Super-efficiency of automatic differentiation for functions defined as a minimum

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Abstract

In min-min optimization or max-min optimization, one has to compute the gradient of a function defined as a minimum. In most cases, the minimum has no closed-form, and an approximation is obtained via an iterative algorithm. There are two usual ways of estimating the gradient of the function: using either an *analytic* formula obtained by assuming exactness of the approximation, or *automatic* differentiation through the algorithm. In this paper, we study the asymptotic error made by these estimators as a function of the optimization error. We find that the error of the automatic estimator is close to the square of the error of the analytic estimator, reflecting a *super-efficiency* phenomenon. The convergence of the automatic estimator greatly depends on the convergence of the Jacobian of the algorithm. We analyze it for gradient descent and stochastic gradient descent and derive convergence rates for the estimators in these cases. Our analysis is backed by numerical experiments on toy problems and on Wasserstein barycenter computation. Finally, we discuss the computational complexity of these estimators and give practical guidelines to chose between them.

1. Introduction

In machine learning, many objective functions are expressed as the minimum of another function: functions ℓ defined as

$$\ell(x) = \min_{z \in \mathbb{R}^m} \mathcal{L}(z, x), \tag{1}$$

where $\mathcal{L} : \mathbb{R}^m \times \mathbb{R}^n \to \mathbb{R}$. Such formulation arises for instance in dictionary learning, where x is a dictionary, z a sparse code, and $\mathcal{L}$ is the Lasso cost (Mairal et al., 2010). In this case, ℓ measures the ability of the dictionary x to encode the input data. Another example is the computation of the Wassertein barycenter of distributions in optimal transport (Agueh and Carlier, 2011): x represents the barycenter, ℓ is the sum of distances to x, and the distances themselves are defined by minimizing the transport cost. In the field of optimization, formulation (1) is also encountered as a smoothing technique, for instance in reweighted least-squares (Daubechies et al., 2010) where $\mathcal{L}$ is smooth but not ℓ. In game theory, such problems naturally appear in two-players maximin games(von Neumann, 1928), with applications for instance to generative adversarial nets (Goodfellow et al., 2014). In this setting, ℓ should be maximized.

A key point to optimize ℓ – either maximize or minimize – is usually to compute the gradient of ℓ, $g^*(x) \triangleq \nabla \ell(x)$. If the minimizer $z^*(x) = \arg\min_z \mathcal{L}(z, x)$ is available, the first order optimality conditions impose that $\nabla_1 \mathcal{L}(z^*(x), x) = 0$ and the gradient is given by

$$g^*(x) = \nabla_2 \mathcal{L}(z^*(x), x) \quad . \tag{2}$$

However, in most cases the minimizer $z^*(x)$ of the function is not available in closed-form. It is approximated via an iterative algorithm, which produces a sequence of iterates $z_t(x)$. There are then three ways to estimate $g^*(x)$:

The **analytic** estimator corresponds to plugging the approximation $z_t(x)$ in (2)

$$g_t^1(x) \triangleq \nabla_2 \mathcal{L}(z_t(x), x) \quad . \tag{3}$$

The **automatic** estimator is $g_t^2(x) \triangleq \frac{d}{dx}\left[\mathcal{L}(z_t(x), x)\right]$, where the derivative is computed with respect to $z_t(x)$ as well. The chain rule gives

$$g_t^2(x) = \nabla_2 \mathcal{L}(z_t(x), x) + \frac{\partial z_t}{\partial x} \nabla_1 \mathcal{L}(z_t(x), x) \quad . \tag{4}$$

This expression can be computed efficiently using automatic differentiation (Baydin et al., 2018), in most cases at a cost similar to that of computing $z_t(x)$.

If $\nabla_{11}^2 \mathcal{L}(z^*(x), x)$ is invertible, the implicit function theorem gives $\frac{\partial z^*(x)}{\partial x} = \mathcal{J}(z^*(x), x)$ where

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$\mathcal{J}(z,x) \triangleq -\nabla^2_{21}\mathcal{L}(z,x)\left[\nabla^2_{11}\mathcal{L}(z,x)\right]^{-1}$. The **implicit** estimator is

$$g^3_t(x) \triangleq \nabla_2\mathcal{L}(z_t(x),x) + \mathcal{J}(z_t(x),x)\nabla_1\mathcal{L}(z_t(x),x). \quad (5)$$

This estimator can be more costly to compute than the previous ones, as a $m \times m$ linear system has to be solved.

These estimates have been proposed and used by different communities. The analytic one corresponds to alternate optimization of $\mathcal{L}$, where one updates x while considering that z is fixed. It is used for instance in dictionary learning (Olshausen and Field, 1997; Mairal et al., 2010) or in optimal transport (Feydy et al., 2019). The second is common in the deep learning community as a way to differentiate through optimization problems (Gregor and Le Cun, 2010). Recently, it has been used as a way to accelerate convolutional dictionary learning (Tolooshams et al., 2018). It has also been used to differentiate through the Sinkhorn algorithm in optimal transport applications (Boursier and Perchet, 2019; Genevay et al., 2018). It integrates smoothly in a machine learning framework, with dedicated libraries (Abadi et al., 2016; Paszke et al., 2019). The third one is found in bi-level optimization, for instance for hyperparameter optimization (Bengio, 2000). It is also the cornerstone of the use of convex optimization as layers in neural networks (Agrawal et al., 2019).

Contribution In this article, we want to answer the following question: *which one of these estimators is the best?* The central result, presented in Sec.2, is the following convergence speed, when $\mathcal{L}$ is differentiable and under mild regularity hypothesis (Prop.2.1, 2.2 and 2.3)

$$\begin{aligned}
|g^1_t(x) - g^*(x)| &= O\left(|z_t(x) - z^*(x)|\right) \quad , \\
|g^2_t(x) - g^*(x)| &= o\left(|z_t(x) - z^*(x)|\right) \quad , \\
|g^3_t(x) - g^*(x)| &= O\left(|z_t(x) - z^*(x)|^2\right) \quad .
\end{aligned}$$

This is a super-efficiency phenomenon for the automatic estimator, illustrated in Fig.1 on a toy example. As our analysis reveals, the bound on g^2 depends on the convergence speed of the Jacobian of z_t, which itself depends on the optimization algorithm used to produce z_t. In Sec.3, we build on the work of Gilbert (1992) and give accurate bounds on the convergence of the Jacobian for gradient descent (Prop.3.2) and stochastic gradient descent (Prop.3.5 and 3.6) in the strongly convex case. We then study a simple case of non-strongly convex problem (Prop.3.9). To the best of our knowledge, these bounds are novel. This analysis allows us to refine the convergence rates of the gradient estimators. In Sec.4, we start by recalling and extending the consequence of using wrong gradients in an optimization algorithm (Prop.4.1 and 4.2). Then, since each gradient estimator comes at a different cost, we put the convergence bounds developed in the paper in perspective with a complexity analysis. This leads to practical and principled guidelines about which estimator should be used in which case. Finally, we provide numerical illustrations of the aforementioned results in Sec.5.

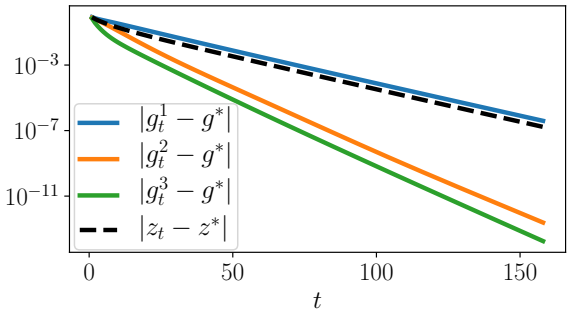

Figure 1. Convergence of the gradient estimators. $\mathcal{L}$ is strongly convex, x is a random point and $z_t(x)$ corresponds to t iterations of gradient descent. As t increases, z_t goes to z^* at a linear rate. g^1_t converges at the same rate while g^2_t and g^3_t are twice as fast.

Notation The ℓ^2 norm of $z \in \mathbb{R}^m$ is $|z| = \sqrt{\sum_{i=1}^m z_i^2}$. The operator norm of $M \in \mathbb{R}^{m\times n}$ is $\|M\| = \sup_{|z|=1}|Mz|$ and the Frobenius norm is $\|M\|_F = \sqrt{\sum_{i,j} M_{ij}^2}$. The vector of size n full of $1'$s is $\mathbb{1}_n$. The Euclidean scalar product is $\langle\cdot,\cdot\rangle$. The derivative of $\mathcal{L}$ with respect to its first variable (resp. second variable) is $\nabla_1\mathcal{L} \in \mathbb{R}^m$ (resp $\nabla_2\mathcal{L} \in \mathbb{R}^n$). The second derivative of $\mathcal{L}$ with respect to its variable $i = 1,2$ and variable $j = 1,2$ is denoted $\nabla^2_{ij}\mathcal{L}$. For sequences $x_t, y_t \in \mathbb{R}$ indexed by t, we denote $x_t = O(y_t)$ when there exists $C > 0$ such that $|x_t| \leq C|y_t|$ for t large enough. We denote $x_t = o(y_t)$ when $\frac{x_t}{y_t} \to 0$ when $t \to +\infty$. Finally, we use the Landau notation Θ to report computation and memory complexity magnitude. The proofs are only sketched in the article, full proofs are deferred to appendix.

2. Convergence speed of gradient estimates

We consider a compact set $K = K_z \times K_x \subset \mathbb{R}^m \times \mathbb{R}^n$. We make the following assumptions on $\mathcal{L}$.

H1: $\mathcal{L}$ is twice differentiable over K with second derivatives $\nabla^2_{21}\mathcal{L}$ and $\nabla^2_{11}\mathcal{L}$ respectively L_{21} and L_{11}-Lipschitz.

H2: For all $x \in K_x$, $z \to \mathcal{L}(z,x)$ has a unique minimizer $z^*(x) \in \text{int}(K_z)$. The mapping $z^*(x)$ is differentiable, with Jacobian $J^*(x) \in \mathbb{R}^{n\times m}$.

H1 implies that $\nabla_1\mathcal{L}$ and $\nabla_2\mathcal{L}$ are Lipschitz, with constants L_1 and L_2. The Jacobian of z_t at $x \in K_x$ is $J_t \triangleq \frac{\partial z_t(x)}{\partial x} \in \mathbb{R}^{n\times m}$. For the rest of the section, we consider a point $x \in K_x$, and we denote $g^* = g^*(x)$, $z^* = z(x)$ and $z_t = z_t(x)$.

2.1. Analytic estimator g^1

The analytic estimator (3) approximates g^* *as well as* z_t approximates z^* by definition of the L_2-smoothness.

Proposition 2.1 (Convergence of the analytic estimator)**.** *The analytic estimator verifies* $|g_t^1 - g^*| \leq L_2|z_t - z^*|$.

2.2. Automatic estimator g^2

The automatic estimator (4) can be written as

$$g^2 = g^* + R(J_t)(z_t - z^*) + R_{21} + J_t R_{11} \tag{6}$$

where

$$R_{21} \triangleq \nabla_2\mathcal{L}(z_t, x) - \nabla_2\mathcal{L}(z^*, x) - \nabla^2_{21}\mathcal{L}(z^*, x)(z_t - z^*)$$
$$R_{11} \triangleq \nabla_1\mathcal{L}(z_t, x) - \nabla^2_{11}\mathcal{L}(z^*, x)(z_t - z^*) \ .$$

are Taylor's rests and

$$R(J) \triangleq J\nabla^2_{11}\mathcal{L}(z^*, x) + \nabla^2_{21}\mathcal{L}(z^*, x) \ . \tag{7}$$

The implicit function theorem states that $R(J^*) = 0$. Importantly, in a non strongly-convex setting where $\nabla^2_{11}\mathcal{L}(z^*, x)$ is not invertible, it might happen that $R(J_t)$ goes to 0 even though J_t does not converge to J^*. **H1** implies a quadratic bound on the rests

$$|R_{21}| \leq \frac{L_{21}}{2}|z_t - z^*|^2 \text{ and } |R_{11}| \leq \frac{L_{11}}{2}|z_t - z^*|^2. \tag{8}$$

We assume that J_t is bounded $\|J_t\| \leq L_J$. This holds when J_t converges, which is the subject of Sec.3. The triangle inequality in Equation 6 gives:

Proposition 2.2 (Convergence of the automatic estimator)**.** *We define*

$$L \triangleq L_{21} + L_J L_{11} \tag{9}$$

Then $|g_t^2 - g^*| \leq \|R(J_t)\||z_t - z^*| + \frac{L}{2}|z_t - z^*|^2$.

This proposition shows that the rate of convergence of g^2 depends on the speed of convergence of $R(J_t)$. For instance, if $R(J_t)$ goes to 0, we have

$$g_t^2 - g^* = o(|z_t - z^*|) \ .$$

Unfortunately, it might happen that, even though z_t goes to z^*, $R(J_t)$ does not go to 0 since differentiation is not a continuous operation. In Sec.3, we refine this convergence rate by analyzing the convergence speed of the Jacobian in different settings.

2.3. Implicit estimator g^3

The implicit estimator (5) is well defined provided that $\nabla^2_{11}\mathcal{L}$ is invertible. We obtain convergence bounds by making a Lipschitz assumption on $\mathcal{J}(z, x) = -\nabla^2_{21}\mathcal{L}(z, x)\left[\nabla^2_{11}\mathcal{L}(z, x)\right]^{-1}$.

Proposition 2.3. *[Convergence of the implicit estimator] Assume that $\mathcal{J}$ is $L_\mathcal{J}$-Lipschitz with respect to its first argument, and that $\|\mathcal{J}_t\| \leq L_J$. Then, for L as defined in (9),*

$$|g_t^3 - g^*| \leq (\frac{L}{2} + L_\mathcal{J} L_1)|z_t - z^*|^2 \ . \tag{10}$$

Sketch of proof. The proof is similar to that of Prop.2.2, using $\|R(\mathcal{J}(z_t, x))\| \leq L_1 L_\mathcal{J}|z_t - z^*|$. □

Therefore this estimator converges twice as fast as g^1, and at least as fast as g^2. Just like g^1 this estimator does not need to store the past iterates in memory, since it is a function of z_t and x. However, it is usually much more costly to compute.

2.4. Link with bi-level optimization

Bi-level optimization appears in a variety of machine-learning problems, such as hyperparameter optimization (Pedregosa, 2016) or supervised dictionary learning (Mairal et al., 2012). It considers problems of the form

$$\min_{x\in\mathbb{R}^n} \ell'(x) \triangleq \mathcal{L}'\left(z^*(x), x\right) \text{ s.t. } z^*(x) \in \arg\min_{z\in\mathbb{R}^m} \mathcal{L}(z, x), \tag{11}$$

where $\mathcal{L}' : \mathbb{R}^m \times \mathbb{R}^n \to \mathbb{R}$ is another objective function. The setting of our paper is a special instance of bi-level optimization where $\mathcal{L}' = \mathcal{L}$. The gradient of ℓ' is

$$g'^* = \nabla\ell'(x) = \nabla_2\mathcal{L}'(z^*, x) + J^*\nabla_1\mathcal{L}'(z^*, x) \ .$$

When $z_t(x)$ is a sequence of approximate minimizers of $\mathcal{L}$, gradient estimates can be defined as

$$g'^1 = \nabla_2\mathcal{L}'(z_t(x), x),$$
$$g'^2 = \nabla_2\mathcal{L}'(z_t(x), x) + J_t\nabla_1\mathcal{L}'(z_t(x), x),$$
$$g'^3 = \nabla_2\mathcal{L}'(z_t(x), x) + \mathcal{J}(z_t(x), x)\nabla_1\mathcal{L}'(z_t(x), x).$$

Here, $\nabla_1\mathcal{L}'(z^*, x) \neq 0$, since z^* does not minimize $\mathcal{L}'$. Hence, g'^1 does not estimate g'^*. Moreover, in general,

$$\nabla^2_{21}\mathcal{L}'(z^*, x) + J^*\nabla^2_{11}\mathcal{L}'(z^*, x) \neq 0.$$

Therefore, there is no cancellation to allow super-efficiency of g^2 and g^3 and we only obtain linear rates

$$g'^2 - g^* = O(|z_t - z^*|), \ \ g'^3 - g^* = O(|z_t - z^*|) \ .$$

3. Convergence speed of the Jacobian

In order to get a better understanding of the convergence properties of the gradient estimators – in particular g^2 – we analyze it in different settings. A large portion of the analysis is devoted to the convergence of $R(J_t)$ to 0, since it does not directly follow from the convergence of z_t. In most cases, we show convergence of J_t to J^*, and use

$$\|R(J_t)\| \leq L_1\|J_t - J^*\| \tag{12}$$

in the bound of Prop.2.2.

3.1. Contractive setting

When z_t are the iterates of a fixed point iteration with a contractive mapping, we recall the following result due to Gilbert (1992).

Proposition 3.1 (Convergence speed of the Jacobian)**.** *Assume that z_t is produced by a fixed point iteration*

$$z_{t+1} = \Phi\left(z_t, x\right),$$

where $\Phi : K_z \times K_x \to K_z$ is differentiable. We suppose that Φ is contractive: there exists $\kappa < 1$ such that for all $(z, z', x) \in K_z \times K_z \times K_x$, $|\Phi(z, x) - \Phi(z', x)| \leq \kappa |z - z'|$. Under mild regularity conditions on Φ:

- *z_t converges to a differentiable function z^* such that $z^* = \Phi(z^*, x)$, with Jacobian J^*.*
- *$|z_t - z^*| = O(\kappa^t)$ and $\|J_t - J^*\| = O(t\kappa^t)$*

3.2. Gradient descent in the strongly convex case

We consider the gradient descent iterations produced by the mapping $\Phi(z, x) = z - \rho \nabla_1 \mathcal{L}(z, x)$, with a step-size $\rho \leq 1/L_1$. We assume that $\mathcal{L}$ is μ-strongly convex with respect to z, i.e. $\nabla^2_{11}\mathcal{L} \succeq \mu \mathrm{Id}$ for all $z \in K_z, x \in K_x$. In this setting, Φ satisfies the hypothesis of Prop.3.1, and we obtain precise bounds.

Proposition 3.2. *[Convergence speed of the Jacobian of gradient descent in a strongly convex setting] Let z_t produced by the recursion $z_{t+1} = z_t - \rho \nabla_1 \mathcal{L}(z_t, x)$ with $\rho \leq 1/L_1$ and $\kappa \triangleq 1 - \rho\mu$. We have $|z_t - z^*| \leq \kappa^t |z_0 - z^*|$ and $\|J_t - J^*\| \leq t\kappa^{t-1}\rho L |z_0 - z^*|$ where L is defined in (9).*

Sketch of proof (C.1). We show that $\delta_t = \|J_t - J^*\|$ satisfies the recursive inequality $\delta_{t+1} \leq \kappa\delta_t + \rho L |z_0 - z^*| \kappa^t$. □

As a consequence, Prop. 2.1, 2.2, 2.3 together with Eq. (12) give in this case

$$\begin{aligned}
|g^1 - g^*| &\leq L_2 |z_0 - z^*| \kappa^t, \\
|g^2 - g^*| &\leq (\rho L_1 t + \frac{\kappa}{2}) L |z_0 - z^*|^2 \kappa^{2t-1}, \\
|g^3 - g^*| &\leq (\frac{L}{2} + L_{\mathcal{J}} L_1) |z_0 - z^*|^2 \kappa^{2t} \quad .
\end{aligned} \tag{13}$$

We get the convergence speed $g^2 - g^* = O(t\kappa^{2t})$, which is almost twice better than the rate for g^1. Importantly, the order of magnitude in Prop.3.2 is tight, as it can be seen in the appendix Prop.C.1, where we exhibit a function reaching this upper-bound.

3.3. Stochastic gradient descent in z

We provide an analysis of the convergence of J_t in the stochastic gradient descent setting, assuming once again the μ-strong convexity of $\mathcal{L}$. We suppose that $\mathcal{L}$ is an expectation

$$\mathcal{L}(z, x) = \mathbb{E}_\xi [C(z, x, \xi)] \ ,$$

where ξ is drawn from a distribution d, and C is twice differentiable. Stochastic gradient descent (SGD) with steps ρ_t iterates

$$z_{t+1}(x) = z_t(x) - \rho_t \nabla_1 C\left(z_t(x), x, \xi_{t+1}\right) \text{ where } \xi_{t+1} \sim d \ .$$

In the stochastic setting, Prop.2.2 becomes

Proposition 3.3. *Define*

$$\delta_t = \mathbb{E}\left[\|J_t - J^*\|_F^2\right] \text{ and } d_t = \mathbb{E}\left[|z_t - z^*|^2\right] \ . \tag{14}$$

We have $\mathbb{E}[|g^2 - g^*|] \leq L_1 \sqrt{\delta_t} \sqrt{d_t} + \frac{L}{2} d_t$.

Sketch of proof (C.4). We use Cauchy-Schwarz and the norm inequality $\|\cdot\| \leq \|\cdot\|_F$ to bound $\mathbb{E}\left[\|R(J_t)\| |z_t - z^*|\right]$. □

We begin by deriving a recursive inequality on δ_t, inspired by the analysis techniques of d_t.

Proposition 3.4. *[Bounding inequality for the Jacobian] We assume bounded Hessian noise, in the sense that $\mathbb{E}\left[\|\nabla^2_{11} C(z, x, \xi)\|_F^2\right] \leq \sigma_{11}^2$ and $\mathbb{E}\left[\|\nabla^2_{21} C(z, x, \xi)\|_F^2\right] \leq \sigma_{21}^2$. Let $r = \min(n, m)$, and $B^2 = \sigma_{21}^2 + L_J^2 \sigma_{11}^2$. We have*

$$\delta_{t+1} \leq (1 - 2\rho_t\mu)\delta_t + 2\rho_t \sqrt{r} L \sqrt{d_t} \sqrt{\delta_t} + \rho_t^2 B^2. \tag{15}$$

Sketch of proof (C.5). A standard strong convexity argument gives the bound

$$\delta_{t+1} \leq (1 - 2\rho_t\mu)\delta_t + 2\rho_t \sqrt{r} L \mathbb{E}[\|J_t - J^*\|_F |z_t - z_0|] + \rho_t^2 B^2.$$

The middle term is then bounded using Cauchy-Schwarz inequality. □

Therefore, any convergence bound on d_t provides another convergence bound on δ_t by unrolling Eq. (15). We first analyze the fixed step-size case by using the simple "bounded gradients" hypothesis and bounds on d_t from Moulines and Bach (2011). In this setting, the iterates converge linearly until they reach a threshold caused by gradient variance.

Proposition 3.5. *[SGD with constant step-size] Assume that the gradients have bounded variance $\mathbb{E}_\xi[|\nabla_1 C(z, x, \xi)|^2] \leq \sigma^2$. Assume $\rho_t = \rho < 1/L_1$, and let $\kappa_2 = \sqrt{1 - 2\rho\mu}$ and $\beta = \sqrt{\frac{\sigma^2 \rho}{2\mu}}$. In this setting*

$$\delta_t \leq \left(\kappa_2^t \left(\|J^*\|_F + t\alpha\right) + B_2\right)^2 \ ,$$

where $\alpha = \frac{\rho\sqrt{r}L}{\kappa_2} |z^* - z_0|$ and $B_2 = \frac{\rho\sqrt{r}L\beta}{\kappa_2(1-\kappa_2)} + \frac{\rho B}{(1-\kappa_2)}$.

Sketch of proof (C.6). Moulines and Bach (2011) give $d_t \leq \kappa_2^{2t}|z_0 - z^*|^2 + \beta^2$, which implies $\sqrt{d_t} \leq \kappa_2^t|z_0 - z^*| + \beta$. A bit of work on Eq. (15) then gives

$$\sqrt{\delta_{t+1}} \leq \kappa_2\sqrt{\delta_t} + \rho\kappa_2^t + (1-\kappa_2)B_2$$

Unrolling the recursion gives the proposed bound. □

This bound showcases that the familiar "two-stages" behavior also stands for δ_t: a transient linear decay at rate $(1-2\rho\mu)^t$ in the first iterations, and then convergence to a stationary noise level B_2^2. This bound is not tight enough to provide a good estimate of the noise level in δ_t. Let B_3^2 the limit of the sequence defined by the recursion (15). We find

$$B_3^2 = (1-2\rho\mu)B_3^2 + 2\rho\sqrt{r}L\beta B_3 + \rho^2 B^2,$$

which gives by expanding β

$$B_3 = \sqrt{\rho}\frac{\sqrt{r}L\sigma}{(2\mu)^{\frac{3}{2}}}\left(1 + \sqrt{1 + \frac{4\mu^2 B^2}{rL^2\sigma^2}}\right) .$$

This noise level scales as $\sqrt{\rho}$, which is observed in practice. In this scenario, Prop. 2.1, 2.2 and 2.3 show that $g^1 - g^*$ reaches a noise level proportional to $\sqrt{\rho}$, just like d_t, while both $g^2 - g^*$ and $g^3 - g^*$ reach a noise level proportional to ρ: g^2 and g^3 can estimate g^* to an accuracy that can never be reached by g^1. We now turn to the decreasing step-size case.

Proposition 3.6. *[SGD with decreasing step-size] Assume that $\rho_t = \rho_0 t^{-\alpha}$ with $\alpha \in (0,1)$. Assume a bound on d_t of the form $d_t \leq d^2 t^{-\alpha}$. Then*

$$\delta_t \leq 4\frac{\rho_0 B^2\mu + rL^2d^2}{\mu^2}t^{-\alpha} + o(t^{-\alpha}) .$$

Sketch of proof (C.7). We use (15) to obtain a recursion

$$\delta_{t+1} \leq \left(1 - \mu\rho_0 t^{-\alpha}\right)\delta_t + (B^2\rho_0^2 + \frac{rL^2d^2\rho_0}{\mu})t^{-2\alpha} ,$$

which is then unrolled. □

When $\rho_t \propto t^{-\alpha}$, we have $d_t = O(t^{-\alpha})$ so the assumption $d_t \leq d^2 t^{-\alpha}$ is verified for some d. One could use the precise bounds of (Moulines and Bach, 2011) to obtain non-asymptotic bounds on δ_t as well. The rate $t^{-\alpha}$ in this bound is tight, as we exhibit a function with this rate in the appendix Prop.C.2.

Overall, we recover bounds for δ_t with the same behavior than the bounds for d_t. Pluging them in Prop.3.3 gives the asymptotic behaviors for the gradient estimators.

Proposition 3.7 (Convergence speed of the gradient estimators for SGD with decreasing step)**.** *Assume that $\rho_t = Ct^{-\alpha}$ with $\alpha \in (0,1)$. Then*

$$\mathbb{E}_\xi[|g^1 - g^*|] = O(\sqrt{t^{-\alpha}}),\ \mathbb{E}_\xi[|g^2 - g^*|] = O(t^{-\alpha})$$
$$\mathbb{E}_\xi[|g^3 - g^*|] = O(t^{-\alpha})$$

The super-efficiency of g^2 and g^3 is once again illustrated, as they converge at the same speed as d_t.

3.4. Beyond strong convexity

All the previous results rely critically on the strong convexity of $\mathcal{L}$. A function f with minimizer z^* is p-Łojasiewicz (Attouch and Bolte, 2009) when $\mu(f(z) - f(z^*))^{p-1} \leq \|\nabla f(z)\|^p$ for some $\mu > 0$. Any strongly convex function is 2-Łojasiewicz: the set of p-Łojasiewicz functions for $p \geq 2$ offers a framework beyond strong-convexity that still provides convergence rates on the iterates. The general study of gradient descent on this class of function is out of scope for this paper. We analyze a simple class of p-Łojasiewicz functions, the least mean p-th problem, where

$$\mathcal{L}(z,x) \triangleq \frac{1}{p}\sum_{i=1}^{n}(x_i - [Dz]_i)^p \tag{16}$$

for p an even integer and D is overcomplete ($\text{rank}(D) = n$). In this simple case, $\mathcal{L}(\cdot, x)$ is minimized by cancelling $x - Dz$, and $g^* = (x - Dz^*)^{p-1} = 0$.

In the case of least squares ($p = 2$) we can perfectly describe the behavior of gradient descent, which converges linearly.

Proposition 3.8. *Let z_t the iterates of gradient descent with step $\rho \leq \frac{1}{L_1}$ in (16) with $p = 2$, and $z^* \in \arg\min \mathcal{L}(z,x)$. It holds*

$$g^1 = D(z_t - z^*),\ \ g^2 = D(z_{2t} - z^*)\ \text{ and }\ g^3 = 0.$$

Proof. The iterates verify $z_t - z^* = (I_n - D^\top D)^t(z_0 - z^*)$, and we find $J_t\nabla_1\mathcal{L}(z_t, x) = (I_n - (I_n - D^\top D)^t)(x - Dz_t)$. The result follows. □

The automatic estimator therefore goes exactly twice as fast as the analytic one to g^*, while the implicit estimator is exact. Then, we analyze the case where $p \geq 4$ in a more restrictive setting.

Proposition 3.9. *For $p \geq 4$, we assume $DD^\top = I_n$. Let $\alpha \triangleq \frac{p-1}{p-2}$. We have*

$$|g_t^1| = O(t^{-\alpha}), \quad |g_t^2| = O(t^{-2\alpha}), \quad g_t^3 = 0 .$$

Sketch of proof (C.8). We first show that the residuals $r_t = x - Dz_t$ verify $r_t = \left(\frac{1}{\rho(p-2)t}\right)^{\frac{1}{p-2}}(1 + O(\frac{\log(t)}{t}))$, which

gives the result for g^1. We find $g_t^2 = M_t r_t^{p-1}$ where $M_t = I_n - J_t D^\top$ verifies $M_{t+1} = M_t(I_n - (p-1)\rho \text{diag}(r_t^{p-2}))$. Using the development of r_t and unrolling the recursion concludes the proof. □

For this problem, g^2 is of the order of magnitude of g^1 squared and as $p \to +\infty$, we see that the rate of convergence of g^1 goes to t^{-1}, while the one of g^2 goes to t^{-2}.

4. Consequence on optimization

In this section, we study the impact of using the previous inexact estimators for first order optimization. These estimators nicely fit in the framework of inexact oracles introduced by Devolder et al. (2014).

4.1. Inexact oracle

We assume that ℓ is μ_2-strongly convex and L_2-smooth with minimizer x^*. A (δ, μ, L)-inexact oracle is a couple (ℓ_δ, g_δ) such that $\ell_\delta : \mathbb{R}^m \to \mathbb{R}$ is the inexact value function, $g_\delta : \mathbb{R}^m \to \mathbb{R}^m$ is the inexact gradient and for all x, y

$$\frac{\mu}{2}|x-y|^2 \leq \ell(x) - \ell_\delta(y) - \langle g_\delta(y) | x-y \rangle \leq \frac{L}{2}|x-y|^2 + \delta \ . \tag{17}$$

Devolder et al. (2013) show that if the gradient approximation g^i verifies $|g^*(x) - g^i(x)| \leq \Delta_i$ for all x, then (ℓ, g^i) is a $(\delta_i, \frac{\mu_2}{2}, 2L_2)$-inexact oracle, with

$$\delta_i = \Delta_i^2 (\frac{1}{\mu_2} + \frac{1}{2L_2}) \ . \tag{18}$$

We consider the optimization of ℓ with inexact gradient descent: starting from $x_0 \in \mathbb{R}^n$, it iterates

$$x_{q+1} = x_q - \eta g_t^i(x_q) \ , \tag{19}$$

with $\eta = \frac{1}{2L_2}$, a fixed t and $i = 1, 2$ or 3.

Proposition 4.1. *[Devolder et al. 2013, Theorem 4] The iterates x_q with estimate g^i verify*

$$\ell(x_q) - \ell(x^*) \leq 2L_2 (1 - \frac{\mu_2}{4L_2})^q |x_0 - x^*|^2 + \delta_i$$

with δ_i defined in (18).

As q goes to infinity, the error made on $\ell(x^*)$ tends towards $\delta_i = O(|g_t^i - g^*|^2)$. Thus, a more precise gradient estimate achieves lower optimization error. This illustrates the importance of using gradients estimates with an error Δ_i as small as possible.

We now consider stochastic optimization for our problem, with loss ℓ defined as

$$\ell(x) = \mathbb{E}_\upsilon[h(x, \upsilon)] \text{ with } h(x, \upsilon) = \min_z H(z, x, \upsilon) \ .$$

Table 1. Computational and memory costs for a quadratic loss $\mathcal{L}$. Here $c \geq 1$ is to the relative cost of automatic differentiation.

Estimator	Computational cost	Memory cost
g_t^1	$\Theta(mnt)$	$\Theta(m)$
g_t^2	$\Theta(cmnt)$	$\Theta(mt)$
g_t^3	$\Theta(mnt + m^3 + m^2 n))$	$\Theta(m(m+n))$

Stochastic gradient descent with constant step-size $\eta \leq \frac{1}{2L_2}$ and inexact gradients iterates

$$x_{q+1} = x_q - \eta g_t^i(x_q, \upsilon_{q+1}) \ ,$$

where $g_t^i(x_q, \upsilon_{q+1})$ is computed by an approximate minimization of $z \to H(z, x_q, \upsilon_{q+1})$.

Proposition 4.2. *We assume that H is μ_2-strongly convex, L_2-smooth and verifies*

$$\mathbb{E}[|\nabla h(x, \upsilon) - \nabla \ell(x)|^2] \leq \sigma^2.$$

The iterates x_q of SGD with approximate gradient g^i and step-size η verify

$$\mathbb{E}|x_q - x^*|^2 \leq (1 - \frac{\eta\mu_2}{2})^q |x_0 - x^*| + \frac{2\eta}{\mu_2}\sigma^2 + \frac{4}{\mu_2}\delta_i$$

with $\delta_i = \Delta_i^2 (\frac{1}{\mu_2} + \frac{1}{2L_2} + 2\eta)$.

The proof is deferred to Appendix D. In this case, it is pointless to achieve an estimation error on the gradient Δ_i smaller than some fraction of the gradient variance σ^2.

As a final note, these results extend without difficulty to the problem of maximizing ℓ, by considering gradient ascent or stochastic gradient ascent.

4.2. Time and memory complexity

In the following, we put our results in perspective with a computational and memory complexity analysis, allowing us to provide practical guidelines for optimization of ℓ.

Computational complexity of the estimators The cost of computing the estimators depends on the cost function $\mathcal{L}$. We give a complexity analysis in the least squares case (16) which is summarized in Table 1. In this case, computing the gradient $\nabla_1 \mathcal{L}$ takes $\Theta(mn)$ operations, therefore the cost of computing z_t with gradient descent is $\Theta(mnt)$. Computing g_t^1 comes at the same price. The estimator g^2 requires a reverse pass on the computational graph, which costs a factor $c \geq 1$ of the forward computational cost: the final cost is $\Theta(cmn)$. Griewank and Walther (2008) showed that typically $c \in [2, 3]$. A popular technique to alleviate the cost of back-propagation is to only backpropagate through the last k iterations of the algorithm, which it equivalent to assuming $J_{t-k} = 0$ (Shaban et al., 2019). This technique trades gradient accuracy for time and memory complexity.

While it is beyond the scope of this paper, one could analyse this method using the tools developed in Sec.3, where the recursive inequalities in the proof of Prop.3.2 or in Prop.3.4 should be unrolled k times. Finally, computing g^3 requires a costly $\Theta(m^2n)$ Hessian computation, and a $\Theta(m^3)$ linear system inversion. The final cost is $\Theta(mnt + m^3 + m^2n)$. The linear scaling of g_t^1 and g_t^2 is highlighted in Fig.A.3.

Linear convergence: a case for the analytic estimator In the time it takes to compute g_t^2, one can at the same cost compute g_{ct}^1. If z_t converges linearly at rate κ^t, Prop.2.1 shows that $g_{ct}^1 - g^* = O(\kappa^{ct})$, while Prop.2.2 gives, at best, $g_t^2 - g^* = O(\kappa^{2t})$: g_{ct}^1 is a better estimator of g^* than g_t^2, provided that $c \geq 2$. In the quadratic case, we even have $g_t^2 = g_{2t}^1$. Further, computing g^2 might requires additional memory: g_{ct}^1 should be preferred over g_t^2 in this setting. However, our analysis is only asymptotic, and other effects might come into play to tip the balance in favor of g^2.

As it appears clearly in Table 1, choosing g^1 over g^3 depends on t: when $mnt \gg m^3 + m^2n$, the additional cost of computing g^3 is negligible, and it should be preferred since it is more accurate. This is however a rare situation in a large scale setting.

Sublinear convergence We have provided two settings where z_t converges sub-linearly. In the stochastic gradient descent case with a fixed step-size, one can benefit from using g^2 over g^1, since it allows to reach an accuracy that can never be reached by g^1. With a decreasing step-size, reaching $|g_t^1 - g^*| \leq \varepsilon$ requires $\Theta(\varepsilon^{-2/\alpha})$ iterations, while reaching $|g_t^2 - g^*| \leq \varepsilon$ only takes $\Theta(\varepsilon^{-1/\alpha})$ iterations. For ε small enough, we have $c\varepsilon^{-1/\alpha} < \varepsilon^{-2/\alpha}$: it is always beneficial to use g^2 if memory capacity allows it.

The story is similar for the simple non-strongly convex problem studied in Sec.3.4: because of the slow convergence of the algorithms, g_t^2 is *much* closer to g^* than g_{ct}^1. Although our analysis was carried in the simple least mean p-th problem, we conjecture it could be extended to the more general setting of p-Łojasiewicz functions (Attouch and Bolte, 2009).

Memory footprint of the estimators Another critical aspect when choosing between these estimators is their memory footprint. While g^1 does not require extra memory compared to computing the loss, computing g^2 usually requires to store in memory all intermediate variables, which might be a burden as it requires memory $\Theta(mt)$. Checkpointing can reduce the memory cost for g^2 to $\Theta(m\sqrt{t})$ but with a computational complexity twice as large (Hascoet and Araya-Polo, 2006). Also, some optimization algorithms are *invertible*, such as SGD with momentum (Maclaurin et al., 2015). Using these algorithms removes the need to store each intermediate variable, since they can be recomputed on the fly. Practical implementations of this method still requires a small memory per iteration in order to enforce numerical stability of the inversion. Note that truncated backpropagation (Shaban et al., 2019) can also be used to reduce the memory cost of using automatic differentiation, with approximation. Finally, the main memory cost for estimator g^3 is storing the second order Hessian of size $\Theta(m(m+n))$.

5. Experiments

All experiments are performed in Python using `pytorch` (Paszke et al., 2019). The code to reproduce the figures is available online.[1]

5.1. Considered losses

In our experiments, we considered several losses with different properties. For each experiments, the details on the size of the problems are reported in Sec.A.1.

Regression For a design matrix $D \in \mathbb{R}^{n \times m}$ and a regularization parameter $\lambda > 0$, we define

$$\mathcal{L}_1(z, x) = \frac{1}{2}|x - Dz|^2 + \frac{\lambda}{2}|z|^2 \ ,$$
$$\mathcal{L}_2(z, x) = \sum_{i=1}^{n} \log\left(1 + e^{-x_i [Dz]_i}\right) + \frac{\lambda}{2}|z|^2 \ ,$$
$$\mathcal{L}_3(z, x) = \frac{1}{p}|x - Dz|^p; \quad p = 4 \ .$$

$\mathcal{L}_1$ corresponds to Ridge Regression, which is quadratic and strongly convex when $\lambda > 0$. $\mathcal{L}_2$ is the Regularized Logistic Regression. It is strongly convex when $\lambda > 0$. $\mathcal{L}_3$ is studied in Sec.3.4, and defined with $DD^\top = I_n$.

Regularized Wasserstein Distance The Wasserstein distance defines a distance between probability distributions. In Cuturi (2013), a regularization of the problem is proposed, which allows to compute it efficiently using the Sinkhorn algorithm, enabling many large scale applications. As we will see, the formulation of the problem fits nicely in our framework. The set of histograms is $\Delta_+^m = \{a \in \mathbb{R}_+^m | \ \sum_{i=1}^m a_i = 1\}$. Consider two histograms $a \in \Delta_+^{m_a}$ and $b \in \Delta_+^{m_b}$. The set of couplings is $U(a, b) = \{P \in \mathbb{R}_+^{m_a \times m_b} | \ P\mathbb{1}_{m_b} = a, \ P^\top \mathbb{1}_{m_a} = b\}$. The histogram a (resp. b) is associated with set of m_a (resp. m_b) points in dimension k, $(X_1, \dots, X_{m_a}) \in \mathbb{R}^k$ (resp $(Y_1, \dots, Y_{m_b})$). The cost matrix is $C \in \mathbb{R}^{m_a \times m_b}$ such that $C_{ij} = |X_i - Y_j|^2$. For $\epsilon > 0$, the entropic regularized Wasserstein distance is $W_\epsilon^2(a, b) = \min_{P \in U(a,b)} \langle C, P \rangle + \epsilon \langle \log(P), P \rangle$. The dual formulation of the previous variational formulation is (Peyré and Cuturi, 2019, Prop. 4.4.):

$$W_\epsilon^2(a, b) = \min_{z_a, z_b} \underbrace{\langle a, z_a \rangle + \langle b, z_b \rangle + \epsilon \langle e^{-z_a/\epsilon}, e^{-C/\epsilon} e^{-z_b/\epsilon} \rangle}_{\mathcal{L}_4((z_a, z_b), a)} \tag{20}$$

[1] See `https://github.com/tomMoral/diffopt`.

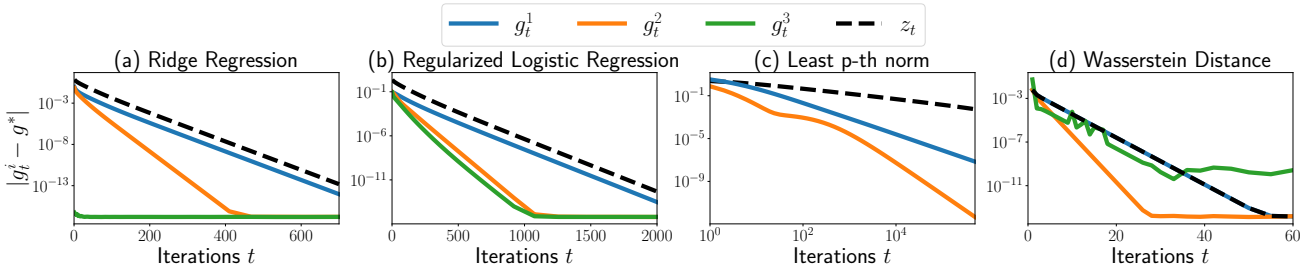

Figure 2. Evolution of $|g_t^i - g^*|$ with the number of iteration t for (a) the Ridge Regression $\mathcal{L}_1$, (b) the Regularized Logistic Regression $\mathcal{L}_2$, (c) the Least Mean p-th Norm $\mathcal{L}_3$ in *log-scale* and (d) the Wasserstein Distance $\mathcal{L}_4$. In all cases, we can see the asymptotic super-efficiency of the g_2 estimator compared to g_1. The g_3 estimator is better in most cases but it is unstable in (d). It is not included in (c) as it is equal to 0 due to the particular shape of $\mathcal{L}_3$.

This loss is strongly convex up to a constant shift on z_a, z_b. The Sinkhorn algorithm performs alternate minimization of $\mathcal{L}_4$:

$$z_a \leftarrow \epsilon(\log(e^{-C/\epsilon}e^{-z_b/\epsilon}) - \log(a)),$$
$$z_b \leftarrow \epsilon(\log(e^{-C^\top/\epsilon}e^{-z_a/\epsilon}) - \log(b)) \ .$$

This optimization technique is not covered by the results in Sec.3, but we will see that the same conclusions hold in practice.

5.2. Examples of super-efficiency

To illustrate the tightness of our bounds, we evaluate numerically the convergence of the different estimators g^1, g^2 and g^3 toward g^* for the losses introduced above. For all problems, g^* is computed by estimating $z^*(x)$ with gradient descent for a very large number of iterations and then using (2).

Gradient Descent Fig.2 reports the evolution of $|g_t^i - g^*|$ with t for the losses $\{\mathcal{L}_j\}_{j=1}^4$, where z_t is obtained by gradient descent for $\mathcal{L}_1, \mathcal{L}_2$ and $\mathcal{L}_3$, and by Sinkhorn iterations for $\mathcal{L}_4$. For the strongly convex losses (a),(b), $|g_t^1 - g^*|$ converges linearly with the same rate as $|z_t - z^*|$ while $|g_t^2 - g^*|$ converges about twice as fast. This confirms the theoretical findings of Prop.3.1 and (13). The estimator g^3 also converges with the predicted rates in (a),(b), however, it fails in (d) as the Hessian of $\mathcal{L}_4$ is ill-conditionned, leading to numerical instabilities. For the non-strongly convex loss $\mathcal{L}_3$, Fig.2.(c) shows that the rates given in Prop.3.9 are correct as g_1 converges with a rate $t^{-\frac{3}{2}}$ while g_t^2 converges as t^{-3}. Here, we did not include g_t^3 as it is exact due to the particular form of $\mathcal{L}_3$.

Stochastic Gradient Descent In Fig.3, we investigate the evolution of expected performances of g^i for the SGD, in order to validate the results of Sec.3.3. We consider $\mathcal{L}_2$. The left part (a) displays the asymptotic expected performance $\mathbb{E}[|g_t^i - g^*|]$ in the fixed step case, as a function of the step ρ, computed by running the SGD with sufficiently many iterations to reach a plateau. As predicted in Sec.3.3, the noise level scales as $\sqrt{\rho}$ for g^1 while it scales like ρ for g^2 and g^3. The right part (b) displays the evolution of $\mathbb{E}[|g_t^i - g^*|]$ as a function of t, where the step-size is decreasing $\rho_t \propto t^{-\alpha}$. Here again, the asymptotic rates predicted by Prop.3.7 is showcased: $g^1 - g^*$ is $O(\sqrt{t^{-\alpha}})$ while $g^2 - g^*$ and $g^3 - g^*$ are $O(t^{-\alpha})$.

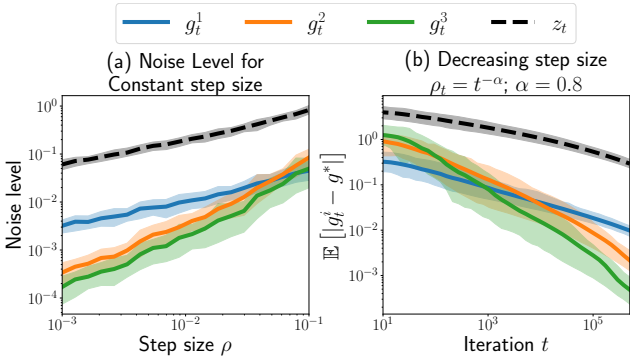

Figure 3. Expected performances of g^i for the SGD; (a) noise level as $t \to +\infty$ for a constant step-size ρ; (b) Expected error as a function of the number of iteration for decreasing step-size $\rho_t = Ct^{-0.8}$. The solid line displays the mean values and the shaded area the first and last decile.

5.3. Example on a full training problem

We are now interested in the minimization of ℓ with respect to x, possibly under constraints. We consider the problem of computing Wasserstein barycenters using mirror descent, as proposed in (Cuturi and Doucet, 2014). For a set of histograms $b_1, \dots, b_N \in \Delta_+^m$ and a cost matrix $C \in \mathbb{R}^{n \times m}$, the entropic regularized Wasserstein barycenter of the b_i's is

$$x \in \arg\min_{x \in \Delta_+^n} \ell(x) = \sum_{i=1}^N W_\epsilon^2(x, b_i) \ ,$$

where W_ϵ^2 is defined in (20), and we have:

$$\ell(x) = \min_{z_x^1, \dots, z_x^N, z_b^1, \dots, z_b^N} \sum_{i=1}^N \mathcal{L}_4\left((z_x^i, z_b^i), x\right) \ . \qquad (21)$$

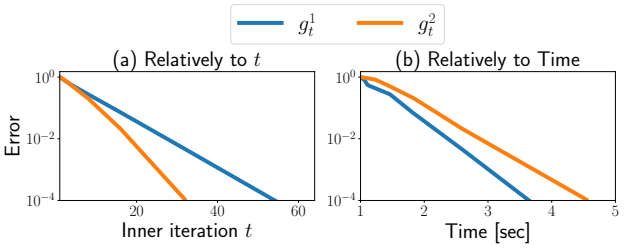

Figure 4. Final optimization error δ_i relatively to (*a*) the number of inner iterations used to estimation g^i; (*b*) the time taken to reach this optimization error level.

The dual variables z_x^i, z_b^i are obtained with t iterations of the Sinkhorn algorithm. In this simple setting, $\nabla_2 \mathcal{L}_4 \left((z_x, z_b), x\right) = z_x$. The cost function is then optimized by mirror descent, with approximate gradient g^i: $x_{q+1} = P_\Delta(\exp(-\eta g^i) x_q)$, where $P_\Delta(x) = x / \sum_{i=1}^n x_i$ is the projection on Δ_+^n. Fig.4 displays the scale of the error $\delta_i = \ell(x_q) - \ell(x^*)$. We excluded g^3 here as the computation were unstable – as seen in Fig.2.(c) – and too expensive. The error decreases much faster with number of inner iteration t by using g_t^2 compared to g_t^1. However, when looking at the time taken to reach the asymptotic error, we can see that g^1 is a better estimator in this case. This illustrates the fact that while g^2 is almost twice as good at approximating g^* as g^1, it is at least twice as expensive, as discussed in Sec.4.2.

6. Conclusion

In this work, we have described the asymptotic behavior of three classical gradient estimators for a special instance of bi-level estimation. We have highlighted a super-efficiency phenomenon of automatic differentiation. However, our complexity analysis shows that it is faster to use the standard analytic estimator when the optimization algorithm converges linearly, and that the super-efficiency can be leveraged for algorithms with sub-linear convergence. This conclusion should be taken with caution, as our analysis is only asymptotic. This suggests a new line of research interested in the non-asymptotic behavior of these estimators. Extending our results to a broader class of non-strongly convex functions would be another interesting direction, as we observe empirically that for logistic-regression, $g_2 - g^* \simeq (g_1 - g^*)^2$. However, as the convexity alone does not ensure the convergence of the iterates, it raises interesting question for the gradient estimation. Finally, it would also be interesting to extend our analysis to non-smooth problems, for instance when z_t is obtained with the proximal gradient descent algorithm as in the case of ISTA for dictionary learning.

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