bound the two terms separately. Let c_* denotes the coefficients of the polynomial $p_*^C = \underset{\substack{p\in\mathbb{R}_k[X]\\ p(1)=1\\ \|p\|_1\leq C}}{\text{argmin}} \max_{x\in[0,\rho]}|p(x)|$, we proceed as follows:

$$\left\|\sum_{i=0}^k \tilde{c}_i(x_{i+1}-x_i)\right\| \leq \left\|\sum_{i=0}^k c_i^*(x_{i+1}-x_i)\right\| \text{ since } c_* \text{ feasible for problem (1.2)},$$

and then

$$\begin{aligned}
&\left\|\sum_{i=0}^k c_i^*(x_{i+1}-x_i)\right\| \\
&= \Bigg\|\sum_{i=0}^k c_i^* G^i(G-I)(x_0-x_*) + (G-I)\sum_{i=0}^k c_i^*\sum_{j=0}^{i-1} G^{i-1-j}(\xi(x_j)-\xi(x_*)) \\
&\quad + \sum_{i=0}^k c_i^*(\xi(x_i)-\xi(x_*))\Bigg\| \\
&= \Bigg\|\sum_{i=0}^k c_i^* G^i\left[(G-I)(x_0-x_*)+\xi(x_0)-\xi(x_*)\right] + (G-I)\sum_{i=0}^k c_i^*\sum_{j=0}^{i-1} G^{i-1-j}(\xi(x_j)-\xi(x_*)) \\
&\quad + \sum_{i=0}^k c_i^*\left[\xi(x_i)-\xi(x_*)-G^i(\xi(x_0)-\xi(x_*))\right]\Bigg\| \\
&\leq \left\|\sum_{i=0}^k c_i^* G^i\left[(F-I)(x_0)\right]\right\| \\
&\quad + \left\|(G-I)\sum_{i=1}^k c_i^*\sum_{j=0}^{i-1} G^{i-1-j}(\xi(x_j)-\xi(x_*)) + \sum_{i=1}^k c_i^*\left[\xi(x_i)-\xi(x_*)-G^i(\xi(x_0)-\xi(x_*))\right]\right\| \\
&\leq \left\|p_*^C(G)\right\|\,\|(F-I)(x_0)\| + \left\|\sum_{i=1}^k c_i^*\left[\sum_{j=1}^i G^{i-j}(\xi(x_j)-\xi(x_*)) - \sum_{j=0}^{i-1} G^{i-1-j}(\xi(x_j)-\xi(x_*))\right]\right\| \\
&\leq \left\|p_*^C(G)\right\|\,\|(F-I)(x_0)\| + \left\|\sum_{i=1}^k c_i^*\sum_{j=0}^{i-1} G^{i-j-1}\left[\xi(x_{j+1})-\xi(x_j)\right]\right\| \\
&\leq \left\|p_*^C(G)\right\|\,\|(F-I)(x_0)\| + \alpha\sum_{i=1}^k |c_i^*|\sum_{j=0}^{i-1}\rho^{i-j-1}\rho^j\,\|(F-I)(x_0)\| \\
&\leq \left(\left\|p_*^C(G)\right\| + \alpha\sum_{i=1}^k |c_i^*|\rho^{i-1}i\right)\|(F-I)(x_0)\| \\
&\leq \left(\left\|p_*^C(G)\right\| + \alpha k\|c^*\|_1\right)\|(F-I)(x_0)\|
\end{aligned}$$

$$\leq \left(\left\|p_*^C(G)\right\| + \alpha k C\right) \|(F-I)(x_0)\| .$$

One can bound $\|p_*^C(G)\|$ with standard arguments: Since $0 \preccurlyeq G \preccurlyeq \rho I$, there exist an orthogonal matrix O and a diagonal matrix D such that $G = O^t D O$. Therefore, we get $\|p_*(G)\| = \|O^t p_*^C(D) O\| \leq \|p_*^C(D)\|$. One can then notice that $\|p_*^C(D)\| = \max_{\lambda \in Sp(G)} |p_*^C(\lambda)| \leq \max_{x \in [0,\rho]} |p_*^C(x)|$, where $Sp(G)$ is the set of eigenvalues of G. Let us bound the second term of the right hand side in (A.1)

$$\begin{aligned}
\|\xi(x_e) - \sum_{i=0}^k \tilde{c}_i \xi(x_i)\| &\leq \|\xi(x_e) - \xi(x_k)\| + \|\xi(x_k) - \sum_{i=0}^k \tilde{c}_i \xi(x_i)\| \\
&\leq \alpha \left(\|x_e - x_k\| + \sum_{i=0}^k |\tilde{c}_i| \|x_k - x_i\| \right) \\
&\leq 2\alpha \sum_{i=0}^{k-1} |\tilde{c}_i| \|x_k - x_i\| \\
&\leq 2\alpha \sum_{i=0}^{k-1} |\tilde{c}_i| \rho^i \|x_{k-i} - x_0\| \\
&\leq 2\alpha \sum_{i=0}^{k-1} |\tilde{c}_i| \rho^i \sum_{j=0}^{k-1-i} \|x_{j+1} - x_j\| \\
&\leq 2\alpha \sum_{i=0}^{k-1} |\tilde{c}_i| \rho^i (k-i) \|(F-I)(x_0)\| \\
&\leq 2\alpha k \|\tilde{c}\|_1 \|(F-I)(x_0)\| \\
&\leq 2\alpha k C \|(F-I)(x_0)\|.
\end{aligned}$$

Combining the two previous bounds allows reaching (2.1).

Let Assumption 1.2 hold, we can then pick $G = F'(x_0)$ and $\xi = F - F'(x_0)$ (note that $F'(x_0)$ is symmetric positive semidefinite by assumption and that $\|F'(x_0)\| \leq \rho$ when F is ρ-Lipschitz). In computations of the previous bounds, Lischitzness was only used on the convex set $B_C = \{\sum_{i=0}^k c_i x_i : \|c\|_1 \leq C, \sum_{i=0}^k c_i = 1\}$. Let us bound $\|D\xi(x)\|$ for $x = \sum_{i=0}^k c_i x_i$ in B_C.

$$\begin{aligned}
\|D\xi(x)\| &= \|F'(x) - F'(x_0)\| \\
&\leq \eta \|x - x_0\| = \eta \left\| \sum_{i=0}^k c_i (x_i - x_0) \right\| \\
&\leq \eta \sum_{i=1}^k |c_i| \left\| \sum_{j=0}^{i-1} x_{j+1} - x_j \right\| \\
&\leq \eta \sum_{i=1}^k |c_i| \sum_{j=0}^{i-1} \rho^j \|x_1 - x_0\|
\end{aligned}$$

$$\leq \eta C k \left\| F(x_0) - x_0 \right\|.$$

Using the mean value theorem, we conclude that $\xi(x)$ is $\eta C k \left\| F(x_0) - x_0 \right\|$-Lipschitz on B_C.

Appendix B. Some Properties of Chebyshev Polynomials. Unspecified facts on Chebyshev polynomials of the first kind are borrowed from [23].

Proposition B.1. *Let $k \in \mathbb{N}$ and $a > 1$, we have*

$$\frac{T_k}{T_k(a)} = \underset{\substack{p \in \mathbb{R}_k[X] \\ p(a)=1}}{\operatorname{argmin}} \max_{x \in [-1,1]} |p(x)|, \tag{B.1}$$

where T_k is the first kind Chebyshev polynomials of order k.

Proof. A proof of this result can be found in [13, Equation 10]. ∎

The following result is classically used for analyzing Anderson acceleration [17, Section 3].

Proposition B.2. *Let $k \in \mathbb{N}^*$, and $\rho \in]0, 1[$. It holds that*

$$\frac{T_k(\frac{2X-\rho}{\rho})}{T_k(\frac{2-\rho}{\rho})} = \underset{\substack{p \in \mathbb{R}_k[X] \\ p(1)=1}}{\operatorname{argmin}} \max_{x \in [0,\rho]} |p(x)|,$$

where T_k is the first kind Chebychev polynomials of order k. Furthermore,

$$\max_{x \in [0,\rho]} \left| \frac{T_k(\frac{2X-\rho}{\rho})}{T_k(\frac{2-\rho}{\rho})} \right| = \frac{2\beta^k}{1+\beta^{2k}},$$

with $\beta = \frac{1-\sqrt{1-\rho}}{1+\sqrt{1-\rho}}$.

Proof. We have

$$\min_{\substack{p \in \mathbb{R}_k[X] \\ p(1)=1}} \max_{x \in [0,\rho]} |p(x)| = \min_{\substack{p \in \mathbb{R}_k[X] \\ p(1)=1}} \max_{y \in [-1,1]} |p(\rho \tfrac{y+1}{2})| = \min_{\substack{q \in \mathbb{R}_k[X] \\ q(\frac{2-\rho}{\rho})=1}} \max_{y \in [-1,1]} |q(y)|.$$

Thus, if p_* is solution of the left hand side problem, $q_*(y) = p_*(\rho \frac{y+1}{2})$ is solution of the right hand side one. This last problem is solved using Proposition B.1 with $a = \frac{2-\rho}{\rho} > 1$. This gives us the solution $q_*(y) = T_k(y) \Big/ T_k(\frac{2-\rho}{\rho})$, and thus the solution to the original problem $p_*(x) = T_k(\frac{2x-\rho}{\rho}) \Big/ T_k(\frac{2-\rho}{\rho})$.

For the value of the max, we know that $\max_{y \in [-1,1]} |T_k(y)| = 1$, therefore

$$\max_{x \in [0,\rho]} \left| \frac{T_k(\frac{2X-\rho}{\rho})}{T_k(\frac{2-\rho}{\rho})} \right| = \frac{1}{T_k(\frac{2-\rho}{\rho})}.$$

Since $\frac{2-\rho}{\rho} > 1$ one can use the formulas for $T_k(x)$ for $|x| \geq 1$ (see e.g [23, Eq 1.49]):

$$T_k(x) = \frac{1}{2}\left(\left(x - \sqrt{x^2-1}\right)^k + \left(x + \sqrt{x^2-1}\right)^k\right) \text{ when } |x| \geq 1.$$

It follows that

$$\begin{aligned}
T_k(\tfrac{2-\rho}{\rho}) &= \tfrac{1}{2}\left(\left(\tfrac{2-\rho}{\rho} - \sqrt{(\tfrac{2-\rho}{\rho})^2 - 1}\right)^k + \left(\tfrac{2-\rho}{\rho} + \sqrt{(\tfrac{2-\rho}{\rho})^2 - 1}\right)^k\right) \\
&= \tfrac{1}{2}\left(\left(\tfrac{2-\rho-2\sqrt{1-\rho}}{\rho}\right)^k + \left(\tfrac{2-\rho+2\sqrt{1-\rho}}{\rho}\right)^k\right) \\
&= \tfrac{1}{2}\frac{\left(\left(1-\sqrt{1-\rho}\right)^{2k} + \left(1+\sqrt{1-\rho}\right)^{2k}\right)}{\rho^k} \\
&= \tfrac{1}{2}\frac{\left(\left(1-\sqrt{1-\rho}\right)^{2k} + \left(1+\sqrt{1-\rho}\right)^{2k}\right)}{(1-\left(\sqrt{1-\rho}\right)^2)^k} \\
&= \tfrac{1}{2}\frac{\left(\left(1-\sqrt{1-\rho}\right)^{2k} + \left(1+\sqrt{1-\rho}\right)^{2k}\right)}{\left(1-\sqrt{1-\rho}\right)^k\left(1+\sqrt{1-\rho}\right)^k} \\
&= \tfrac{1}{2}\frac{\frac{\left(1-\sqrt{1-\rho}\right)^{2k}}{\left(1+\sqrt{1-\rho}\right)^{2k}} + 1}{\frac{\left(1-\sqrt{1-\rho}\right)^{k}}{\left(1+\sqrt{1-\rho}\right)^{k}}} = \frac{1+\beta^{2k}}{2\beta^k}.
\end{aligned}$$

■

In the following, we focus on problems where ε is close to 0.

Lemma B.3. *Let $k > 0$ and $\rho \in [0, 1[$. For $\varepsilon \in [0, \tilde{\varepsilon}]$ with $\tilde{\varepsilon} = \rho\frac{1+\cos(\frac{2k-1}{2k}\pi)}{1-\cos(\frac{2k-1}{2k}\pi)}$ we have the following properties of $R_k^{[-\varepsilon,\rho]} = \frac{T_k(\frac{2(X+\varepsilon)}{\rho+\varepsilon}-1)}{T_k(\frac{2(1+\varepsilon)}{\rho+\varepsilon}-1)}$.*

(i) $\left|R_k^{[-\varepsilon,\rho]}(X)\right|$ is maximal on the $m_i = \frac{(\rho+\varepsilon)\cos(\frac{i\pi}{k})+\rho-\varepsilon}{2} \in [-\varepsilon, \rho]$ for $i = 0, \dots, k$ and $\operatorname{sign}(R_k^{[-\varepsilon,\rho]}(m_i)) = (-1)^i$.

(ii) Let $c \in \mathbb{R}^{k+1}$ such that $R_k^{[-\varepsilon,\rho]}(X) = \sum_{i=0}^k c_i X^i$. Then $\operatorname{sign}(c_i) = (-1)^{k-i}$ for $i = 1, \dots, k$ and $(-1)^k c_0 \geq 0$.

Proof. The Chebyshev polynomial of first kind $T_k(X)$ is defined such that

$$T_k(\cos(\theta)) = \cos(k\theta) \text{ for all } \theta \in \mathbb{R}.$$

Using this property, *(i)* is obtained by observing that $\max_{x\in[-1,1]} |T_k(x)| = 1$ is attained for $x_i = \cos(\frac{i\pi}{k})$ with $i = 0, \dots, k$. In particular $T_k(x_i) = (-1)^i$. Thus $|R_k^{[-\varepsilon,\rho]}|$ has its maxima on

$$m_i = \frac{(\rho+\varepsilon)\cos(\frac{i\pi}{k})+\rho-\varepsilon}{2}, \quad i = 0, \dots, k$$

and $R_k^{[-\varepsilon,\rho]}(m_i) = (-1)^i$.

Let us now prove *(ii)*. From the definition of T_k, we get that the roots of T_k are the $(z_i)_{i\in[0,k-1]} = (\cos\left(\frac{2i+1}{2k}\pi\right))_{i\in[0,k-1]} \in [-1,1]$. The roots of $R_k^{[-\varepsilon,\rho]}(X)$ are the z_i^ε defined such that $\frac{2z_i^\varepsilon}{\rho+\varepsilon} - \frac{\rho-\varepsilon}{\rho+\varepsilon} = z_i$. This corresponds to

$$z_i^\varepsilon = \tfrac{(\rho+\varepsilon)z_i+\rho-\varepsilon}{2} \in [-\varepsilon,\rho], \quad i = 0,\dots,k-1.$$

The smallest root $z_{k-1}^\varepsilon = \frac{(\rho+\varepsilon)\cos(\frac{2k-1}{2k}\pi)+\rho-\varepsilon}{2}$ is nonnegative for $\varepsilon \in [0, \rho\frac{1+\cos(\frac{2k-1}{2k}\pi)}{1-\cos(\frac{2k-1}{2k}\pi)}] = [0,\tilde{\varepsilon}]$. This means that this for choice of ε, all the roots of $R_k^{[-\varepsilon,\rho]}$ are in $[0,\rho]$.

One can thus express $R_k^{[-\varepsilon,\rho]}$ using its roots as $R_k^{[-\varepsilon,\rho]}(x) = a\prod_{i=0}^{k-1}(x - z_i^\varepsilon)$ with a the leading coefficients. Using that the leading coefficient of T_k is 2^{k-1} and that $T_k(\frac{2(1+\varepsilon)}{\rho+\varepsilon} - 1) > 0$ since $\frac{2(1+\varepsilon)}{\rho+\varepsilon} - 1 > 1$, we have $a > 0$. By developing the product we have

$$R_k^{[-\varepsilon,\rho]}(x) = a\left(\sum_{j=1}^{k}(-1)^{k-j}x^j \sum_{0<i_0<\dots<i_{k-j}} z_{i_0}^\varepsilon \cdots z_{i_{k-j}}^\varepsilon + x^k\right),$$

which gives us (ii). ■

Appendix C. Proof of Theorem 3.9.

In order to prove Theorem 3.9, we use some intermediary results on rescaled Chebyshev polynomials, listed on the following Lemma.

Lemma C.1. *Let $k > 0$ and $0 \le \varepsilon \le \tilde{\varepsilon}$, suppose that there exists a nonzero polynomial $h \in \mathbb{R}_k[X]$ satisfying*

$$\begin{aligned}
&(i) && h(1) = 0.\\
&(ii) && \max_{x\in[0,\rho]}|h(x)| \le \tfrac{1}{2}\max_{x\in[0,\rho]}|R_k^{[-\varepsilon,\rho]}(x)|.\\
&(iii) && \max_{x\in[0,\rho]}|R_k^{[-\varepsilon,\rho]}(x) + h(x)| < \max_{x\in[0,\rho]}|R_k^{[-\varepsilon,\rho]}(x)|.
\end{aligned}$$

Then, h possesses k distinct roots in $]0,1]$, $(-1)^k h(-1) > 0$ and $(-1)^k h(0) > 0$.

Proof. From Lemma B.3 we know that $|R_k^{[-\varepsilon,\rho]}|$ is maximal on $[-\varepsilon,\rho]$ at the $m_i = \frac{(\rho+\varepsilon)\cos(\frac{i\pi}{k})+\rho-\varepsilon}{2}$ for $i = 0,\dots,k$ and $\mathrm{sign}(R_k^{[-\varepsilon,\rho]}(m_i)) = (-1)^i$. In addition, $m_i \in]0,\rho]$ for $i = 0,\dots,k-1$. Indeed the m_i are in decreasing order and $m_{k-1} = \frac{(\rho+\varepsilon)\cos(\frac{(k-1)\pi}{k})+\rho-\varepsilon}{2} > \frac{(\rho+\varepsilon)\cos(\frac{(2k-1)\pi}{2k})+\rho-\varepsilon}{2} \ge \frac{(\rho+\tilde{\varepsilon})\cos(\frac{(2k-1)\pi}{2k})+\rho-\tilde{\varepsilon}}{2} = 0$ since $\varepsilon \in [0,\tilde{\varepsilon}]$.

It follows from (ii) that $|h(m_i)| \le \frac{1}{2}|R_k^{[-\varepsilon,\rho]}(m_i)|$ for $i = 0,\dots,k-1$ which implies that $|R_k^{[-\varepsilon,\rho]}(m_i) + h(m_i)| = |R_k^{[-\varepsilon,\rho]}(m_i)| + \mathrm{sign}(R_k^{[-\varepsilon,\rho]}(m_i))h(m_i) = |R_k^{[-\varepsilon,\rho]}(m_i)| + (-1)^i h(m_i)$. Together with (iii) this leads to $(-1)^i h(m_i) < 0$ for $i = 0,\dots,k-1$.

Because h alternates sign between m_i's, the mean value theorem implies that h possesses a root inside each interval $]m_{i+1}, m_i[\subset]0,1[$ for $i = 0,\dots,k-2$. Along with (i), this shows that

h has k distinct roots in $]m_{k-1}, 1] \subset]0,1]$. Furthermore, h keeps the same sign on $]-\infty, m_{k-1}]$ (since it already has k roots) which is $(-1)^k$. In particular, it implies that $(-1)^k h(-1) > 0$ and $(-1)^k h(0) > 0$ reaching the desired statements. ■

Proof of Theorem 3.9.

Proof. We proceed by contradiction: we assume that $R_k^{[-\varepsilon,\rho]}$ is not a solution to the constrained Chebyshev problem and show that it leads to a contradiction.

Assume that $R_k^{[-\varepsilon,\rho]}$ is not a global minimum of (Cstr-Cheb), $R_k^{[-\varepsilon,\rho]}$ is not a local minimum either, therefore for all $\delta > 0$, there exists a nonzero polynomial $h \in \mathbb{R}_k[X]$ such that

$$\begin{array}{lll} (i) & R_k^{[-\varepsilon,\rho]}(1) + h(1) = 1. & \text{(feasibility)} \\ (ii) & \left\| R_k^{[-\varepsilon,\rho]} + h \right\|_1 \leq \left\| R_k^{[-\varepsilon,\rho]} \right\|_1. & \text{(feasibility)} \\ (iii) & \max\limits_{x\in[0,\rho]} |h(x)| \leq \delta. & \text{(not a local minimum)} \\ (iv) & \max\limits_{x\in[0,\rho]} |R_k^{[-\varepsilon,\rho]}(x) + h(x)| < \max\limits_{x\in[0,\rho]} |R_k^{[-\varepsilon,\rho]}(x)|. & \text{(not a minimum).} \end{array}$$

For $\delta < \frac{1}{2} \max_{x\in[0,\rho]} |R_k^{[-\varepsilon,\rho]}(x)|$, (i), (iii) and (iv) correspond to the assumptions of Lemma C.1 for h. This implies that it possesses k roots in $]0,1[$, $(-1)^k h(-1) > 0$ and $(-1)^k h(0) > 0$.

Then, writing $R_k^{[-\varepsilon,\rho]}(x) = \sum_{i=0}^k c_i x^i$ and $h(x) = \sum_{i=0}^k h_i x^i$, Lemma B.3 allows concluding that

$$\begin{array}{ll} (v) & c_i \neq 0 \text{ and } \operatorname{sign}(c_i) = (-1)^{k+i} \text{ for } i = 1, \dots, k \\ (vi) & (-1)^k c_0 \geq 0. \end{array}$$

From (vi) and the fact that $(-1)^k h(0) > 0$, we have $|c_0 + h_0| = (-1)^k(c_0 + h_0) = |c_0| + (-1)^k h_0$. Hence, for δ small enough, it follows that $0 < \max_{i=1,\dots,k} |h_i| < \min_{i=1,\dots,k} |c_i|$ and we obtain

$$|c_i + h_i| = |c_i| + \operatorname{sign}(c_i) h_i = |c_i| + (-1)^{k+i} h_i,$$

where the second equality follows from (v).

It remains to express the ℓ_1 norm of $R_k^{[-\varepsilon,\rho]} + h$ as

$$\begin{aligned} \left\| R_k^{[-\varepsilon,\rho]} + h \right\|_1 &= \sum_{i=0}^k |c_i + h_i| = \sum_{i=0}^k |c_i| + (-1)^{k+i} h_i \\ &= \left\| R_k^{[-\varepsilon,\rho]} \right\|_1 + (-1)^k h(-1). \end{aligned}$$

Combining (ii) with the previous equality leads to $(-1)^k h(-1) \leq 0$ which is in contradiction with $(-1)^k h(-1)$ obtained earlier.

Therefore, $R_k^{[-\varepsilon,\rho]}$ has to be a solution of (Cstr-Cheb), reaching the desired claim. ■

Appendix D. Ordering of the C_i.

Lemma D.1. *Let $k \in \mathbb{N}$, $\rho < 1$, C_* is defined in* (3.4) *(an explicit value is provided in Remark* 3.11*) and C_2 in* (3.6)*. It holds that*

$$C_1 = \tfrac{2+\rho^k}{2-\rho^k} \leq C_2 \text{ for } k > 1 \text{ and } C_2 \leq C_* \text{ for } k \geq 1.$$

Proof. We start from the expression of C_2

$$C_2 = \frac{(1-\sqrt{1+\rho^2})^k+(1+\sqrt{1+\rho^2})^k}{(1-\sqrt{1-\rho^2})^k+(1+\sqrt{1-\rho^2})^k} = \frac{\sum_{i=0}^{\lfloor k/2 \rfloor} \binom{k}{2i}(1+\rho^2)^i}{\sum_{i=0}^{\lfloor k/2 \rfloor} \binom{k}{2i}(1-\rho^2)^i}.$$

For obtaining $C_2 \geq \frac{2+\rho^k}{2-\rho^k}$ we need to show

$$(2-\rho^k)\sum_{i=0}^{\lfloor k/2 \rfloor}\binom{k}{2i}(1+\rho^2)^i - (2+\rho^k)\sum_{i=0}^{\lfloor k/2 \rfloor}\binom{k}{2i}(1-\rho^2)^i \geq 0,$$

and in particular we study

$$(2-\rho^k)(1+\rho^2)^i - (2+\rho^k)(1-\rho^2)^i.$$

When $i=0$, this is equal to $-2\rho^k$, and when $i=1$ this is equal to $4\rho^2-2\rho^k$. In addition, one can easily observe that it is an increasing function of i. Hence, it is nonnegative when $i \geq 1$. For $k \geq 2$, we can further write

$$\begin{aligned}(2-\rho^k)\sum_{i=0}^{\lfloor k/2 \rfloor}\binom{k}{2i}(1+\rho^2)^i - (2+\rho^k)\sum_{i=0}^{\lfloor k/2 \rfloor}\binom{k}{2i}(1-\rho^2)^i &\geq -2\rho^k + \binom{k}{2}(-2\rho^k+4\rho^2)\\ &\geq 4\rho^2(1-\rho^{k-2})\\ &\geq 0 \text{ strict inequality when } k>2,\end{aligned}$$

and then

$$\boxed{C_2 \geq \frac{2+\rho^k}{2-\rho^k}} \text{ with strict inequality when } k>2.$$

Finally, we show the second inequality between C_* and C_2.

$$C_* = \frac{\left(2+\rho-2\sqrt{1+\rho}\right)^k+\left(2+\rho+2\sqrt{1+\rho}\right)^k}{\left(2-\rho-2\sqrt{1-\rho}\right)^k+\left(2-\rho+2\sqrt{1-\rho}\right)^k} = \frac{\sum_{i=0}^{\lfloor k/2 \rfloor}\binom{k}{2i}(1+\frac{\rho}{2})^{k-2i}(1+\rho)^i}{\sum_{i=0}^{\lfloor k/2 \rfloor}\binom{k}{2i}(1-\frac{\rho}{2})^{k-2i}(1-\rho)^i}.$$

When $k \geq 1$, $(1+\frac{\rho}{2})^{k-2i}(1+\rho)^i > (1+\rho^2)^i$ and $(1-\frac{\rho}{2})^{k-2i}(1-\rho)^i < (1-\rho^2)^i$ for $i \in [0, \lfloor \frac{k}{2} \rfloor]$ and thus

$$\boxed{C_* > C_2} \text{ when } k \geq 1,$$

reaching the desired conclusion. ■