# Acceleration of Descent-based Optimization Algorithms via Carathéodory’s Theorem

## Abstract

We propose a new technique to accelerate algorithms based on Gradient Descent using Carathéodory’s Theorem. In the case of the standard Gradient Descent algorithm, we analyse the theoretical convergence of the approach under convexity assumptions and empirically display its ameliorations. As a core contribution, we then present an application of the acceleration technique to Block Coordinate Descent methods. Experimental comparisons on least squares regression with a LASSO regularisation term show remarkably improved performance on LASSO than the ADAM and SAG algorithms.

## 1 Introduction

A common problem in machine learning tasks is the optimization

$$\arg \min_\theta E[L_\theta(X,Y)],$$

where $L_\theta$ is a generic loss function and the expectation is taken with respect to the joint distribution of $(X,Y)$; e.g. $L_\theta(x,y) = (x^T \theta - y)^2 + \lambda |\theta|_1$ for LASSO. In practice, the distribution of $(X,Y)$ is not known and one approximates it with the empirical measure $\mu = \frac{1}{N} \sum_{i=1}^N \delta_{(x_i,y_i)}$ built from $N$ samples $(x_i,y_i)$ of the pair $(X,Y)$. That is, one minimizes the so-called empirical risk

$$\theta^* := \arg \min_\theta E[L_\theta(Z)] = \frac{1}{N} \sum_{i=1}^N L_\theta(x_i,y_i).$$ (1)

where $Z$ denotes the discrete random variable that takes the values $z_i = (x_i,y_i)$ with equal probability. If $L$ is smooth with bounded derivatives and convex, standard gradient descent (GD),

$$\theta_{j+1} - \theta_j = -\frac{\gamma}{N} \sum_{i=1}^N \nabla_\theta L_\theta(x_i,y_i) \bigg|_{\theta=\theta_j}$$ (2)

converges if the learning rate $\gamma$ is appropriately chosen, $\lim_{j \to \infty} \theta_j = \theta^*$, see [1]. However, for large scale problems when the number of samples $N$ is huge, the evaluation of the gradient in (2) in every iteration step is prohibitive. Arguably the most popular approach to address this are so-called stochastic gradient descent (SGD) algorithms, where the gradient is approximated by selecting at each iteration step $j$ a subset of the $N$ points at random.

## Contribution and outline

We propose an alternative to SGD, based on classic results of Carathéodory and Tchakaloff [2]. Instead of approximating the empirical measure $\mu$ that is supported on $N$ atoms by subsampling, we replace $\mu$ (resp. $Z$) at certain steps in the GD iteration with a carefully...
constructed probability measure $\hat{\mu}$ (resp. $\hat{Z}$) that is supported on a very small subset of the original $N$ atoms but matches certain statistical functions of the empirical measure $\mu$ (resp. $Z$). In general, such approaches to simplify measures are known as quadrature and cubature formulas but for the special case of discrete measures this is also known as recombination problem and efficient algorithms are nowadays available to solve the recombination problem. Although it can be relatively costly to carry out the recombination at a given step, in return the gradient is perfectly matched at this step and the expectation can be computed as a sum over $n$ weighted points rather than $N \gg n$ uniformly weighted points. We balance this tradeoff by combining two techniques, namely (i) using an approximation to the Hessian to derive a control statistic that tells use when to carry out the recombination, (ii) using Block coordinate descent (BCD) to carry out the reduction only for $n = 2$ coordinates of the gradient, which makes recombination step cheap. Section 2 introduces the theoretical background on recombination, Section 3 provides the main theoretical results and a first application of (i) to logistic regression; Section 4 then adds technique (ii) and benchmarks the result Carathéodory BCD (CaBCD) against classic SGD algorithms SAG and ADAM. The proofs of the technical results are in the Appendix.

Related work. Solving the minimization problem via (S)GD has a long history and is a research topic that is still rapidly evolving; we refer to [11] for a general overview. Similarly, the recombination problem for discrete measures has a long history, see [6]. While algorithms to construct the reduced measure by solving a constrained linear system have been known for a long time [6], more recently more efficient algorithms have been developed [7, 8, 9, 10]. Concretely, we use the recent randomized Algorithm [10] since it has shown better performance when $n$ is “low” and $N$ is considerable big, i.e. the setting of this work. However, we emphasize that the main ideas are independent of the concrete recombination algorithm used, in return, any advance on recombination algorithms can be used for our CaBCD.

2 The Recombination Problem

We now recall a classic result which shows that for any discrete random variable that can take $N$ different values, there exists another discrete random variable that only takes values in a subset of $n + 1$ of the original $N$ points that has the same statistics as defined by $n$ functions $f_1, \ldots, f_n$.

Theorem 1 (Carathéodory [11]). Given a set of $N > n + 1$ points in $\mathbb{R}^n$ and a point $z$ that lies in the convex hull of these $N$ points, $z$ can be expressed as a convex combination of maximum $n + 1$ points.

As is well-known, this implies Tchakaloff’s Theorem [2] for the special case of discrete measures: given $n$ functions $f_1, \ldots, f_n : \mathcal{X} \to \mathbb{R}^n$ define $F : \mathcal{X} \to \mathbb{R}^n$ as $F(z) := (f_1(z), \ldots, f_n(z))$. Now given a discrete probability measure $\mu$ on $\mathcal{X}$ that is supported on $N$ atoms $z_1, \ldots, z_N \in \mathcal{X}$, it follows that $\mathbb{E}_{Z \sim \mu}[F(Z)] = \sum_{i=1}^{N} F(z_i) \mu(z_i)$. Since this finite sum defines a point within the convex hull of the set of $N$ points $z := (F(z_i))_{i=1}^{N}$, it follows by Carathéodory’s Theorem that this point can be equivalently expressed as a convex combination of a subset $\hat{Z}$ of $z$ comprising at most $n + 1$ points. As first shown by Tchakaloff, this shows that Theorem 1 implies the following recombination result.

Theorem 2 (Tchakaloff [2]). Let $Z$ be a discrete random variables that can take $N$ values $\{z_1, \ldots, z_N\}$. For any set $\{f_1, \ldots, f_n\}$ of $n$ real-valued functions there exists a random variable $\hat{Z}$ such that $\mathbb{E}[f_i(Z)] = \mathbb{E}[f_i(\hat{Z})]$ for every $i = 1, \ldots, n$.

and $\hat{Z}$ only takes values in a subset of $\{z_1, \ldots, z_N\}$ of cardinality at most $n + 1$.

Tchakaloff [2] showed a more general version for continuous random variable, but for us the above result for the discrete setting is sufficient. In our context of the optimization problem (1), we will apply it with $Z = (X, Y)$ denoting a pair consisting of observations $X$ and labels $Y$.

Algorithms. The above derivation already implies an algorithm to calculate $\hat{Z}$, by finding the subset $\hat{z}$ that solves $N - n - 1$ times a constrained linear system, see [6] for details. More recently, algorithms have been devised that exploit a divide and conquer strategy which reduce the complexity of the needed calculations drastically, but they all require $O((Nn + \log(N/n)n^4)$ [7,9] resp. $O((Nn + \log(N/n)n^3)$ [8] where for the latter the question of numerical stability is less clear. Throughout, we use Algorithm 2 from [10] that construct $\hat{\mu}$ by a geometric greedy sampling which is advantageous when $N \gg n$.
which is the regime we care most about in this work. However, the ideas below are independent of
the choice of the concrete reduction algorithm.

3 Carathéodory Gradient Descent

Given a dataset \( \{(x_i, y_i) : i = 1, \ldots, N\} \) consisting of \( N \) observations \( x_i \) with labels \( y_i \), we denote with \( Z \) the discrete random variable that takes the value \( z = (x_i, y_i) \) with probability \( \frac{1}{N} \). That is, the empirical risk (1) at \( \theta \) equals \( \mathbb{E}[L_\theta(Z)] \). Further, denote with \( G(\theta, z) := \nabla_\theta L_\theta(z) \in \mathbb{R}^n \) the gradient at \( \theta \) and with \( H(\theta, z) := \nabla_\theta^2 L_\theta(z) \) the Hessian. With this notation, the usual GD iteration reads as

\[
\theta_{j+1} := \theta_j - \gamma \mathbb{E}[G(\theta_j, Z)].
\]

and converges under assumption which we recall below to the minimum \( \theta^* \) as given in (1). However, in every step \( j \) the evaluation of the sum \( \mathbb{E}[G(\theta_j, Z)] = \frac{1}{N} \sum_{i=1}^N G(\theta_j, (x_i, y_i)) \) is costly. Below we use Theorem 2 to derive a similar iteration \( (\hat{\theta}_j) \), that also converges to \( \theta^* \), which however avoids the evaluation of \( \mathbb{E}[G(\theta_j, Z)] \) at most of the steps.

The first recombination. Initialize \( \theta_0 \in \mathbb{R}^n \) as before in (S)GD, but before the first step, apply Theorem 2 to \( Z \) and the \( n \) coordinate functions of the gradient \( z \mapsto G(\theta_0, z) \) to produce a discrete random variable \( \hat{Z}_0 \). Now define

\[
\hat{\theta}_1 := \theta_0 - \gamma \mathbb{E}[G(\theta_0, \hat{Z}_0)].
\]

Since by construction, \( \mathbb{E}[G(\theta_0, Z)] = \mathbb{E}[G(\theta_0, \hat{Z}_0)] \), it follows that \( \hat{\theta}_1 = \theta_1 \). In general \( \mathbb{E}[G(\hat{\theta}_1, Z)] \neq \mathbb{E}[G(\hat{\theta}_1, \hat{Z}_0)] \) but we expect \( \mathbb{E}[G(\hat{\theta}_1, \hat{Z}_0)] \) to be a good approximation of \( \mathbb{E}[G(\hat{\theta}_1, Z)] \) for reasonable choices of \( \gamma \). Hence, we continue to iterate

\[
\hat{\theta}_{j+1} := \hat{\theta}_j - \gamma \mathbb{E}[G(\hat{\theta}_j, \hat{Z}_0)].
\]

until the first time \( \tau_1 \) a control statistic tells us that the gradient error has become too big.

A control statistic. Let \( L \) be convex, twice differentiable, and its gradient to be Lipschitz, we show in the appendix that a natural choice for control statistic is the quantity

\[
\Delta_{j,0} := \mathbb{E}[G(\theta_0, \hat{Z}_0)] : (\hat{\theta}_j - \theta_0) + \frac{c}{2} \| \hat{\theta}_j - \theta_0 \|^2.
\]

(4)

where \( c \) is such that \( v^\top H(\theta, z)v \leq c \) for every \( v \in \mathbb{R}^n \); the existence of such a \( c \) is justified by the assumptions on \( L \). More precisely, \( \Delta_{j,0} < \Delta_{j-1,0} \) guarantees that the loss function \( L \) continues to decrease. Hence, we follow the iteration (3) until \( \Delta_{j,0} < \Delta_{j-1,0} \), that is until step \( \tau_1 := \inf \{ j > 0 : \Delta_{j,0} < \Delta_{j-1,0} \} \), where we fix \( \Delta_{0,0} := 0 \).

Gradient descent by recombination. At time \( \tau_1 \) we then simply update \( \hat{Z}_0 \) to \( \hat{Z}_1 \) so that the gradients are matched at the point \( \hat{\theta}_{\tau_1-1} \), that is \( \hat{Z}_1 \) is such that \( \mathbb{E}[G(\hat{\theta}_{\tau_1-1}, Z)] = \mathbb{E}[G(\hat{\theta}_{\tau_1-1}, \hat{Z}_1)] \), and then we continue as before. To sum up, we set \( \tau_0 := 0, \Delta_{0,0} = 0, \) and construct \( \hat{Z}_0 \) such that \( \mathbb{E}[G(\theta_0, Z)] = \mathbb{E}[G(\theta_0, \hat{Z}_0)] \). We then update, for \( j \geq 0 \),

\[
\hat{\theta}_{j+1} := \hat{\theta}_j - \gamma \mathbb{E}[G(\hat{\theta}_j, \hat{Z}_0)]
\]

as long as \( \Delta_{j,0} < \Delta_{j-1,0} \).

where \( \Delta_{j,0} := \mathbb{E}[G(\hat{\theta}_{\tau_j}, \hat{Z}_0)] : (\hat{\theta}_j - \theta_0) + \frac{c}{2} \| \hat{\theta}_j - \theta_0 \|^2 \). At time \( \tau_1 := \inf \{ j > 0 : \Delta_{j,0} < \Delta_{j-1,0} \} \) we compute \( \hat{Z}_1 \) such that

\[
\mathbb{E}[G(\hat{\theta}_{\tau_1-1}, Z)] = \mathbb{E}[G(\hat{\theta}_{\tau_1-1}, \hat{Z}_1)]
\]

and update for \( j \geq \tau_1 - 1 \)

\[
\hat{\theta}_{j+1} := \hat{\theta}_j - \gamma \mathbb{E}[G(\hat{\theta}_j, \hat{Z}_1)],
\]

as long as \( \Delta_{j,1} < \Delta_{j-1,1} \), where \( \Delta_{j,1} := \mathbb{E}[G(\hat{\theta}_{\tau_j}, \hat{Z}_1)] : (\hat{\theta}_j - \hat{\theta}_{\tau_{j-1}}) + \frac{c}{2} \| \hat{\theta}_j - \hat{\theta}_{\tau_{j-1}} \|^2 \) and \( \Delta_{\tau_1-1,1} = 0 \). At time \( \tau_2 := \inf \{ j > \tau_1 : \Delta_{j,1} \geq \Delta_{j-1,1} \} \) we compute \( \hat{Z}_2 \) such that \( \mathbb{E}[G(\hat{\theta}_{\tau_2-1}, Z)] = \mathbb{E}[G(\hat{\theta}_{\tau_2-1}, \hat{Z}_2)] \), etc.
Carathéodory Gradient descent (CaGD). The above is already the main structure of our first algorithm. However, we add three modifications: (i) stop as soon as the gradient or the value of the loss function is smaller than a given \( \varepsilon \) since this means we are already close enough to the minimum; (ii) bound the number of iterations between two recombinations by a constant, that is \( \tau_{k+1} - \tau_k \leq \text{it\_max\_Ca} \) to avoid pathological cases, see Appendix 6 and the proof of Theorem 3 for more details; (iii) allow to match a general oracle direction \( D_j \) at step \( j \). In Algorithm 1 we write \( D_j(\{ \theta \}, Z) \) to express its dependencies on the data \( Z \) and the sequence \( \{ \theta \} \) computed up to the step \( j \), although it could depend also on the loss function \( L \), in particular it could depend on its derivatives \( G, H, \) etc. The choice \( D_j = -\mathbb{E}[G(\hat{\theta}_j, Z)] \) is the most relevant for this section, but in Section 4 we will use more involved choices (such as momentum strategies). This leads to Algorithm 1 as stated below. Theorem 3 shows that it converges whenever we match oracle directions, and Theorem 4 gives the convergence rate for the choice \( D_j = -\mathbb{E}[G(\hat{\theta}_j, Z)] \).

**Algorithm 1 Carathéodory Acceleration**

1: Initialize \( \hat{\theta}_0 \)
2: \( j \leftarrow 1, k \leftarrow 0 \) \quad \triangleright j \) counts steps, \( k+1 \) the number of recombinations
3: \( \tau_k \leftarrow 0 \) \quad \triangleright \( \tau_k \) is the step we made with the \((k+1)\)th recombination
4: \( \Delta_{0,0} \leftarrow 0 \)
5: \( \text{Grad}_0 \leftarrow \mathbb{E}[G(\hat{\theta}_0, Z)] \)
6: \( \textbf{while} (\| \text{Grad}_k \| > \varepsilon_1 \text{ or } |L(\hat{\theta}_k, Z)| > \varepsilon_2) \text{ and } j \leq \text{it\_max} \textbf{do} \)
7: \( \text{Compute } \hat{Z}_k \text{ such that } \mathbb{E}[D_{\hat{\theta}_k}(\{ \hat{\theta} \}, \hat{Z}_k)] = \mathbb{E}[D_{\hat{\theta}_k}(\{ \hat{\theta} \}, Z)] \quad \triangleright \text{Solve a RP to reduce } Z \text{ to } \hat{Z}_k \)
8: \( \textbf{while } \Delta_{j,k} \leq \Delta_{j-1,k} \text{ and } j - \tau_k \leq \text{it\_max\_Ca} \textbf{ do} \)
9: \( \hat{\theta}_j \leftarrow \hat{\theta}_{j-1} + \gamma \mathbb{E}[D_{\hat{\theta}_{j-1}}(\{ \hat{\theta} \}, \hat{Z}_j)] \)
10: \( \Delta_{j,k} \leftarrow \text{Grad}_{\hat{\theta}_k}(\hat{\theta}_j - \hat{\theta}_{\tau_k}) + \frac{\gamma}{2} \| \hat{\theta}_j - \hat{\theta}_{\tau_k} \|^2 \)
11: \( j \leftarrow j + 1 \)
12: \( \textbf{end while} \)
13: \( \textbf{if } j - \tau_k \neq \text{it\_max\_Ca} \textbf{ then} \)
14: \( \tau_k, j \leftarrow j - 1 \)
15: \( \textbf{else} \)
16: \( \tau_k, j \leftarrow j \)
17: \( \textbf{end if} \)
18: \( \text{Grad}_{\hat{\theta}_{\tau_k}} \leftarrow \mathbb{E}[G(\hat{\theta}_{\tau_k}, Z)], \quad \Delta_{\tau_k,k} \leftarrow 0 \)
19: \( k \leftarrow k + 1 \)
20: \( \textbf{end while and return } j, \hat{\theta}_j \)

**Theorem 3.** Let \( L_0 \) be convex, twice differentiable in \( \theta \) and its gradient \( G \) be Lipschitz. If the quantities \( \{ \theta \} \) defined as

\[ \theta_j - \theta_{j-1} = \gamma \mathbb{E}[D_{\hat{\theta}_{j-1}}(\{ \hat{\theta} \}, Z)] \]

converge to the minimum \( \theta^* \), i.e. \( \lim_{j \rightarrow \infty} \theta_j = \theta^* \), then also the sequence of \( \{ \hat{\theta} \} \) computed via Algorithm 1 converges to \( \theta^* \), \( \lim_{j \rightarrow \infty} \hat{\theta}_j = \theta^* \).

Theorem 3 can be easily extended to the case where the learning rate \( \gamma \) is not fixed.

**Theorem 4.** Let \( L_0 \) be convex, twice differentiable in \( \theta \) and its gradient \( G \) be Lipschitz. Then if \( D_j = -G(\hat{\theta}_j, Z) \), Algorithm 1 converges to \( \theta^* \), and its convergence rate is

\[ |L(\hat{\theta}_j) - L(\theta^*)| \leq \frac{1}{2\gamma} \frac{\| \hat{\theta}_0 - \theta^* \|^2}{j}, \quad (5) \]

where \( j \) is the number of iterations, and \( J \) is the number of times the reduced measure is used (as per Algorithm 1 we can conservatively bound \( J < \text{it\_max\_Ca} \)).

**Variations.** First note, that the bound in Equation (5) assumes that when we use the reduced measures the objective function does not decrease, thanks to Equation (4). Secondly, note that the constant \( c \) in Equation (4) in practice might be unknown and expensive to compute, and even when known it might be quite conservative. In our implementation we use an approximation of the second
derivative, so that $\Delta_{j,k}$ in Equation (4) becomes

$$\Delta_{j,k} := \mathbb{E}(G(\hat{\theta}_j, \mathbb{Z}_k)) \cdot (\hat{\theta}_j - \bar{\theta}_k) + \frac{1}{2} (\hat{\theta}_j - \bar{\theta}_k)^T \cdot \mathcal{H}_k \cdot (\hat{\theta}_j - \bar{\theta}_k), \quad j \geq \tau_k,$$

where $\mathcal{H}_k := [\mathbb{E}(G(\hat{\theta}_j, \mathbb{Z}_k)) - \mathbb{E}(G(\hat{\theta}_j, \mathbb{Z}))]^T \cdot [1/(\hat{\theta}_k - \bar{\theta}_{k-1})]$ and $[1/x]$ denotes a vector whose elements are the reciprocals of those in $[x]$. To compute the terms $\Delta_{j,k}$ we modify Algorithm 1 doing two iterations where $\mathbb{E}(G(\theta, Z))$ is computed – see Algorithms 2 in the next section or Algorithm 3 in the Appendix for the cases discussed in Section 4. We do not discuss how to optimally select $\gamma$, since there exists a broad literature about the optimal selection of the step $\gamma$, which is not core to this work.

### 3.1 A first comparison of CaGD and GD: logistic regression

Comparing the complexity of Algorithm 1 to standard GD is not trivial, since the number of recomputations of the reduced measure is not known a-priori. However, the intuition is that for large $N$ the cost for carrying out recombinations becomes negligible compared to a full evaluation of the sum. In this Section, we present three numerical experiments to test this intuition. We use classic logistic regression for binary classification (it is easy to check that the assumptions of Theorem 4 are fulfilled in this case, see [12, Exercise 8.3]) and use synthetic data which allows to study various regimes of $N$. We run both GD and CaGD until either the norm of the gradient is less than $1 \times 10^{-3}$, or the number of iterations is greater than $1 \times 10^4$.

Figure 1: Synthetic data generated by sampling from (i) a uniform distribution, classified with a sine function, (ii) a shifted exponential, classified as 1 in the third octant, and 0 otherwise, (iii) a uniform distribution, classified with a logistic model with parameter $(-5; 2)$. The top row shows samples with $N = 5,000$. The bottom row shows the ratios of running times between standard GD and CaGD, as a function of the step size for various sample sizes $N$.

Figure 1 indicates that the improvement in the running time is up to 35-fold, and generally the improvement increases as the number of points becomes larger and when the step is small; recall that the step of the GD must be small enough for the algorithm to converge to a minimum. Further, CaGD reaches lower gradient values than GD, because in Algorithm 1 the “true” gradient $\mathbb{E}(G(\theta, Z))$ is only computed at the step 18 but we modify $\hat{\theta}_j$ at step 9. In these instances we have employed $\text{it}_{\text{max}} = \max \{10/\text{step}, 10^4\}$.

### 4 Carathéodory Block Coordinate Descent

The computational bottleneck of CaGD is in step 9 where a recombination algorithm is run to compute $\mathbb{Z}$. For example, using a deterministic algorithm the complexity of this step is $O(Nn + n^3 \log(N/n))$

\footnote{All experiments have been run on a MacBook Pro, CPU: i7-7920HQ, RAM: 16 GB, 2133 MHz LPDDR3.}
whether or not we can afford to compute the full gradient: if we can, then the GS rule is expected where BCD appears to be more effective (we analyse this problem in the next subsection). A well-known procedure is the Modified Gauss-Southwell (GS) rule, defined as
\[ \theta_{j+1} = \theta_j - \gamma \nabla E[B_j](\theta, Z), \]
where \( B_j \) denotes a set of coordinates, and \( G^{B_j}(\theta) \) denotes the function that returns the gradient for the coordinate in \( B_j \), and sets the other coordinates equal to 0. If the problem we want to solve is of the form
\[ \min_{\theta} L_\theta = \min_{\theta} (f(\theta) + g(\theta)), \]
where \( f \) is convex and \( g \) is (block) separable, i.e. \( g = \sum_{m=1}^b g_m : \mathbb{R}^{n_m} \to \mathbb{R} \) and \( \sum_m n_m \leq n, b \leq n \), then BCD converges to a minimum and the rate of convergence is that of standard GD, up to some constants depending on different factors, e.g. the number of directions we update at any step, the strategy to choose such directions, the separability of the objective function \( g \); see [13, 14] for a detailed study. Notable examples of optimisation problems with functions \((f, g)\) abiding by the previous condition are least-squares problems with LASSO regularisation \([14, 15, 16]\), which is where BCD appears to be more effective (we analyse this problem in the next subsection). A well-studied aspect of BCD is its parallelisation \([16, 17, 18]\), which can be studied in terms of the spectral radius of the data \([18]\). In the following, we focus on the simplest application of BCD to highlight the improvements that are due to CaBCD, rather than BCD optimizations.

Choosing the descent directions. An important aspect is how to select the directions for the descent \([19]\), and how many directions: cyclic versus acyclic, deterministic versus random, or via the Gauss-Southwell (GS) rule (discussed below). The main differences amongst these options hinge on whether or not we can afford to compute the full gradient: if we can, then the GS rule is expected to be the best strategy; if we cannot, then the random strategy seems to perform better than the deterministic cyclic ones. Quite importantly, these strategies can be implemented in parallel, exploiting multiple processors. We focus on the following two acyclic strategies, whose respective procedures are presented in Algorithm 2 and Algorithm 3:

- **Modified Gauss-Southwell (GS).** If we can compute the full gradient, then we can select directions where the gradient is larger in absolute value. A rule of thumb is to consider only a percentage of the “total” value of the gradient (in our experiments we consider 75%):
  
  (a) Let us call \( \nabla_S \) the vector with the absolute value of the directions of the GD sorted in descending order, i.e. \( |\nabla L(\psi_s^{(r)})| \geq |\nabla L(\psi_s^{(r)})| \) if \( r \leq q \);
  
  (b) We consider the directions where the gradient is bigger in absolute value, namely the first \( \hat{n} \) components of \( \nabla_S \), where \( \hat{n} := \inf \left\{ q : \sum_{r=1}^q |\nabla L(\psi_s^{(r)})| > \text{Percentage} \right\} \);
  
  (c) We split the \( \hat{n} \) directions in \( b = \hat{n}/s \) blocks of size \( s \), respecting the ordering.

- **Random.** If we cannot compute the full gradient, then we can group the directions into \( n/s \) blocks of size \( s \), and perform BCD over the blocks. In the experiments of the next subsection we randomly group half of the directions per iteration.

In \([15, 16]\), the selection of the coordinate step \( \gamma \) is given as sub-optimisation problem, which for simplicity we skip in the following. Furthermore, \([15]\) shows that a momentum application to the single block of directions can improve the rate of convergence: knowing the convexity of the function to be optimised, it is possible to obtain an accelerated method with an improved rate of convergence \( O(1/j^2) \), where \( j \) is the number of iterations, in the same spirit of \([20]\). Our implementation has been done in a synchronous and parallel manner (cf. discussion above).
We consider a least-squares problem with LASSO regularisation, i.e.

\[
\min_{\theta} \frac{1}{N} \sum_{i=1}^{N} (x_i^T \theta - y_i)^2 + \lambda |\theta|_1.
\]

Datasets. We have used the following datasets: (i) Household power consumption \[21\] which consists of \(N = 2075259\) data points. We want to predict the Voltage given active power, reactive power, intensity. We have raised to the tensor power of \(5\), scaled the data, and applied PCA to reduce the number of features to 7. (ii) 3D Road Network \[22\] which consists of \(N = 434874\) data points. We want to predict the Altitude, given Longitude, Latitude. We have raised to the tensor power of \(5\), scaled the data, and applied PCA to reduce the number of features to 7. (iii) NYC Taxi Trip Duration \[23\] which consists of \(N = 1458644\) data points. We want to predict the trip duration,
given pickup time/longitude/latitude and dropoff longitude/latitude. We consider only the time of the feature pickup_datetime, without the date. We have raised to the tensor power of 3, scaled the data, and applied PCA to reduce the number of features to 8. In this case we have considered as outliers the points such that $y_i > 10000$, this amounts to 2123 points (0.14%). In all datasets the variance reduction by PCA is greater than 99.9%, which results from eliminating the symmetries introduced via the tensor power. Throughout we have chosen $\lambda = 0.01$ for the Lasso regularisation.

**Benchmarks.** We have implemented the CaBCD with Gauss-Southwell rule (CaBCD GS), CaBCD with a momentum strategy and the GS rule (CaBCD mom GS), and with the Random rule (CaBCD mom random). For the momentum strategy we have chosen the momentum parameter $\beta = 0.9$. As benchmarks we used ADAM [24] and SAG [25] with standard mini-batches with size of 256. The learning rate for the CaBCD Algorithms and ADAM is $1 \times 10^{-3}$, as suggested in [24]; we picked $\text{it}_{\text{max,Ca}} = 1/\gamma/10 = 100$. SAG was more sensitive to the step size and we decreased it to $1 \times 10^{-6}$ to preserve the convergence. BCD was not competitive to any of the above so we omit it for brevity.

**Discussion of results.** The results are summarized in Figure 2. Let us make some observations:

(i) the size of the blocks $s$ has been fixed to two. Experimentally we have observed that if the block’s size is between 2 and 5 the reduced measure is used for longer, i.e. the algorithm does more steps with the reduced measure, thus decreasing the runtime; (ii) in the case of CaBCD algorithms we count 1 iteration when a full gradient has been computed, while we count the size of the blocks $s$ (i) the size of the blocks $s$ has been fixed to two. Experimentally we have observed that if the block’s size is between 2 and 5 the reduced measure is used for longer, i.e. the algorithm does more steps with the reduced measure, thus decreasing the runtime; (ii) in the case of CaBCD algorithms we count 1 iteration when a full gradient has been computed, while we count the size of the blocks $s$ (i) the size of the blocks $s$ has been fixed to two. 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Experimentally we have observed that if the block’s size is between 2 and 5 the reduced measure is used for longer, i.e. the algorithm does more steps with the reduced measure, thus decreasing the runtime; (ii) in the case of CaBCD algorithms we count 1 iteration when a full gradient has been computed, while we count the size of the blocks $s$ (i) the size of the blocks $s$ has been Fixed for any iteration done with the reduced measure (if the size of the block is $s$ the reduced measure has support on $s + 1$ points, see Theorem [1]); (iii) note that the CaBCD algorithms for the first two iterations are “slower”, which is due to the fact that we compute $\mathcal{H}$, i.e. the approximation of the second derivative; (iv) using the GS rule, the parallelisation of the code has often no effect because the directions to optimise belong to only one block. The code can be found at [Github Link].

### 5 Summary

We introduced a new approach to accelerate GD methods that falls outside the usual SGD paradigm. In contrast to SGD approaches, we perform recombination steps in which a small, weighted summary of the data is constructed and subsequently the gradient is only computed under this simpler summary until a control statistic tells us to recombine again. To deal with high-dimensional optimization problems we then leveraged the strengths of this approach with BCD. Our experiments show that this can lead to remarkable improvements compared to competitive baselines such as ADAM and SAG. Many extensions are possible, e.g. studying the behaviour under non-convex losses, combination with Quasi-Newton methods, or developing BCD rules that are specialized to CaBCD. Independently of these, any improvement for recombination algorithms can lead to a further speed up of CaGD/BCD.
Acknowledgements and Disclosure of Funding

The authors want to thank The Alan Turing Institute and the University of Oxford for the financial support given. FC is supported by The Alan Turing Institute, TU/C/000021, under the EPSRC Grant No. EP/N510129/1. HO is supported by the EPSRC grant “Datasig” [EP/S026347/1], The Alan Turing Institute, and the Oxford-Man Institute.

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Algorithm 1, we can conservatively bound $J < \infty$, the number of times the reduced measure is used (as per Theorem 1). Let $L_\theta$ be convex, twice differentiable in $\theta$ and its gradient $G$ be Lipschitz. If the quantities $\{\theta_j\}$ defined as

\[
\theta_j - \theta_{j-1} = \gamma E[D_{j-1}(\{\theta\}, Z)]
\]

converge to the minimum $\theta^*$, i.e. $\lim_{j \to \infty} \theta_j = \theta^*$, then also the sequence of $\{\hat{\theta}\}$ computed via Algorithm converges to $\theta^*$, $\lim_{j \to \infty} \hat{\theta}_j = \theta^*$.

Proof. Thanks to the hypothesis there exists $c$ s.t.

\[
E[L(\hat{\theta}, Z)] = E[L(\hat{\theta}_0, Z)] + E[G(\hat{\theta}_0, Z) \cdot (\hat{\theta} - \hat{\theta}_0)] + \frac{1}{2} (\hat{\theta} - \hat{\theta}_0)^T \cdot E[H(\hat{\theta}, Z)] \cdot (\hat{\theta} - \hat{\theta}_0)
\]

where $\tau$ is a convex combination of $\hat{\theta}_j$ and $\hat{\theta}_0$. It is now easy to see that we have a condition to check to rebuild the measure: we update the measure after $\tau_1$ steps, where

\[
\tau_1 := \inf \{ j \geq 1 : \Delta_j,0 \geq \Delta_{j-1},0 \}
\]

\[
\Delta_j,0 := E[G(\hat{\theta}_0, Z)] \cdot (\hat{\theta}_j - \hat{\theta}_0) + \frac{C}{2} \| \hat{\theta}_j - \hat{\theta}_0 \|^2,
\]

note that $\Delta_0,0 = 0$. We have that $\{\Delta_0,0, \Delta_1,0, \ldots\}$ is a negative decreasing sequence and therefore

\[
E[L(\hat{\theta}_{q-1}, Z)] \leq E[L(\hat{\theta}_0, Z)].
\]

In particular, note that $\Delta_{j,0} \leq 0$, since $\hat{\theta}_1 = \theta_1 := \hat{\theta}_0 + \gamma E[D_0(\{\theta\}, Z)]$, thanks to Theorem 1 and the definition of $Z_0$, therefore $\tau_1 \geq 2$. $\tau_1 - 1 = 1$ means that the reduced r.v. $Z_0$ computed has been useless, i.e. we have done only one step with the reduced measure that we could have done directly using $E[D_0(\{\theta\}, Z)]$ without computing the reduced measure.

The reasoning can be easily generalized: we can define for $k > 1$, $j \geq \tau_{k-1}$

\[
\Delta_j,k := E[G(\hat{\theta}_{q-1}, Z)] \cdot (\hat{\theta}_j - \hat{\theta}_{q-1}) + \frac{C}{2} \| \hat{\theta}_j - \hat{\theta}_{q-1} \|^2
\]

\[
\tau_k := \inf \{ j \geq \tau_{k-1} : \Delta_j,k \geq \Delta_{j-1,k} \},
\]

where note that $\Delta_{q-1,k} = 0$. The proof of the convergence follows since if $\tau_k - \tau_{k-1} = 2$ we follow the directions $D_j(\{\theta\}, Z)$ which converge for hypothesis, if $\tau_k - \tau_{k-1} \geq 2$ the value of $L$ decreases,

\[
E[L(\hat{\theta}_{q-1}, Z)] \leq E[L(\hat{\theta}_{q-1}, Z)].
\]

Moreover, to avoid pathological cases, e.g. $\Delta_{1,k} < \Delta_{2,k} < \ldots < \gamma - a$, $a > 0$ in which cases $L(\hat{\theta}_j, Z)$ cannot decrease “enough”, we impose a number of maximum iterations that the Algorithm can do with the reduced measure.

Theorem 4. Let $L_\theta$ be convex, twice differentiable in $\theta$ and its gradient $G$ be Lipschitz. Then if $D_j = -G(\hat{\theta}_j, Z)$, Algorithm converges to $\theta^*$, and its convergence rate is

\[
|L(\hat{\theta}_j) - L(\theta^*)| \leq \frac{1}{2\gamma} \frac{\| \hat{\theta}_0 - \theta^* \|^2}{j},
\]

where $j$ is the number of iterations, and $J$ is the number of times the reduced measure is used (as per Algorithm we can conservatively bound $J < \text{it}_{\text{max}} \cdot Ca$).

Proof. The convergence is a simple application of Theorem 3. We can show that Algorithm does not reduce the order of convergence of the standard GD. Let us call $\hat{\theta}_i$ the sequence of weights obtained by Algorithm in chronological order

\[
\{\hat{\theta}_0, \hat{\theta}_1, \ldots, \hat{\theta}_{q-1}, \hat{\theta}_q, \ldots, \hat{\theta}_{2q-1}, \hat{\theta}_{2q}, \ldots\},
\]
where for $k > 1$ ($k = 1$) $\tau_k$ indicates the number of times we use the reduced measure computed using $\theta_{t_k - 1}^{-1}$ ($\theta_0$). Moreover, let us suppose that for any step $j$ we have a map $S$ that tells us the step where we had recomputed the measure the last time, so $S(j) = \max\{k : \tau_k \leq j\}$. Let us recall that if the function is convex we have that

$$L(\theta) \leq L(\theta^*) + \nabla L(\theta)(\theta - \theta^*)$$

where $\theta^*$ is the minimum, moreover if $\{\theta_i\}$ are the weights computed using the standard GD, we can say that

$$L(\theta_{i+1}) \leq L(\theta_i) - \frac{1}{2} \gamma \|\nabla L(\theta_i)\|^2,$$

if $\gamma$ respects the usual conditions, i.e. $\gamma \leq \frac{1}{\text{Lip}(L)}$, where $\text{Lip}(L)$ indicates the Lipschitz constant of $L$. We know that $L(\hat{\theta}_j) \leq L(\hat{\theta}_{S(j) - 1}) + \Delta_j, S(j)$ therefore, since $\Delta_j, S(j) \leq 0$

$$L(\hat{\theta}_j) \leq L(\hat{\theta}_{S(j)}) \leq L(\theta^*) + \nabla L(\hat{\theta}_{S(j) - 1})(\hat{\theta}_{S(j) - 1} - \theta^*) - \frac{1}{2} \gamma \|\nabla L(\hat{\theta}_{S(j) - 1})\|^2,$$

which rearranging the terms and using that $\hat{\theta}_{S(j)} - \hat{\theta}_{S(j) - 1} = \mathbb{E}[G(\hat{\theta}_{S(j) - 1}, Z)] = \mathbb{E}[G(\hat{\theta}_{S(j) - 1}, \hat{Z}_{S(j) - 1})]$ becomes

$$L(\hat{\theta}_j) - L(\theta^*) \leq \frac{1}{2 \gamma} \left( \|\hat{\theta}_{S(j) - 1} - \theta^*\|^2 - \|\hat{\theta}_{S(j)} - \theta^*\|^2 \right).$$

Thus,

$$\sum_{i=1}^{j} L(\hat{\theta}_i) - L(\theta^*) \leq \frac{1}{2 \gamma} \sum_{i=1}^{j} \left( \|\hat{\theta}_{S(j) - 1} - \theta^*\|^2 - \|\hat{\theta}_{S(j)} - \theta^*\|^2 \right)$$

$$= \frac{1}{2 \gamma} \sum_{i=1}^{j} \left( \tau_k - \tau_{k-1} \right) \left( \|\hat{\theta}_{S(j) - 1} - \theta^*\|^2 - \|\hat{\theta}_{S(j)} - \theta^*\|^2 \right)$$

$$\leq \frac{1}{2 \gamma} \max \{ \tau_k - \tau_{k-1} \} \sum_{k: \tau_k \leq j} \left( \|\hat{\theta}_{S(j) - 1} - \theta^*\|^2 - \|\hat{\theta}_{S(j)} - \theta^*\|^2 \right)$$

$$\leq \frac{1}{2 \gamma} \max \{ \tau_k - \tau_{k-1} \} \|\hat{\theta}_0 - \theta^*\|^2.$$

Therefore it holds that

$$L(\hat{\theta}_j) - L(\theta^*) \leq \frac{1}{j} \sum_{i=1}^{j} L(\hat{\theta}_i) - L(\theta^*) \leq \frac{1}{2 \gamma} \max \{ \tau_k - \tau_{k-1} \} \frac{\|\hat{\theta}_j - \theta^*\|^2}{j}.$$

\[\square\]

### 7 More experiments

In Section 3.1 and 4.1 we have given a detailed comparison between Standard Algorithms in the literature and the acceleration techniques via the Caratheodory’s Theorem\[1\]. In this section we want to present the different paths done by the sequence $\{\hat{\theta}\}$ computed with the acceleration both in the case of the CaGD both the CaBCD.

![Figure 3](image_url)

Figure 3: Paths generated by CaGD (Theorem\[4\]) and GD, for the experiments of Figure\[1\] same order.
Figure 4: Samples of paths followed by the GD and the CaBCD over the parameters space. The dotted blue paths and the continuous orange paths converge to the same desired minimum, though via different paths. The CaBCD, between change of directions, uses only a subset of the total points $N$, namely $s + 1$ if the size of the selected block is $s$. This Figure has been obtained using the data of Figure 1(center) in the multi-dimensional case.

8 Algorithm - Random rule

In the definition of the Random rule, we assume that we cannot compute the full gradient, therefore the condition to terminate now depends “only” on the loss function $L$.

Algorithm 3 Carathéodory BCD - Random

1: Initialize $\hat{\theta}_0$
2: $j \leftarrow 1$, $k \leftarrow 0$  
\hspace{.7cm} $\triangleright \hspace{.2cm} j$ counts steps, $\sum_{l=0}^{k} b_j$ counts the number of recombinations
3: \hspace{1cm} while $|L(\theta_{j-1}, Z)| > \varepsilon$ and $j \leq \text{it}_{\text{max}}$ do
4: \hspace{2cm} Build $b$ blocks $B(m, k)$, $m = 1, \ldots, b$ using the Random rule
5: \hspace{2cm} for $m = 1, \ldots, b$, in parallel do
6: \hspace{3cm} $\nabla_j G_m(\hat{\theta}_{j-1}, Z)$
7: \hspace{3cm} $\hat{\theta}_j(m) \leftarrow \nabla_j G(m) \hat{\theta}_{j-1} + \gamma \mathbb{E}[D_j^m(\theta_j, Z)]$
8: \hspace{3cm} $\nabla_j \tau_k \leftarrow j$
9: \hspace{2cm} $j_m \leftarrow j + 1$, $\Delta_{m-k} \leftarrow 0$  
\hspace{.7cm} $\triangleright \hspace{.2cm} j_m - 1 = \tau_k$
10: \hspace{2cm} Hessian$_k^m \leftarrow \left[\nabla_j G_m - \nabla_j G_{m-1}\right]^\top \left[1/(\hat{\theta}_k^m - \hat{\theta}_q^m)\right]$
11: \hspace{2cm} Compute $Z_k^m$ s.t. $\mathbb{E}[D_k^m(\theta_j^k, Z)] = \mathbb{E}[D_k^m(\theta_j^k, Z)]$
12: \hspace{2cm} while $\Delta_{m-k} \leq \Delta_{m-1,k}$ and $j_m - \tau_k \leq \text{it}_{\text{max Ca}}$ do
13: \hspace{3cm} $\hat{\theta}_j(m) \leftarrow \hat{\theta}_j(m) + \mathbb{E}[D_{j_m-1}(\theta_j, Z_k^m)]$
14: \hspace{3cm} $\delta_{j_m,k} \leftarrow \hat{\theta}_j(m) - \hat{\theta}_q^m$
15: \hspace{3cm} $\Delta_{m-k} \leftarrow \text{Grad}^m_{\text{Ca}} \cdot \delta_{j_m,k}^m + \left(\delta_{j_m,k}^m\right)^\top \cdot \text{Hessian}^m_{\text{Ca}} \cdot \delta_{j_m,k}^m$
16: \hspace{3cm} $j_m \leftarrow j_m + 1$
17: \hspace{2cm} end while
18: \hspace{2cm} if $j_m - \tau_k \neq \text{it}_{\text{max Ca}}$ then
19: \hspace{3cm} $\tau_{m,k+1} \leftarrow j_m - 1$  
\hspace{.7cm} $\triangleright \hspace{.2cm} \tau_{m,k+1} - \tau_k$ steps in $(k+1)$th recombination relative to $B(m, j)$
20: \hspace{3cm} else
21: \hspace{3cm} $\tau_{m,k+1} \leftarrow j_m$
22: \hspace{3cm} end if
23: \hspace{2cm} end for
24: \hspace{2cm} $j \leftarrow j + \sum_{k} \tau_{m,k+1}$
25: \hspace{2cm} $\hat{\theta}_j(m) \leftarrow \hat{\theta}_j(m)$, $\forall m$  
\hspace{.7cm} $\triangleright \hspace{.2cm}$ synchronise and update $\hat{\theta}$
27: \[ k \leftarrow k + 1, \quad j \leftarrow j + 1 \]
28: \textbf{end while and return} \( j, \hat{\theta}_j \)

We write \( .(m) \) in place of \((B(m,k))\) to indicate the restriction to the components of \( . \) in the blocks \( B(m,k) \).