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Easy and Fast Computation of Approximate Smallest Enclosing Balls

by

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Easy and Fast Computation of Approximate Smallest Enclosing Balls

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***Abstract*— Badoiu and Clarkson [1] introduced an extremely simple incremental algorithm which finds the smallest enclosing ball around points with ϵ precision in at most $\mathcal{O}(\epsilon^{-2})$ iteration steps. A simplified proof for this quadratic scaling is given. Based on this proof it is shown that the number of steps in fact increases only like $\mathcal{O}(\epsilon^{-1})$. This new bound leads to a new optimal step size of the algorithm. With this new step size one can even expect a $\mathcal{O}(\epsilon^{-1/2})$ scaling.**

I. Introduction

In many applications it is necessary to find the smallest enclosing ball (SEB) around a set S of n points $\mathbf{x} \in \mathbb{R}^d$. See, e.g., references in Kumar et al. [3]. There are more or less elaborate combinatorial algorithms which provide exact solutions, also in high dimensions (see e.g. [2]), but without a polynomial worst-case bound. Badoiu and Clarkson [1] introduced a very simple, gradient based "three-liner" which provides ϵ-approximate solutions in at most $\mathcal{O}(\frac{nd}{\epsilon^2})$ time. This iterative algorithm works as follows: Let $\mathbf{c}$ be the unknown center of the SEB of S, and R its radius. Let $\mathbf{c}_t$ be the guess for the center at step t. Set $\mathbf{c}_0 = \mathbf{0}$, and iterate according to

$$\mathbf{c}_{t+1} = \mathbf{c}_t + \frac{1}{1+t}(\mathbf{x}_t - \mathbf{c}_t), \qquad (1)$$

with $\mathbf{x}_t$ as the point of S which is furthest away from $\mathbf{c}_t$. At the latest after $1/\epsilon^2$ iterations $||\mathbf{c}_t - \mathbf{c}||/R \leq \epsilon$ and $(R_t - R)/R \leq \epsilon$ is valid, with R_t as the radius of the smallest enclosing ball around $\mathbf{c}_t$ [1].

We show that in fact the precision of the solution increases like $\mathcal{O}(t^{-1})$ with the number of iteration steps. Based on this new bound a step size different from $1/(1+t)$ can be derived which achieves a precision increase of even $\mathcal{O}(t^{-2})$.

II. A New Bound

Theorem: An ϵ-approximate SEB is obtained in at most $\min(a/\epsilon, 1/\epsilon^2)$ iteration steps, with a as a constant which depends on S. This requires at most $\mathcal{O}\left(\min(a, 1/\epsilon)\frac{nd}{\epsilon}\right)$ time.

First we give an alternative proof for the $1/\sqrt{t}$ convergence bound of $||\mathbf{c}_t - \mathbf{c}||/R$. Then we show that $||\mathbf{c}_t - \mathbf{c}||/R$ also converges at least as a/t.

Without loss of generality we can set $\mathbf{c} = \mathbf{0}$ and $R = 1$. We introduce $\mathbf{u}_t = t\mathbf{c}_t$. The iteration rule yields $\mathbf{u}_{t+1} = \mathbf{u}_t + \mathbf{x}_t$, and the change of the length of $\mathbf{u}_t$ obeys

$$\mathbf{u}_{t+1}^2 - \mathbf{u}_t^2 = 2\mathbf{u}_t^T\mathbf{x}_t + \mathbf{x}_t^2 \leq 1 , \qquad (2)$$

since according to Lemma 2.1 in [1] always $\mathbf{u}_t^T\mathbf{x}_t \leq 0$. But then $||\mathbf{u}_t||^2 \leq t$, and we obtain

$$\frac{||\mathbf{c}_t - \mathbf{c}||}{R} = \frac{||\mathbf{u}_t||}{t} \leq \frac{\sqrt{t}}{t} = \frac{1}{\sqrt{t}} \qquad (t > 0) .$$

A $\mathcal{O}(1/t)$ convergence is given, if $\mathbf{u} = \sum_{\tau=0}^{t-1}\mathbf{x}_\tau$ stays bounded. This is indeed the case. After a finite number of iterations t^* each $\mathbf{x}_t$ will lie on the surface of the SEB, i.e. $||\mathbf{x}_t|| = 1$. The set of points on the surface we denote by S'. With $\mathbf{u}'_t$ we introduce the projection of $\mathbf{u}_t$ onto the subspace spanned by these $\mathbf{x} \in S'$. If $\mathbf{u}'_t$ stays bounded, then also $\mathbf{u}$. From t^* on, the $\mathbf{x}_t \in S$ for which $(\mathbf{x}_t - \mathbf{c}_t)^2$ is maximal is the $\mathbf{x}_t \in S'$ for which ${\mathbf{u}'}_t^T\mathbf{x}_t$ is minimal. For $\mathbf{x} \in S'$ $\mathbf{u}_t^T\mathbf{x}_t = {\mathbf{u}'}_t^T\mathbf{x}_t \leq 0$ is valid. We discriminate two cases:

i) $\max_{||\mathbf{u}'||=1}\min_{\mathbf{x}\in S'}({\mathbf{u}'}^T\mathbf{x}) < 0$
ii) $\max_{||\mathbf{u}'||=1}\min_{\mathbf{x}\in S'}({\mathbf{u}'}^T\mathbf{x}) = 0$

Note that $\mathbf{u}'$ with $||\mathbf{u}'|| = 1$ varies only within the subspace spanned by the $\mathbf{x} \in S'$. If this subspace is of dimension one, only i) can occur. For i) it can easily be proven that ${\mathbf{u}'}_t$ remains bounded. Case ii) can be redirected to i), which is a little bit more tedious.

i) There is a $\delta > 0$ such that for each iteration step ${\mathbf{u}'}_t^T\mathbf{x}_t \leq -\delta||{\mathbf{u}'}_t||$. Analog to Equation (2) we obtain

$$\begin{aligned} {\mathbf{u}'}_{t+1}^2 - {\mathbf{u}'}_t^2 &= 2{\mathbf{u}'}_t^T\mathbf{x}_t + \mathbf{x}_t^2 \\ &\leq -2\delta||{\mathbf{u}'}_t|| + 1 . \end{aligned}$$

The negative contribution to the change of $||{\mathbf{u}'}_t||$ increases with $||{\mathbf{u}'}_t||$ and keeps it bounded.

ii) We redirect this case to i). Let ${\mathbf{u}'}_*$, $||{\mathbf{u}'}_*|| = 1$ maximize $\min_{\mathbf{x}\in S'}({\mathbf{u}'}^T\mathbf{x})$. The set of those $\mathbf{x} \in S'$ with ${\mathbf{u}'}_*^T\mathbf{x} = 0$ we denote by S''. Since ${\mathbf{u}'}_*$ is spanned by the $\mathbf{x} \in S'$, there is at least one $\mathbf{x} \in S'$ for which ${\mathbf{u}'}_*^T\mathbf{x} > 0$. The hyperplane defined by ${\mathbf{u}'}_*$ separates all those $\mathbf{x} \in S'$ which do not belong to S'' from the origin by a positive margin. Note that $\mathbf{u}'$ changes according to the perceptron learning rule [4]. Hence, after a finite number of learning steps $\mathbf{x}_t$ will always be an element of S''. Then the $\mathbf{x}_t \in S'$ that minimizes ${\mathbf{u}'}_t^T\mathbf{x}$ is identical to the $\mathbf{x}_t \in S''$ that minimizes ${\mathbf{u}''}_t^T\mathbf{x}$, where ${\mathbf{u}''}_t$ is the projection of ${\mathbf{u}'}_t$ onto the subspace spanned by the $\mathbf{x} \in S''$. Note that the dimension of S'' is reduced by at least one compared to S'. For $\mathbf{x} \in S''$ again $\mathbf{u}_t^T\mathbf{x}_t = {\mathbf{u}'}_t^T\mathbf{x}_t = {\mathbf{u}''}_t^T\mathbf{x}_t \leq 0$ is valid. $\mathbf{u}'$

remains bounded, if $\mathbf{u}''$ remains bounded. We have the same problem as in the beginning, but within a reduced subspace. Either case i) or ii) applies. After a finite number of these recursions the dimension of the respective subspace will be one. Then only case i) can apply and, hence, $||\mathbf{u}||$ will stay bounded.

With $a = ||\mathbf{u}_{max}||$, we finally obtain

$$\frac{||\mathbf{c}_t - \mathbf{c}||}{R} \leq \min\left(\frac{a}{t}, \frac{1}{\sqrt{t}}\right). \quad (3)$$

Figure 1 shows the convergence of the algorithm for 5.000 points in 100 dimensions, (a) homogeneously distributed on a ball of unit radius and (b) uniformly distributed on the vertices of a unit hypercube. Two points were prespecified to lie on opposite sites, respectively, to know the exact solution for the precision measurement. Usually a is smaller in the scenario (a) than in (b). Computer experiments and intuition, but not yet a proof, suggest that $a \leq \sqrt{2d}$ can be assumed as a very conservative bound. Since everything happens in a subspace of at most $(n-1)$ dimensions, we obtain $a \leq \min(\sqrt{2d}, \sqrt{2n})$. Usually a is much smaller, for the scenario (a) sometimes even smaller than 1.

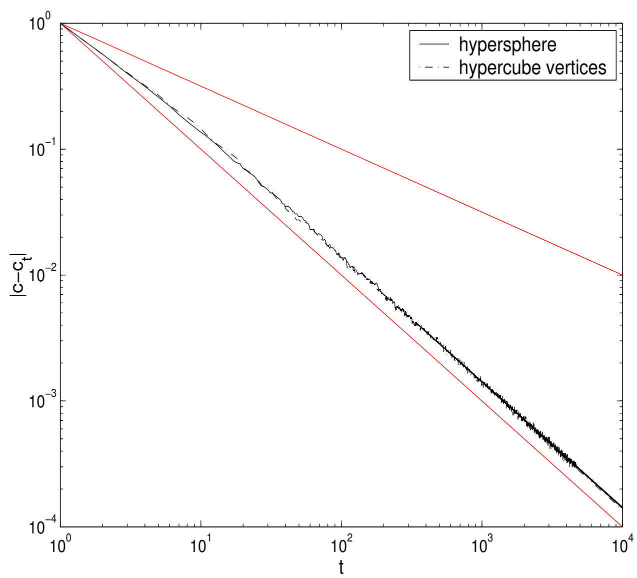

Fig. 1. Double-logarithmic plot of the deviation from the exact SEB center with the number of iteration steps ($n = 5.000$, $d = 100$). This deviation decreases to zero along a line of slope -1, which demonstrates the $\mathcal{O}(t^{-1})$ convergence we have proven. The line of slope $-1/2$ gives the old upper bound.

III. A New Step Size

Now we know that always $||\mathbf{c}_t - \mathbf{c}||/R \leq \Delta_t$ with $\Delta_t = \min\left(a/t, 1/\sqrt{t}\right)$ is valid. With this improved bound we can improve the step size of algorithm (1). The worst case at step t is $||\mathbf{c}_t - \mathbf{c}||/R = \Delta_t$ together with $(\mathbf{x}_t - \mathbf{c})(\mathbf{c}_t - \mathbf{c}) = 0$. The step size which then minimizes $(\mathbf{c}_{t+1} - \mathbf{c})^2 - (\mathbf{c}_t - \mathbf{c})^2$ is given by $1/(1 + \Delta_t^{-2})$. As long as $t \leq a^2$, the better bound is $\Delta_t = 1/\sqrt{t}$ with the step size $1/(1+t)$. As soon as $t > a^2$, however, the a/t bound is better and we should take the step size $1/(1 + t^2/a^2)$.

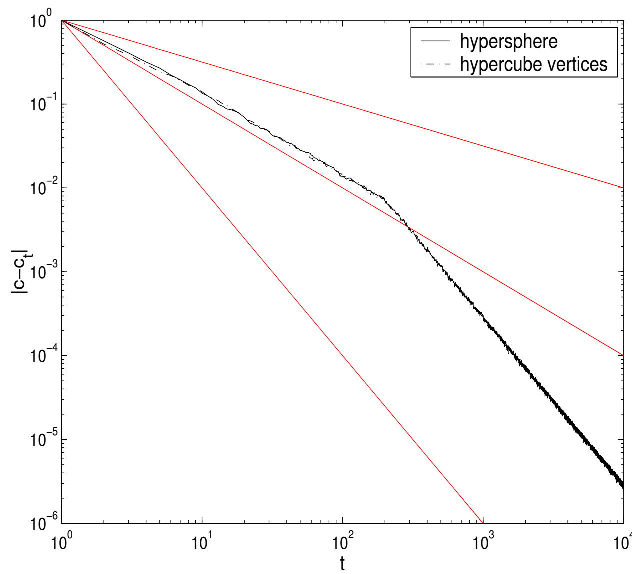

Fig. 2. Double-logarithmic plot of the deviation from the exact SEB center with the number of iteration steps if the improved step size is used ($n = 5.000$, $d = 100$). Compared to Fig. 1 We obtain a drastically improved convergence. It seems that one can expect a $\mathcal{O}(t^{-2})$ decrease.

Figure 2 shows that this modified step size scheduling indeed leads to an improved convergence of the algorithm. We took the same scenario as in Fig. 1 and $a = \min(\sqrt{2d}, \sqrt{2n})$. In the double-logarithmic plot the deviation of $\mathbf{c}_t$ from the exact SEB center decreases along a line of slope -2. It seems that instead of $\mathcal{O}(t^{-1})$ we now can expect even a $\mathcal{O}(t^{-2})$ convergence. After 10^4 steps we are two orders of magnitude more precise than in Fig. 1.

IV. Discussion

Combined with core sets [1], [3] we obtain the bound $\mathcal{O}\left(\frac{nd}{\epsilon} + \min(a, 1/\epsilon)\frac{d}{\epsilon^3}\right)$. Obviously, this is advantageous only for $n \geq \epsilon^{-2}$. With a bound on a we can apply the improved step size scheduling. The next step would be to prove the observed $\min(b/t^2, a/t, 1/\sqrt{t})$ convergence for this scheduling. With this bound one could improve the step size scheduling even further and would again get a better bound for a further step size improvement. The extension of Badoiu's and Clarkson's algorithm and our convergence analysis to smallest enclosing balls around balls (SEBB) is straightforward.

References

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