Convergence diagnostics for stochastic gradient descent with constant step size

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Abstract

Iterative procedures in stochastic optimization are typically comprised of a transient phase and a stationary phase. During the transient phase the procedure converges towards a region of interest, and during the stationary phase the procedure oscillates in a convergence region, commonly around a single point. In this paper, we develop a statistical diagnostic test to detect such phase transition in the context of stochastic gradient descent with constant step size. We present theoretical and experimental results suggesting that the diagnostic behaves as intended, and the region where the diagnostic is activated coincides with the convergence region. For a class of loss functions, we derive a closed-form solution describing such region, and support this theoretical result with simulated experiments. Finally, we suggest an application to speed up convergence of stochastic gradient descent by halving the learning rate every time convergence is detected. This leads to remarkable speed gains that are empirically comparable to state-of-art procedures.

1 Introduction

We consider the classical problem in stochastic optimization stated as

$$\theta_* = \arg \min_{\theta \in \Theta} \mathbb{E}(\ell(y, x^\top \theta)),$$

(1)

where $\ell$ is the loss function, $y \in \mathbb{R}$ denotes the response, $x \in \mathbb{R}^p$ are the features, and $\theta$ are parameters in $\Theta \subseteq \mathbb{R}^p$. For example, the quadratic loss function is defined as $\ell(y, x^\top \theta) =$
$(1/2)(y - x^T\theta)^2$. In estimation problems we typically have a finite data set $\{(x_i, y_i)\}$, for $i = 1, 2, \ldots, N$, from which we wish to estimate $\theta^\star$ by solving the empirical version of Eq. (1):

$$
\hat{\theta} = \arg \min_{\theta \in \Theta} \frac{1}{N} \sum_{i=1}^{N} \ell(y_i, x_i^T \theta).
$$

When data size, $N$, and parameter size, $p$, are large classical methods for computing $\hat{\theta}$ fail. Stochastic gradient descent (SGD) is a powerful alternative (Zhang, 2004; Bottou, 2010, 2012; Touli and Airoldi, 2015) because it solves the problem in an iterative fashion through the procedure:

$$
\theta_n = \theta_{n-1} - \gamma \nabla \ell(y_n, x_n^T \theta_{n-1}).
$$

Here, $\theta_{n-1}$ is the estimate of $\theta^\star$ prior to the $n$th iteration, $(x_n, y_n)$ is a random sample from the data, and $\nabla \ell$ is the gradient of the loss with respect to $\theta$. Classical stochastic approximation theory (Robbins and Monro, 1951; Benveniste et al., 1990; Borkar, 2008) suggests that SGD converges to a value $\theta^\infty$ such that $E(\nabla \ell(y, x^T \theta^\infty)) = 0$, which under typical regularity conditions is equal to $\theta^\star$ when $N$ is infinite (streaming setting), or is equal to $\hat{\theta}$ when $N$ is finite. Going forward we assume the streaming setting for simplicity, but our results hold for finite-$N$ settings as well.

Typically, stochastic iterative procedures start from some starting point and then move through a transient phase and towards a stationary phase (Murata, 1998). In stochastic gradient descent this behavior is largely governed by parameter $\gamma > 0$, which is known as the learning rate, and can be either decreasing over $n$ (e.g., $\propto 1/n$), or constant. In the decreasing rate case, the transient phase is usually long, and can be impractically so if the rate is slightly misspecified (Nemirovski et al., 2009; Touli and Airoldi, 2015), whereas the stationary phase involves SGD converging in quadratic mean to $\theta^\star$. In the constant rate
case the transient phase is much shorter and less sensitive to the learning rate, whereas the stationary phase involves SGD oscillating within a region that contains $\theta_*$. As such, in this paper we focus on constant rate SGD because it is in this context where the diagnostic can be utilized to identify when there is no benefit in running the procedure longer. Furthermore, we can utilize the speed of constant rate SGD in combination with the diagnostic to implement SGD procedures that converge in linear time, as in Section 1.2.

More generally, understanding when a stochastic procedure, such as stochastic gradient descent, reaches the stationary phase is crucial for implementation and for understanding its empirical performance. The main approach to this problem in current practice is through heuristics. In this paper, we develop a principled statistical diagnostic to detect stationarity in SGD with constant learning rate. We illustrate the use of this diagnostic through extensive theory and simulated experiments in the quadratic loss model and extensions. As an additional illustration of the diagnostic’s use, we suggest a new variant of SGD, where we halve the learning rate each time stationarity is detected. This variant combines effectively the speed of constant rate SGD with the convergence property of decreasing rate SGD and exhibits state-of-art performance.

1.1 Related work and contributions

The idea that SGD methods are roughly composed of a transient phase and a stationary phase (also known as search phase and convergence phase, respectively), has been expressed before (Murata, 1998). However, no principled statistical methods have been developed to address stationarity issues, and thereby guide empirical practice of SGD. Currently, guidance is based on heuristics originating from optimization theory that aim to evaluate the magnitude of SGD updates. For example, a popular method is to stop when $||\theta_n - \theta_{n-1}||$ is small according to some threshold, or when updates of the loss function have reached machine precision (Ermoliev and Wets, 1988; Bottou et al., 2016). These methods, however,
do not take into account the sampling variation in SGD estimates, which implies that the aforementioned thresholds depend on the learning rate and the underlying data variation, and are thus suited for deterministic procedures but not stochastic ones.

A more statistically motivated approach is to monitor the test error of SGD iterates on a hold-out validation test, concurrently with the main SGD iteration \cite{Blum99,Bottou12}. One idea here is to stop the procedure when the validation error starts increasing. An important problem with this approach is that the validation error is also a stochastic process, and estimating when it actually starts increasing presents similar, if not greater, challenges to the original problem of detecting convergence to stationary phase. Furthermore, cross validation can be computationally costly in large data sets.

Interestingly, statistically principled methods to detect stationarity can be traced back to classical theory of stopping times in stochastic approximation \cite{Yin89,Pflug90}, of which SGD is a special case. One important method, which also forms the basis of our own work, is Pflug’s procedure \cite{Pflug90} that keeps a running average of the inner product of successive gradients \(\nabla n - 1 \ell^\top \nabla n \ell\), where \(\nabla j \ell = \nabla \ell(y_j, x_j^\top \theta_j - 1)\). The underlying idea is that in the transient phase SGD moves towards \(\theta^\star\) and on average the stochastic gradients point to the same direction, and thus their inner product is positive. In the stationary phase, however, SGD with constant rate moves more haphazardly around \(\theta^\star\), and so the gradients point to different directions making their inner product negative. Despite the solid mathematical underpinnings of this idea, so far it has not been analyzed or implemented in settings of SGD-based stochastic optimization.

### 1.1.1 Overview of results and contributions

Our contributions in this paper can be summarized as follows. In Section 2 we develop the convergence diagnostic test for SGD, which combines Pflug’s stopping time procedure \cite{Pflug90} with SGD in Eq. 2 to detect when SGD exits the transient phase and enters to the
stationary phase. We note that by convergence of SGD with constant rate we do not mean convergence to a single point but convergence to the stationarity region. In Theorem 2 we prove under relatively mild assumptions that the diagnostic is activated almost surely. We obtain this result by examining the expected value of change (increase or decrease) in the diagnostic as a function of \( \theta \). We then illustrate the use of the diagnostic through a simulated example where conditional on the diagnostic being activated, the distance to true parameter value, \( ||\theta_n - \theta_*|| \), is uncorrelated with the starting distance \( ||\theta_0 - \theta_*|| \), which implies that the diagnostic captures the transition from transient to stationary phase well. In Section 3 we develop theory for quadratic loss, and derive a closed-form solution describing the region where the diagnostic is activated, which we support with visual empirical evidence. In Section 4.1 we present extensions beyond the quadratic loss. In Section 4.2 we suggest an application of the diagnostic in speeding up SGD by halving the learning rate each time convergence is detected. This leads to a new SGD procedure, named SGD\(^{1/2} \), with impressive speed gains that we compare against state-of-art procedures, such as variance-reduced SGD (Johnson and Zhang 2013, SVRG) and averaged SGD (Bottou 2010; Xu 2011), in Sections 4.3 and 4.4.

2 Convergence diagnostic

In this section, we focus on the SGD procedure in Eq. (2) and develop the diagnostic for detecting when \( \theta_n \) has escaped the transient phase and is in the stationary phase. Before we develop the diagnostic we note that the existence of the two phases is suggested from existing analyses of the SGD procedure in Eq. (2). Such analyses operate under different assumptions, but invariably suggest that the mean squared error of SGD has a bias term from distance to the starting point, and a variance term from noise in stochastic gradients that becomes dominant for large \( n \). The following meta-theorem summarizes this finding.
Theorem 1 ((Moulines and Bach, 2011; Needell et al., 2014)) Under certain assumptions on the loss function, there are positive constants $A_\gamma, B$ such that, for every $n$, it holds that

$$\mathbb{E}(||\theta_n - \theta_*||^2) \leq \mathbb{E}(||\theta_0 - \theta_*||^2)e^{-A_\gamma n} + B\gamma.$$  

**Remarks.** The constants $A_\gamma, B$ differ depending on the analysis. For example, Bach and Moulines (Moulines and Bach, 2011) use $A_\gamma \approx \gamma \mu / 4 - \gamma^2 L^2$, where $\mu$ is the strong convexity constant of expected loss $f(\theta) = \mathbb{E}(\ell(y, x^\top \theta))$, and $L$ is the Lipschitz constant of $\nabla \log \ell(y, x^\top \theta)$; and $B = \sigma^2 / \mu$, where $\sigma^2$ is an upper bound for the variance of $||\nabla \log \ell(y, x^\top \theta)||^2$. Needell and Srebro (Needell et al. 2014), under different assumptions, use $A_\gamma \approx 2\gamma \mu - 2\gamma^2 \mu L$ and $B = \sigma^2 / \mu(1 - \gamma L)$.

Despite differences, all analyses suggest that the SGD procedure with constant rate goes through a transient phase exponentially fast during which it forgets the initial conditions $\mathbb{E}(||\theta_0 - \theta_*||^2)$, and then enters a stationary phase during which it oscillates around $\theta_*$, roughly at a region of radius $R_\gamma = O(\sqrt{\gamma})$. We note that a trade-off exists here: reducing $\gamma$ will make the oscillation radius, $R_\gamma$, smaller but escaping the transient phase becomes much slower—in the extreme case where $\gamma = 0$, for instance, the procedure will never exit the transient phase.

Despite the theoretical insights it offers, Theorem 1 has limited practical utility for estimating the phase transition in SGD. For example, consider one approach where we find the value of $n$ for which $\mathbb{E}(||\theta_0 - \theta_*||^2)e^{-A_\gamma n} = 0.01B\gamma$, that is, the initial conditions have been discounted to 1% of the oscillation (squared) radius of the stationarity region. That, however, requires estimating quantities such as $\mu, L, \sigma^2$, and $\mathbb{E}(||\theta_0 - \theta_*||^2)$, which is challenging. In the following section, we develop a concrete statistical diagnostic to estimate the phase transition and detect convergence of SGD in a much simpler way.
2.1 Pflug diagnostic

In this section, we develop a convergence diagnostic for SGD procedures that relies on Pflug’s procedure ([Pflug, 1992] in stochastic approximation. The diagnostic is presented as Algorithm 1 and concrete instances under quadratic loss along with theoretical analysis are presented in Section 3 with extensions in Section 4.

The diagnostic is defined by a random variable, $S_n$, that keeps the running sum of the inner product of successive stochastic gradients, as shown in Line 5. The idea is that in the transient phase SGD moves towards $\theta^\star$ by discarding initial conditions, and so the stochastic gradients point to the same direction, on average. This implies that the inner product of successive stochastic gradients is likely positive in the transient phase. In the stationary phase, however, SGD is oscillating around $\theta^\star$ at a distance bounded by Theorem 1, and so the gradients point to different directions. This implies a negative inner product on average during the stationary phase. When the statistic $S_n$ changes sign from positive to negative, this is probably a good signal that the procedure has exited the transient phase.

Since our testing diagnostic is iterative we need to show that it eventually terminates with an answer. Our first theoretical result is Theorem 2 where we prove that $\mathbb{E}(S_n - S_{n-1}) < 0$ as $n \to \infty$, and so the algorithm indeed terminates almost surely. For brevity, we state the theorem without technical details. The full assumptions and proof are in the supplementary material.

**Theorem 2** Under certain assumptions, the convergence diagnostic in Algorithm 1 for constant rate SGD procedure in Eq. (2) satisfies $\mathbb{E}(S_n - S_{n-1}) < 0$ as $n \to \infty$, and so the algorithm terminates almost surely.

**Remarks.** Theorem 2 shows that the inner product of successive gradients is negative in expectation as the iteration number increases. Roughly, when $\theta_n$ is very close to $\theta^\star$, the dominant force is the variance in the stochastic gradient pulling away the next iterates;
Algorithm 1  Pflug diagnostic for convergence of stochastic gradient descent.

**Input:** starting point $\theta_0$, data $\{(y_1, x_1), (y_2, x_2), \ldots\}$, $\gamma > 0$, burnin > 0.

**Output:** Iteration when SGD in Eq. (2) is estimated to have entered stationary phase.

1: $S_0 \leftarrow 0$
2: $\theta_1 \leftarrow \theta_0 + \gamma \nabla \ell(y_1, x_1^\top \theta_0)$
3: for all $n \in \{2, 3, \cdots\}$ do
4: Sample $(x_n, y_n)$
5: Define $\nabla \ell_n = \nabla \ell(y_n, x_n^\top \theta_{n-1})$.
6: $\theta_n \leftarrow \theta_{n-1} + \gamma \nabla \ell_n$.
7: $S_n \leftarrow S_{n-1} + \nabla \ell_n^\top \nabla \ell_{n-1}$.
8: if $n > \text{burnin}$ and $S_n < 0$ then
9:    return $n$
10: end if
11: end for

when $\theta_n$ is far from $\theta_*$ the dominant force is the bias in the stochastic gradient pulling in the next iterates towards $\theta_*$. This implies that the running average of successive gradients will eventually become negative at a finite iteration, and so by the law of large numbers the diagnostic returns a value almost surely.

### 3 Quadratic loss model

In this section, we focus on the quadratic loss function, where $\ell(y, x^\top \theta) = (1/2)(y - x^\top \theta)^2$ and $\nabla \ell(y, x^\top \theta) = -(y - x^\top \theta)x$. In this context we will obtain theoretical and empirical results that will illustrate the performance of the Pflug diagnostic in Algorithm 1. In Section 4 we discuss extensions to other models.

For a first intuition on how the test works consider the case where $\theta_0 = \theta_*$, i.e., the procedure starts in the stationary region. Let $y_n = x_n^\top \theta_* + \varepsilon_n$, where $\varepsilon_n$ are zero-mean
random variables, $\mathbb{E}(\varepsilon_n|x_n) = 0$. Then,

$$\theta_1 = \theta_* + \gamma(y_1 - x_1^\top \theta_*)x_1 = \theta_* + \gamma \varepsilon_1 x_1,$$

from which it follows that

$$S_2 - S_1 = (y_2 - x_2^\top \theta_1)(y_1 - x_1^\top \theta_0)x_2^\top x_1$$

$$= (\varepsilon_2 - \gamma \varepsilon_1 x_2^\top x_1)\varepsilon_1 x_2^\top x_1.$$

$$\mathbb{E}(S_2 - S_1) = -\gamma \mathbb{E}(\varepsilon_1^2)\mathbb{E}((x_2^\top x_1)^2) < 0. \quad (3)$$

Thus, when the procedure starts at the truth, $\theta_*$, the diagnostic is decreased in expectation, and eventually, by the law of large numbers, at some iteration $\tau$ the statistic $S_\tau$ becomes negative and the diagnostic is activated returning value $\tau$. We generalize this result in the following theorem.

**Theorem 3** Suppose that the loss is quadratic, $\ell(y, x^\top \theta) = (1/2)(y - x^\top \theta)^2$. Let $x_1$ and $x_2$ be two iid vectors from the distribution of $x$, and define: $\sigma^2 = \mathbb{E}((y - x^\top \theta_*)^2)$; $c^2 = \mathbb{E}((x_1^\top x_2)^2)$; $C = \mathbb{E}(x_1x_2^\top (x_1^\top x_2))$; $D = \mathbb{E}(x_1x_1^\top (x_1^\top x_2)^2)$, and suppose that all such constants are finite. Then, for $\gamma > 0$,

$$\Delta_n(\theta) = \mathbb{E}(S_{n+2} - S_{n+1} | \theta_n = \theta)$$

$$= (\theta - \theta_*)^\top (C - \gamma D)(\theta - \theta_*) - \gamma c^2 \sigma^2.$$

**Remarks.** Theorem 3 shows that the boundary surface that separates the two regions where the test statistic $S_n$ increases or decreases in expectation looks like an ellipse, for large enough $\gamma$. Regardless of the choice of $\gamma$, when $\theta_n$ is close enough to $\theta_*$, the diagnostic is guaranteed to decrease in expectation since the only remaining term is $-\gamma c^2 \sigma^2 < 0$. 

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The result also shows the various competing forces between bias and variance in the stochastic gradients as they relate to how the diagnostic behaves. For instance, when $\theta_n$ is very close $\theta_*$, larger $\sigma^2$ (noise in stochastic gradient) contributes faster decrease of the diagnostic in expectation, but at the cost of higher variance. The contribution of the other term, $c^2$, is less clear. For instance, $c$ is large when there is strong collinearity in features $x$, which may contribute to decreasing $S_n$. But strong collinearity also implies that $C$ is almost positive definite which contributes positive values to $S_n$, thus counteracting the contribution of $c$. Note that $D$ is a positive definite matrix but $C$ may not be. This implies that careful selection of $\gamma$ may be necessary for the diagnostic to work well. For example, when $\gamma$ is very small and $C$ is positive definite, then $S_n$ will converge to a negative number slowly. One way to alleviate this sensitivity to the learning rate is through implicit updates (Toulis et al., 2014), which we explore in Section 3.3.

In the following sections we illustrate the main result of Theorem 3 and also the performance of the Pflug diagnostic in detecting convergence of SGD.

3.1 Illustration

Here, we illustrate the main results of Theorem 3 through Figure 1 which can be described as follows. The dark shaded area in the figure corresponds to the region where the Pflug diagnostic is decreased in expectation if the SGD iterate falls in the region. We call this the Pflug region. Outside of the Pflug region the diagnostic is increased in expectation, and the farther we move away from the center of that region, which roughly coincides with $\theta_*$, the larger the expected increase of the diagnostic becomes. The polygon shaded with diagonal lines corresponds to empirical estimations of the convergence region of SGD, where SGD iterates have oscillated around over 1000 simulations. In addition to the result in Theorem 3 about the shape of the region this shows that the Pflug region approximates very well the convergence region of SGD. This is remarkable because the Pflug region is implementable...
from data, whereas the SGD convergence region is not since by Theorem 1 it depends on unknown quantities.

### 3.2 Simulated example

Next, we apply the Pflug convergence diagnostic on a simulated example to investigate empirically whether it estimates the phase transition well. The experimental setup is as follows. We set $p = 20$ as the parameter dimension, and $N = 5000$ as the data set size. We fix $\theta_* \in \mathbb{R}^p$
with \( \theta_{\ast,j} = 10e^{-0.75j} \)—this ensures some variation and sparsity in the parameter values. We sample features as \( x_i \sim \mathcal{N}_p(0, I) \), where \( \mathcal{N}_p \) denotes a \( p \)-variate normal distribution, and \( I \) is the identity matrix, and \( i = 1, 2, \ldots N \). We sample outcomes as \( y_i = x_i^\top \theta_{\ast} + \mathcal{N}(0, \sigma^2) \), \( \sigma = 3 \).

For a given \( \gamma \) we run Algorithm 1 with \( \text{burnin} = 0.1N \), for various values of the starting point \( \theta_0 \) sampled as \( \mathcal{N}_p(\theta_{\ast}, \sigma_0^2 I) \), where \( \sigma_0 = 2 \). Let \( E_n = ||\theta_n - \theta_{\ast}||^2 \), then for each run we store the tuple

\[
(\gamma, \tau, E_0, E_{\tau/2}, E_{2\tau}),
\]

where \( \tau \) is the output of Algorithm 1, i.e., the iteration at which the Pflug diagnostic detected convergence. The idea in this experimental evaluation is that if the convergence diagnostic detects convergence accurately, the iterates \( \theta_{\tau/2} \) will depend on the initial conditions \( \theta_0 \) more than the iterates \( \theta_{2\tau} \). Thus, for given \( \gamma \) and \( \tau \), we should expect a much higher correlation between \( E_{\tau/2} \) and \( E_0 \) than between \( E_{2\tau} \) and \( E_0 \). To test this hypothesis, for a given value of \( \gamma \) we draw 100 independent samples of \( (E_0, E_{\tau/2}, E_{2\tau}) \). With these samples we regress \( E_{\tau/2} \) on \( E_0 \) and \( E_{2\tau} \) on \( E_0 \) in two normal linear regression models. Table 1 summarizes the experimental results. In the second and third column of Table 1 we report the regression coefficients of \( E_0 \) in the two model fits, respectively, and also report statistical significance.

Table 1: Experimental evaluation of convergence diagnostic over 100 runs per learning rate value. Significance levels: *** = < 0.1%; ** = 1%; * = 5%; . = 10%
From the table, we see that the regression coefficient corresponding to $E_{\tau/2}$ is always positive and statistically significant, whereas the coefficient is mostly not significant for $E_{2\tau}$. This suggests that $E_{\tau/2}$ depends on initial conditions $E_0$, and thus stationarity has not yet been reached at iteration $\tau/2$. In contrast, $E_{2\tau}$ does not depend on initial conditions $E_0$, and thus stationarity has likely occurred after iteration $\tau$. This is evidence indicating that the Pflug diagnostic performs reasonably well in estimating the switch of SGD from its transient phase to its stationary phase. We note that in the regression evaluation we had to control for $\tau$ (by using it as a regressor) because the iteration number is correlated with mean-squared error (larger values for $\tau$ are correlated with smaller error).

### 3.3 Implicit update

As mentioned in the remarks of Theorem 3 the Pflug diagnostic is sensitive to the choice of learning rate $\gamma$. For example, when $\gamma$ is small and $C$ is positive definite, $S_n$ will be mostly increasing during the transient phase, which makes convergence slower. But choosing a large learning rate can easily lead to numerical instability. One way to alleviate such sensitivity to the learning rate is to use the SGD procedure with an implicit update:

$$
\theta_n = \theta_{n-1} + \gamma \nabla \ell(y_n, x_n^\top \theta_n). \tag{4}
$$

Note that $\theta_n$ appears on both sides of the equation. In the quadratic loss model we can solve exactly the implicit equation as follows:

$$
\theta_n = (I + \gamma x_n x_n^\top)^{-1}(\theta_{n-1} + \gamma y_n x_n) \tag{5}
$$

Implementing the procedure in Eq. (5) is fast since it is equivalent to $\theta_n = (\theta_{n-1} + \gamma y_n x_n)/(1 + \gamma ||x_n||^2)$. More generally, the implicit update in Eq. 14 can be computed efficiently through
a one-dimensional root-finding procedure in many settings (Toulis et al., 2014). Previous work on implicit SGD procedures (ISGD) has shown that implicit procedures have similar asymptotic properties with standard SGD procedures with numerical stability as an added benefit. Since most related work on ISGD methods is with respect to decreasing learning rate procedures (Kulis and Bartlett, 2010; Bertsekas, 2011; Toulis et al., 2014, 2017), we provide an analysis for constant rate ISGD as in Eq. (4) in the supplementary material. We note that ISGD procedures are related to proximal updates in stochastic optimization (Parikh and Boyd, 2013; Rosasco et al., 2014; Xiao and Zhang, 2014), but these methods differ from ISGD methods in that they employ a combination of classical SGD with deterministic proximal operators, whereas ISGD’s proximal operator is purely stochastic.

The following theorem shows that the implicit update in the linear model mitigates the sensitivity of the Pflug diagnostic to the choice of the learning rate.

**Theorem 4** Let \( \lambda_\gamma = \mathbb{E}(1/(1 + \gamma||x||^2)) \in (0, 1] \). Under the assumptions of Theorem 3 applied on the implicit procedure in Eq. (14), it holds that

\[
\Delta_{n}^{im}(\theta) = a_\gamma \Delta_n(\theta) + b_\gamma [((\theta - \theta_*)^\top D(\theta - \theta_*) + \sigma^2 c^2],
\]

where \( a_\gamma = \lambda_\gamma^2 \), \( b_\gamma = \gamma \lambda_\gamma^2 (1 - \lambda_\gamma) \).

**Remarks.** Theorem 4 shows that the diagnostic is more stable with the ISGD procedure rather than the classical SGD procedure. Take, for example, the case where \( \gamma = \infty \) so that \( \lambda_\gamma = 0 \). In the classical SGD setting, Theorem 3 suggests that the diagnostic increases without bound and convergence fails. In the ISGD setting, however, it holds that \( \Delta_{n}^{im}(\theta) \approx 0 \), and convergence may happen. In contrast, when \( \gamma \approx 0 \) then \( \lambda_\gamma \approx 1 \) and so \( \Delta_{n}^{im}(\theta) \approx \Delta_n(\theta) \), which implies that the diagnostic behaves in the implicit procedure as it behaves in the explicit one.
4 Extensions and applications

In this section we consider extensions of the \textit{Pflug} diagnostic to a more broad family of loss functions inspired by generalized linear models (GLMs). We also consider an application of the diagnostic to speed up convergence of SGD with constant rate.

4.1 Generalized linear loss

Here, we consider the loss based on the GLM formulation \cite{McCullagh1984, Toulis2014} where $\ell(y, x^\top \theta) = -y \cdot x^\top \theta + f(x^\top \theta)$. For example, the quadratic loss is equivalent to $f(u) = u^2/2$. The logistic loss is when $y$ is binary and $f(u) = \log(1 + e^u)$. In general, $f$ cannot be chosen arbitrarily—one standard choice is to define $f$ such that $e^{-\ell(y,x^\top \theta)}$ is a proper density, i.e., it integrates to one. The following theorem generalizes the results in Section 3 on the quadratic loss.

Theorem 5 Consider the GLM loss defined as $\ell(y, x^\top \theta) = y \cdot x^\top \theta - f(x^\top \theta)$. Let $h(u) = f'(u)$ and suppose that $h'(x^\top \theta) \geq k > 0$, almost surely for all $\theta$. Let $x_1, x_2$ be two iid vectors from the distribution of $x$. Define $\sigma^2 = \mathbb{E}((y - h(x^\top \theta_*)^2); c^2 = \mathbb{E}((x_1^\top x_2)^2); C(\theta, \theta_*) = \mathbb{E}(h(x_1^\top \theta) - h(x_1^\top \theta_*)) x_1); D^2(\theta, \theta_*) = \mathbb{E}((h(x_1^\top \theta) - h(x_1^\top \theta_*))^2(x_1^\top x_2)^2).$ For small enough $\gamma$,

$$\Delta_{n}^{glm}(\theta) = \mathbb{E}(S_{n+2} - S_{n+1}|\theta_n = \theta) \leq ||C(\theta, \theta_*)||^2 - \gamma k [\sigma^2 c^2 + D^2(\theta, \theta_*)].$$

Remarks. The result in Theorem 5 has the same structure as in Theorem 3, so a direct analogy can be helpful. The terms $\sigma^2, c^2$ in the two theorems are identical, if we consider that for the quadratic loss it holds that $h(u) = u$. The term $||C(\theta, \theta_*)||^2$ in Theorem 5 corresponds to the term $(\theta - \theta_*)^\top C(\theta - \theta_*)$ in Theorem 3 and $D^2(\theta, \theta_*)$ corresponds to $(\theta - \theta_*)^\top D(\theta - \theta_*)$, respectively. The terms are equal when we set $h(u) = u$, in which case $k = 1$. Thus,
the diagnostic with the more general GLM loss has familiar properties. For example, when
$\theta \approx \theta_*$, i.e., when SGD is near the truth, $||C(\theta, \theta_*)||^2 \approx 0$ and $D^2(\theta, \theta_*) \approx 0$, in which case
the negative constant term dominates and the test statistic decreases in expectation. One
difference with the quadratic loss, however, is that as we move farther from $\theta_*$ the statistic
may change in a nonlinear way. Therefore the boundary separating the positive and negative
regions of the diagnostic will generally not have the nice, smooth elliptical shape as in the
quadratic loss (see Figure 1). This may lead to more complex behavior for the diagnostic,
which we aim to analyze fully in future work.

We note that the constraint on $h'$ is not particularly strict because in the GLM formul-
ation $h'$ is guaranteed to be positive. The assumption is made to simplify the analysis but
can be improved by analyzing the quantity $h'(x^T \theta_n)$ through existing analyses of $\theta_n$.

4.2 SGD$^{1/2}$ for fast convergence

We now switch gears from analyzing the behavior of the Pflug diagnostic to using it in
a practical application. Our suggested application is to use the diagnostic within a SGD
loop where the learning rate is halved and the procedure restarted each time convergence is
detected. We note that our goal here is to illustrate the utility of our convergence diagnostic,
and a full analysis of the proposed method will be a subject of future work.

More specifically, note that by Theorem 1 procedure SGD with constant rate has linear
convergence to a stationary distance from $\theta_*$ of $R_\gamma = O(\sqrt{\gamma})$. It would therefore be beneficial
to reduce the learning rate when we know that the SGD iterates are oscillating around $\theta_*$ in a
ball of radius $R_\gamma$, so that the procedure moves to a ball with a smaller radius. To implement
such a procedure, however, would require knowing $\theta_*$, and also knowing all parameters
required to calculate $R_\gamma$. Our solution employs the Pflug convergence diagnostic to detect
stationarity. Algorithm 2 describes such a procedure, named SGD$^{1/2}$, where the learning rate
is halved upon detection of convergence (Line 10).
Algorithm 2 Procedure SGD$^{1/2}$.

**Input:** $\theta_0$, data $\{(y_1, x_1), (y_2, x_2), \ldots\}$, $\gamma > 0$, burnin, maxit > 0.

**Output:** Iteration $\tau > 0$, when SGD is estimated to have converged.

1: $s \leftarrow 0$
2: $\tau \leftarrow 0$
3: $\theta_1 \leftarrow \theta_0 + \gamma \nabla \ell (y_1, x_1^\top \theta_0)$
4: for all $n \in \{2, 3, \ldots\}$ do
5: $\theta_n \leftarrow \theta_{n-1} + \gamma \nabla \ell (y_n, x_n^\top \theta_{n-1})$
6: $s \leftarrow s + (\theta_n - \theta_{n-1})^\top (\theta_{n-1} - \theta_{n-2}) / \gamma^2$
7: if $n > \tau + \text{burnin}$ and $s < 0$ then
8: $\tau \leftarrow n$
9: $s \leftarrow 0$
10: $\gamma \leftarrow \gamma / 2$
11: if $\gamma < 1e^{-10}$ and $n > \text{maxit}$ then
12: return $\theta_n$
13: end if
14: end if
15: end for

Note that implicit updates can be used in this algorithm as well; we call this modified algorithm ISGD$^{1/2}$. In our experiments in the following section, we employ ISGD$^{1/2}$ because of the benefits in numerical stability from using implicit updates.

### 4.3 Simulated data experiments

To evaluate the effectiveness of ISGD$^{1/2}$, we compare to other classical and state-of-the-art SGD methods. We first experiment on simulated data to better understand the performance of ISGD$^{1/2}$ and its competition under various parameter settings. In particular, we compare the performance of our procedure ISGD$^{1/2}$ in Algorithm 2 against SVRG and classical ISGD on simulated data. The classical ISGD uses an optimized learning rate of $O(1/n)$. The basic experimental setup is as follows.

We consider settings of high and low signal to noise ratio (SNR), and high and low dimension and test under the four combinations of these settings. For the high SNR case, we set $SNR = 5$, where $SNR = \text{trace}(\text{Var}(x))/p\text{Var}(y|x)$, and for the low SNR case we
Figure 2: Simulated data experiments, comparing the performance of our procedure $\text{ISGD}^{1/2}$ against SVRG and classical ISGD. The left four plots are with the normal model, the right four plots with the logistic model.

set $SNR = 2$. For the high dimension case we set $p = 150$ as the parameter dimension, and for the low dimension case we set $p = 10$. Given the dimension $p$, we fix $\theta_* \in \mathbb{R}^p$ such that $\theta_{*,j} = 10e^{-0.75j}$. We set $N = 5000$ as the size of the data set. We sample features as $x_i \sim \mathcal{N}_p(0, I)$, where $i = 1, 2, \ldots N$. We sample outcomes as $y_i \sim \mathcal{N}(x_i^T \theta_*, \sigma^2)$ for the normal model, and $y_i \sim \text{Binom}(\exp(x_i^T \theta_*)/(1 + \exp(x_i^T \theta_*)))$ for the logistic model, where $\text{Binom}(q)$ denotes the binomial random variable with mean $q$. The learning parameters for each SGD method were tuned to provide best performance through pre-processing.

From simulations with the normal model in the left half of Figure 2 we see that $\text{ISGD}^{1/2}$ attains a comparable performance to SVRG. In general, SVRG attains an overall better performance for these experiments, which we believe is related to our convergence diagnostic being aggressive in a couple of cases.

From simulations with the logistic model in the right half of Figure 2 we see that $\text{ISGD}^{1/2}$ attains an even better performance than before as there are fewer cases where the diagnos-
tic is aggressive. With high SNR and low dimension parameter settings, ISGD$^{1/2}$ achieves consistently better performance than SVRG. We note that such comparisons do not take into account the sensitivity of SVRG to misspecifications of the learning rate (large enough learning rates can easily make the procedure diverge); or that SVRG requires periodic calculations over the entire data set, which here is easy because we are using only 5,000 data points, but may be a problem in more realistic settings. We also note that there are several improvements available for ISGD$^{1/2}$ by allowing a larger burnin period or by discounting the learning rate less aggressively, but we plan on addressing such tuning issues in future work, both theoretically and empirically.

4.4 Benchmark data sets

In addition to simulated experiments we conduct experiments on benchmark data sets MNIST (binary) and COVERTYPE (binary) to evaluate real world performance. In particular, we perform binary logistic regression using ISGD$^{1/2}$, SVRG, classical ISGD, and averaged ISGD, where averaging iterates theoretically leads to optimal asymptotic errors. We plot the prediction error on a held out test set in Figure 3 relative to the number of passes over the data.

Overall, we see that ISGD$^{1/2}$ convergences very quickly, after going over less than a quarter of the data, and achieves best performance in the COVERTYPE data set. We currently do not have a theoretical justification for this, but we have verified that it is consistently observed across multiple experiments. ISGD$^{1/2}$ was also very stable to specifications of the learning rate parameter, as expected from the analysis of Theorem 4. In contrast, even though SVRG performed comparably to ISGD$^{1/2}$, its performance was unstable, especially in the COVERTYPE data set, and required careful fine tuning of the learning rate through

---

1Data sets can be found at https://archive.ics.uci.edu/ml/databases/mnist/ and https://archive.ics.uci.edu/ml/datasets/covertype, respectively.
Figure 3: Benchmark data sets with binary logistic regression using ISGD$^{1/2}$, SVRG, classical ISGD, and averaged ISGD. Prediction error on a held out test set. MNIST (binary) on the left, COVERTYPE (binary) on the right.

trial and error. Averaged SGD performed well on the MNIST data set, but flattened out very fast in the COVERTYPE data, possibly due to misspecification.

5 Concluding remarks

In this paper we focused on the problem of convergence of SGD to the stationary phase. This is an important task because statistical properties of iterative stochastic procedures are better understood when they have reached stationarity. We borrowed from the theory of stopping times in stochastic approximation to develop a diagnostic that reliably detects the phase transition, as shown theoretically and empirically. Future work can focus on analysis of $||\theta_n - \theta_*||^2$ conditional on the diagnostic being activated. This could show theoretically that the error is uncorrelated with the initial starting point conditional on the test being activated, and so provide a theoretical analysis of the results in Table 1.

In separate work we plan to focus more on the procedure ISGD$^{1/2}$ that worked very well in experiments, and to analyze theoretically its behavior. One idea is to run parallel ISGD$^{1/2}$ chains and aggregate the iterates. At stationarity we expect the iterates from different chains
to be uncorrelated with each other; averaging can help, in a similar way that iterate averaging helps in stochastic approximations [Ruppert, 1988].

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A Proofs of theorems

Theorem 1 ([Moulines and Bach, 2011; Needell et al., 2014]) Under certain assumptions on the loss function, there are positive constants $A\gamma, B$ such that, for every $n$, it holds that

$$
\mathbb{E}(||\theta_n - \theta_*||^2) \leq \mathbb{E}(||\theta_0 - \theta_*||^2)e^{-A\gamma n} + B\gamma.
$$

Theorem 2 Consider SGD with constant rate,

$$
\theta_n = \theta_{n-1} - \gamma \nabla \ell(y_n, x_n^\top \theta_{n-1}).
$$

Suppose that Theorem 1 holds, so that $\mathbb{E}(||\theta_n - \theta_*||^2) \leq \gamma M$, for some positive $M$ and large enough $n$. We make the following additional assumptions:

(a) $\nabla \ell(y, x^\top \theta) = f(x, \theta) + e$, where $f(x, \theta)$ is $L$-Lipschitz, $\mathbb{E}(e|x, \theta) = 0$ and $\mathbb{E}(|e|^2) \geq \tau^2$.

(b) It holds $\mathbb{E}(f(x, \theta - \gamma z)^\top z) \leq \mathbb{E}(f(x, \theta)^\top z) - \gamma K \cdot \mathbb{E}(z^\top C z)$, for any $\theta, z$, for some positive constant $K$, and some positive definite matrix $C$ with minimum eigenvalue $\mu > 0$.

(c) It holds that $\gamma > (L^2 M - \mu K \tau^2)/\mu KL^2 M$.

Then,

$$
\mathbb{E}(\nabla \ell(y_n, x_n^\top \theta_{n-1})^\top \nabla \ell(y_{n+1}, x_{n+1}^\top \theta_n)) < 0.
$$

Proof 2 For brevity let $\tilde{\ell}_i = f(x_{i+1}, \theta_i) + e_i = f_i + e_i$ be the stochastic gradient at iteration $i + 1$. 

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\[ \mathbb{E}(\tilde{\ell}_i^\top \tilde{\ell}_i) = \mathbb{E}[(f_{i-1} + e_{i-1})^\top (f_i + e_i)] = \mathbb{E}[(f_{i-1} + e_{i-1})^\top f_i] \]  
[ because \( e_i \) are zero-mean ]

\[ = \mathbb{E}[(f_{i-1} + e_{i-1})^\top f (\theta_{i-1} - \gamma f_{i-1} - \gamma e_{i-1})] \]  
[ by SGD step for \( \theta_i \) ]

\[ \leq \mathbb{E}(||f_{i-1}||^2) - \gamma K \cdot \mathbb{E}[(f_{i-1} + e_{i-1})^\top C(f_{i-1} + e_{i-1})] \]  
[ by Assumption (b) ]

\[ \leq (1 - \gamma \mu K)\mathbb{E}(||f_{i-1}||^2) - \gamma K \cdot \mathbb{E}(||e_{i-1}||^2_C) + O(\gamma^2) \]

\[ \leq (1 - \gamma \mu K)L^2\mathbb{E}(||\theta_{i-1} - \theta^*||^2) - \gamma \mu K \tau^2 + O(\gamma^2) \]  
[ by Lipschitz Assumption (a) ]

\[ \leq \gamma[(1 - \gamma \mu K)L^2 M - \mu K \tau^2] + O(\gamma^2) \]

\[ < 0. \]  
[ by Assumption (c) and small enough \( \gamma \) ]

\[ (6) \]

**Remarks.** Assumption (b) is a form of strong convexity. For example, suppose that 
\[ y = x^\top \theta^* + e, \] 
then 
\[ f(x, \theta) = xx^\top (\theta - \theta^*) \] 
and 
\[ f(x, \theta - \gamma z)^\top z = f(x, \theta)^\top z - \gamma z^\top \mathbb{E}(xx^\top)z. \]

In this case \( C = \mathbb{E}(xx^\top) \) is the Fisher information matrix and Assumption (b) holds for 
\( K = 1. \) When \( \gamma \) is small enough and a Taylor approximation of \( f(x, \theta - \gamma z) \) is possible, 
the above result still holds for \( K = 1 \) when the Fisher information exists. Assumption (c) 
shows that there is a threshold value for \( \gamma \) below which the diagnostic cannot terminate. For 
example, suppose that error noise is small so that \( \tau^2 \approx 0 \) and \( K = 1, \) as argued before. Then, 
\( \gamma > 1/\mu, \) that is, the learning rate has to exceed the reciprocal of the minimum eigenvalue 
of the Fisher information matrix.

**Theorem 3** Suppose that the loss is quadratic, 
\[ \ell(y, x^\top \theta) = (1/2)(y - x^\top \theta)^2. \] 
Let \( x_1 \) and \( x_2 \) be two iid vectors from the distribution of \( x, \) and define: 
\( \sigma^2 = \mathbb{E}((y - x^\top \theta^*)^2); \) \( c^2 = \mathbb{E}((x_1^\top x_2)^2); \)
\( C = \mathbb{E}(x_1 x_2^\top (x_1^\top x_2)); \) \( D = \mathbb{E}(x_1 x_1^\top (x_1^\top x_2)^2), \) 
and suppose that all such constants are finite.

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Then, for $\gamma > 0$,

$$
\Delta_n(\theta) = \mathbb{E}(S_{n+2} - S_{n+1} | \theta_n = \theta) \\
= (\theta - \theta_\star)\top (C - \gamma D)(\theta - \theta_\star) - \gamma \sigma^2.
$$

**Proof 3** For notational brevity we make the following definitions:

$$
\begin{align*}
\theta^+ &= \theta + \gamma (y_1 - x_1\top \theta)x_1 \\
\theta^{++} &= \theta^+ + \gamma (y_2 - x_2\top \theta^+)x_2,
\end{align*}
$$

where $\theta$ is the current iterate, and $\theta^+$ and $\theta^{++}$ are the next two using iid data $(x_1, y_1)$ and $(x_2, y_2)$. For a fixed $\theta$ we understand the Pflug diagnostic through the function

$$
H(\theta) = S_{++} - S_+ | \theta = \nabla_{++}\ell\top \nabla_+\ell = (\theta^+ - \theta)^\top (\theta^{++} - \theta^+)/\gamma^2
$$

and $\Delta_n(\theta) = \mathbb{E}(H(\theta)) = \mathbb{E}\left((\theta^+ - \theta)^\top (\theta^{++} - \theta^+)/\gamma^2\right)$.  

We use Eq. (7) to derive an expression for $H$:

$$
H(\theta) = (y_1 - x_1\top \theta)(y_2 - x_2\top \theta^+)x_1\top x_2 \\
= (y_1 - x_1\top \theta) [y_2 - x_2\top \theta - \gamma(y_1 - x_1\top \theta)x_1\top x_2] x_1\top x_2 \\
= (y_1 - x_1\top \theta)(y_2 - x_2\top \theta)x_1\top x_2 - \gamma(y_1 - x_1\top \theta)^2(x_1\top x_2)^2.
$$

Let $y_i = x_i\top \theta_\star + \epsilon_i$; we know that $\mathbb{E}((y_i - x_i\top \theta_\star)x_i) = 0$. Now, we analyze each term.
individually:

\[(y_1 - x_1^\top \theta)(y_2 - x_2^\top \theta)x_1^\top x_2 = [x_1^\top (\theta - \theta) + \varepsilon_1][x_2^\top (\theta - \theta) + \varepsilon_2]x_1^\top x_2\]

\[= (\theta - \theta_\star)^\top x_1 x_2^\top (x_1^\top x_2)(\theta - \theta_\star) + \varepsilon_1 W^{(1)} + \varepsilon_2 W^{(2)} + \varepsilon_1 \varepsilon_2 W^{(3)}.\]

The \(W\) variables are conditionally independent of \(\varepsilon\) and so using the law of iterated expectations these terms vanish.

\[\mathbb{E} \left( (y_1 - x_1^\top \theta)(y_2 - x_2^\top \theta)x_1^\top x_2 \right) = (\theta - \theta_\star)^\top \mathbb{E} (x_1 x_2^\top (x_1^\top x_2)) (\theta - \theta_\star) = (\theta - \theta_\star)^\top C(\theta - \theta_\star).\]

Using a similar reasoning, for the second term we have:

\[\left( y_1 - x_1^\top \theta \right)^2 (x_1^\top x_2)^2 = \left[ (x_1^\top (\theta - \theta) + \varepsilon_1 \right]^2 (x_1^\top x_2)^2\]

\[= (\theta - \theta_\star)^\top x_1 x_2^\top (x_1^\top x_2)^2 (\theta - \theta_\star) + \varepsilon_1 W^{(4)} + \varepsilon_1^2 (x_1^\top x_2)^2. \quad (11)\]

In expectation of Eq. (11),

\[\mathbb{E} \left( \left( y_1 - x_1^\top \theta \right)^2 (x_1^\top x_2)^2 \right) = (\theta - \theta_\star)^\top \mathbb{E} (x_1 x_2^\top (x_1^\top x_2)^2) (\theta - \theta_\star) + \varepsilon_1^2 (x_1^\top x_2)^2\]

\[= (\theta - \theta_\star)^\top D(\theta - \theta_\star) + \sigma^2 c^2. \quad (12)\]

By combining all results we finally get:

\[\Delta_n(\theta) = (\theta - \theta_\star)^\top (C - \gamma D)(\theta - \theta_\star) - \gamma \sigma^2 c^2.\]

**Theorem 4** Let \(\lambda_\gamma = \mathbb{E}(1/(1 + \gamma ||x||^2)) \in (0, 1]\). Under the assumptions of Theorem 3

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applied on the implicit procedure in Eq. (14), it holds that

\[ \Delta^\text{im}_n(\theta) = \mathbb{E}(S_{n+2} - S_{n+1}|\theta_n = \theta) \]

\[ = a_\gamma \Delta_n(\theta) + b_\gamma [(\theta - \theta_*)^\top D(\theta - \theta_*) + \sigma^2 c^2], \]

where \( a_\gamma = \lambda_\gamma^2 \), \( b_\gamma = \gamma \lambda_\gamma^2 (1 - \lambda_\gamma) \).

**Proof 4** We derive similar theoretical results for \( H^\text{im}(\theta), \Delta^\text{im}_n(\theta) \) under the linear normal model for implicit updates. We have the implicit updates

\[
\theta^+ = \theta + \gamma (y_1 - x_1^\top \theta^+) x_1 \\
\theta^{++} = \theta^+ + \gamma (y_2 - x_2^\top \theta^{++}) x_2
\]

Also note the collinearity

\[
(y_1 - x_1^\top \theta^+) = \lambda_1 (y_1 - x_1^\top \theta) \\
(y_2 - x_2^\top \theta^{++}) = \lambda_2 (y_2 - x_2^\top \theta^+) \\
= \lambda_2 [y_2 - x_2^\top \theta - \gamma \lambda_1 (y_1 - x_1^\top \theta) x_1^\top x_2],
\]

where \( \lambda_1 = 1/(1 + \gamma \|x_1\|^2) \) and \( \lambda_2 = 1/(1 + \gamma \|x_2\|^2) \). We derive an expression for \( H^\text{im} \), with implicit updates:

\[
H^\text{im}(\theta) = (\theta^+ - \theta)^\top (\theta^{++} - \theta^+)/\gamma^2 \\
= (y_1 - x_1^\top \theta^+) (y_2 - x_2^\top \theta^{++}) x_1^\top x_2 \\
= \lambda_1 \lambda_2 (y_1 - x_1^\top \theta)(y_2 - x_2^\top \theta - \gamma \lambda_1 (y_1 - x_1^\top \theta) x_1^\top x_2) x_1^\top x_2 \\
= \lambda_1 \lambda_2 [H(\theta) + \gamma (1 - \lambda_1)(y_1 - x_1^\top \theta)^2 (x_1^\top x_2)^2] \\
= \lambda_1 \lambda_2 H(\theta) + \gamma \lambda_1 \lambda_2 (1 - \lambda_1)(y_1 - x_1^\top \theta)(x_1^\top x_2)^2,
\]
where \( H \) is the function from the explicit update in Eq. (10). The formula for \( \Delta_{\text{glm}}(\theta) \) follows by applying expectation and the reasoning in Eq. (12). Note that \( \mathbb{E}(\lambda_1\lambda_2) = \lambda_2^2 \) since \( \lambda_1 \) and \( \lambda_2 \) are independent and have marginally identical distributions.

**Theorem 5** Consider the GLM loss defined as \( \ell(y, x^\top \theta) = y \cdot x^\top \theta - f(x^\top \theta) \). Let \( h(u) = f'(u) \) and suppose that \( h'(x^\top \theta) \geq k > 0 \), almost surely for all \( \theta \). Let \( x_1, x_2 \) be two iid vectors from the distribution of \( x \). Define \( \sigma^2 = \mathbb{E}((y - h(x^\top \theta_*))^2); \ c^2 = \mathbb{E}((x_1^\top x_2)^2); \ C(\theta, \theta_*) = \mathbb{E}(|h(x_1^\top \theta) - h(x_1^\top \theta_*)| x_1); \ D^2(\theta, \theta_*) = \mathbb{E}(|h(x_1^\top \theta) - h(x_1^\top \theta_*)|^2 (x_1^\top x_2)^2) \). For small enough \( \gamma \),

\[
\Delta_{\text{glm}}^n(\theta) = \mathbb{E}(S_{n+2} - S_{n+1}|\theta_n = \theta) \\
\leq ||C(\theta, \theta_*)||^2 - \gamma k[\sigma^2 c^2 + D^2(\theta, \theta_*)].
\]

**Proof 5** The updates for the GLM loss are as follows:

\[
\theta^+ = \theta + \gamma (y_1 - h(x_1^\top \theta)) x_1 \\
\theta^{++} = \theta^+ + \gamma (y_2 - h(x_2^\top \theta^+)) x_2,
\]

(13)

Note that \( h(x_2^\top \theta^+) = h(x_2^\top \theta) + \gamma h'(x_2^\top \theta)(y_1 - h(x_1^\top \theta)) x_2^\top x_1 + O(\gamma^2) \). We can now follow the exact same reasoning as in Theorem 3 and that \( h'(x^\top \theta) \geq k \) almost surely.

**B**  
Mean squared error bound for constant rate ISGD

We have the implicit update of SGD (ISGD):

\[
\theta_n = \theta_{n-1} + \gamma \nabla \ell(y_n, x_n^\top \theta_n). \quad (14)
\]

We will operate under the following assumptions:

**Assumption 1** The following assumptions are true with regard to procedure in Eq. (14).
(a) Function $\ell$ is convex, twice differentiable almost surely with respect to $x^\top \theta$.

(b) For the observed Fisher information matrix $\hat{I}_n(\theta) = \nabla^2 \ell(y_n, x_n^\top \theta)$ there exists constants $b > 0$ and $0 < t < \infty$ such that $b \leq \text{trace}(\hat{I}_n(\theta)) \leq t$ almost surely, for all $\theta$. The Fisher information matrix $I(\theta_*) = \mathbb{E}\left(\hat{I}_n(\theta_*)\right)$ has minimum eigenvalue $\lambda > 0$.

(c) There exists $\sigma^2 > 0$ such that, for all $n$, $\mathbb{E}(\|\nabla \ell(y_n, x_n^\top \theta_*)\|^2 | F_{n-1}) \leq \sigma^2$, almost surely.

(d) The function $\theta \mapsto \mathbb{E}(\nabla \ell(y, x^\top \theta))$ is Lipschitz with constant $L$, i.e., for all $n, \theta_1, \theta_2$,

$$\mathbb{E}(\|\nabla \ell(y_n; x_n^\top \theta_1) - \nabla \ell(y_n; x_n^\top \theta_2)\|^2 | F_{n-1}) \leq L^2 \|\theta_1 - \theta_2\|^2.$$

(e) Learning rate $\gamma > 0$ is such that $\gamma L^2 (1 + \gamma t) < \lambda (1 + \gamma b)^2$.

To prove Theorem 8, our result for the upper bound on the MSE for constant learning rate ISGD, we first prove the following results:

**Lemma 6** The gradient $\nabla \ell$ is a scaled version of covariate $x$, i.e., for every $\theta \in \mathbb{R}^p$ there is a scalar $\lambda \in \mathbb{R}$ such that

$$\nabla \ell(y; x^\top \theta) = \lambda x.$$

Thus, the gradient in the implicit update is a scaled version of the gradient calculated at the previous iterate, i.e.,

$$\nabla \ell(y_n; x_n^\top \theta_n) = \lambda_n \nabla \ell(y_n; x_n^\top \theta_{n-1}), \quad (15)$$

where the scalar $\lambda_n$ satisfies

$$\lambda_n \ell'(y_n; x_n^\top \theta_{n-1}) = \ell'(y_n; x_n^\top \theta_{n-1} + \gamma \lambda_n \ell'(y_n; x_n^\top \theta_{n-1}) x_n^\top x_n) \quad (16)$$
Proof 6 From the chain rule $\nabla \ell(y_n; x_n^\top \theta_n) = \ell'(y_n; x_n^\top \theta_n)x_n$, and similarly $\nabla \ell(y_n; x_n^\top \theta_{n-1}) = \ell'(y_n; x_n^\top \theta_{n-1})x_n$. Thus the two gradients are collinear. Therefore there exists a scalar $\lambda_n$ such that

$$\ell'(y_n; x_n^\top \theta_n)x_n = \lambda_n \ell'(y_n; x_n^\top \theta_{n-1})x_n$$  \hspace{1cm} (17)

We also have,

$$\theta_n = \theta_{n-1} + \gamma \nabla \ell(y_n; x_n^\top \theta_n) \quad \text{[by definition of implicit SGD update Eq. (14)\]}$$

$$= \theta_{n-1} + \gamma \lambda_n \ell'(y_n; x_n^\top \theta_{n-1})x_n \quad \text{[by chain rule and Eq. (17)\]} \hspace{1cm} (18)$$

Substituting the expression for $\theta_n$ in Eq. (18) into Eq. (17) we obtain the desired result of the theorem. From Eq. (17) we get the equality

$$\ell'(y_n; x_n^\top \theta_n) = \lambda_n \ell'(y_n; x_n^\top \theta_{n-1})$$  \hspace{1cm} (19)

and substituting we get our desired result

$$\lambda_n \ell'(y_n; x_n^\top \theta_{n-1}) = \ell'(y_n; x_n^\top (\theta_{n-1} + \gamma \lambda_n \ell'(y_n; x_n^\top \theta_{n-1})x_n))$$

$$= \ell'(y_n; x_n^\top \theta_{n-1} + \gamma \lambda_n \ell'(y_n; x_n^\top \theta_{n-1})x_n^\top x_n)$$

Lemma 7 Suppose Assumptions 1 (a), and (b) hold. Then, almost surely it holds

$$\frac{1}{1 + \gamma t} \leq \lambda_n \leq \frac{1}{1 + \gamma b}$$  \hspace{1cm} (20)
Proof 7 From Lemma 6 we have
\[ \ell'(y_n; x_n^\top \theta_n) = \lambda_n \ell'(y_n; x_n^\top \theta_{n-1}), \] (21)

where the derivative of the loss function \( \ell \) is with respect to the natural parameter \( x^\top \theta \).

Using the definition of the implicit update Eq. (14),
\[ \theta_n = \theta_{n-1} + \gamma \lambda_n \ell'(y_n; x_n^\top \theta_{n-1}) x_n. \] (22)

We substitute this definition of \( \theta_n \) into Eq. (21) and perform a Taylor approximation on \( \ell' \). Recall Taylor approximation for a function \( f \),
\[ f(x) = f(a) + f'(\xi)(x - a) \]

where \( \xi \) lies in the closed interval between \( a \) and \( x \). From Eq. (22) we let \( \theta_{n-1} = a \) and \( \gamma \lambda_n \ell'(y_n; x_n^\top \theta_{n-1}) x_n = (x - a) \). Also, by the Chain rule
\[ \frac{\delta}{\delta \theta} \ell'(y; x^\top \theta) = \ell''(y; x^\top \theta) x^\top. \]

Thus we obtain,
\[ \ell'(y_n; x_n^\top \theta_n) = \ell'(y_n; x_n^\top \theta_{n-1}) + \ell''(y_n; x_n^\top \tilde{\theta}) x_n^\top \gamma \lambda_n \ell'(y_n; x_n^\top \theta_{n-1}) x_n \]
\[ = \ell'(y_n; x_n^\top \theta_{n-1}) + \gamma \lambda_n \ell''(y_n; x_n^\top \tilde{\theta}) \ell'(y_n; x_n^\top \theta_{n-1}) x_n x_n \] (23)

where \( \tilde{\theta} = \delta \theta_{n-1} + (1 - \delta)\theta_n \) and \( \delta \in [0, 1] \).

By combining Eq. (21) with Eq. (23) and cancelling out the first derivative term we get
\[ \lambda_n = 1 + \gamma \lambda_n \ell''(y_n; x_n^\top \tilde{\theta}) x_n^\top x_n \]
\[ \lambda_n(1 - \gamma \ell''(y_n; x_n^\top \tilde{\theta}) ||x||^2) = 1 \]
\[ (1 + \gamma \text{trace}(\hat{I}_n(\tilde{\theta}))) \lambda_n \leq 1 \text{ [where } \hat{I} \text{ is the observed Fisher information]} \] (24)
\[ (1 + \gamma b) \lambda_n \leq 1 \text{ [By Assumption 1 (b)]} \] (25)

Now we get the other bound,
\[ (1 + \gamma t) \lambda_n \geq 1 \text{ [By Assumption 1 (b)]} \]
Theorem 8 Suppose that Assumptions 1(a) - (e) hold. Then,

\[
\mathbb{E}(||\theta_n - \theta^*||^2) \leq \left(1 - \frac{2\gamma \lambda}{1 + \gamma t} + \frac{2\gamma^2 L^2}{(1 + \gamma b)^2}\right)^n \mathbb{E}(||\theta_{n-1} - \theta^*||^2)
\]

\[
+ \frac{\gamma^2}{\lambda(1 + \gamma b)^2 - \gamma L^2(1 + \gamma t)}
\]

Proof 8 Starting from the implicit update (14), we have

\[
\theta_n - \theta^* = \theta_{n-1} - \theta^* + \gamma \nabla \ell(y_n; x_n^\top \theta_n)
\]

\[
\theta_n - \theta^* = \theta_{n-1} - \theta^* + \gamma \lambda_n \nabla \ell(y_n; x_n^\top \theta_{n-1}) \quad \text{[By Lemma 6]}
\]

\[
||\theta_n - \theta^*||^2 = ||\theta_{n-1} - \theta^*||^2
\]

\[
+ 2\gamma \lambda_n (\theta_{n-1} - \theta^*)^\top \nabla \ell(y_n; x_n^\top \theta_{n-1})
\]

\[
+ ||\gamma \lambda_n \nabla \ell(y_n; x_n^\top \theta_{n-1})||^2
\]

(28)

To bound the last term,

\[
||\gamma \lambda_n \nabla \ell(y_n; x_n^\top \theta_{n-1})||^2
\]

\[
= \gamma^2 \lambda_n^2 ||\nabla \ell(y_n; x_n^\top \theta_{n-1})||^2
\]

\[
= \gamma^2 \lambda_n^2 ||\nabla \ell(y_n; x_n^\top \theta_{n-1}) - \nabla \ell(y_n; x_n^\top \theta^*) + \nabla \ell(y_n; x_n^\top \theta^*)||^2
\]

\[
\leq 2\gamma^2 \lambda_n^2 ||\nabla \ell(y_n; x_n^\top \theta_{n-1}) - \nabla \ell(y_n; x_n^\top \theta^*)||^2 + 2\gamma^2 \lambda_n^2 ||\nabla \ell(y_n; x_n^\top \theta^*)||^2
\]

\[
\leq 2 \left(\frac{\gamma}{1 + \gamma b}\right)^2 (||\nabla \ell(y_n; x_n^\top \theta_{n-1}) - \nabla \ell(y_n; x_n^\top \theta^*)||^2 + ||\nabla \ell(y_n; x_n^\top \theta^*)||^2)
\]

[By Lemma 7] (29)
Taking expectation of both sides of Eq. (29),

\[
\mathbb{E}(|\gamma_n \nabla \ell(y_n; x_n^\top \theta_{n-1})|^2) \\
\leq 2 \left( \frac{\gamma}{1 + \gamma_b} \right)^2 \left[ \mathbb{E}(||\nabla \ell(y_n; x_n^\top \theta_{n-1}) - \nabla \ell(y_n; x_n^\top \theta_*)||^2) + \mathbb{E}(||\nabla \ell(y_n; x_n^\top \theta_*)||^2) \right] \\
\leq 2 \left( \frac{\gamma}{1 + \gamma_b} \right)^2 \left( L^2 \|\theta_{n-1} - \theta_*\|^2 + \sigma^2 \right) \quad \text{[By Lipschitz and gradient bound, Assumption 1 (c), (d)] (30)}
\]

We can bound the expectation of the second term as

\[
\mathbb{E}(2\lambda_n \gamma (\theta_{n-1} - \theta_*)^\top \nabla \ell(y_n; x_n^\top \theta_{n-1})) \\
\geq \frac{2\gamma}{1 + \gamma_t} \mathbb{E}((\theta_{n-1} - \theta_*)^\top \nabla \ell(y_n; x_n^\top \theta_{n-1})) \quad \text{[By Lemma \[7\]} \\
\geq \frac{2\gamma}{1 + \gamma_t} \mathbb{E}((\theta_{n-1} - \theta_*)^\top \nabla h(\theta_{n-1})) \quad \text{[where } \nabla h(\theta_{n-1}) = \mathbb{E}(\nabla \ell(y_n; x_n^\top \theta_{n-1})|\mathcal{F}_{n-1})\] \\
\leq -\frac{2\gamma \lambda}{1 + \gamma_t} \mathbb{E}(\|\theta_{n-1} - \theta_*\|^2) \quad \text{[By strong convexity, Assumption 1 (b)] (31)}
\]

Taking expectations in (28) and substituting inequalities (30) and (31) into (28), and again taking expectation, yields the recursion,

\[
\mathbb{E}(\|\theta_n - \theta_*\|^2) \leq \left( 1 - \frac{2\gamma \lambda}{1 + \gamma t} + \frac{2\gamma^2 L^2}{(1 + \gamma b)^2} \right) \mathbb{E}(\|\theta_{n-1} - \theta_*\|^2) + 2 \left( \frac{\gamma \sigma}{1 + \gamma b} \right)^2 \quad (32)
\]

Let \( \delta_n \equiv \mathbb{E}(\|\theta_n - \theta_*\|^2) \). We can now derive the bound of the theorem as follows:

\[
\delta_n \leq \left( 1 - \frac{2\gamma \lambda}{1 + \gamma t} + \frac{2\gamma^2 L^2}{(1 + \gamma b)^2} \right)^n \delta_0 + \sum_{k=1}^{\infty} 2 \left( \frac{\gamma \sigma}{1 + \gamma b} \right)^2 \left( 1 - \frac{2\gamma \lambda}{1 + \gamma t} + \frac{2\gamma^2 L^2}{(1 + \gamma b)^2} \right)^k \\
= \left( 1 - \frac{2\gamma \lambda}{1 + \gamma t} + \frac{2\gamma^2 L^2}{(1 + \gamma b)^2} \right)^n \delta_0 + \frac{2 \gamma \sigma^2}{1 + \gamma t} \left( 1 - \frac{2\gamma \lambda}{1 + \gamma t} + \frac{2\gamma^2 L^2}{(1 + \gamma b)^2} \right)^{\frac{1}{1+\gamma t} - 1} \\
= \left( 1 - \frac{2\gamma \lambda}{1 + \gamma t} + \frac{2\gamma^2 L^2}{(1 + \gamma b)^2} \right)^n \delta_0 + \frac{\gamma \sigma^2(1 + \gamma t)}{\lambda(1 + \gamma b)^2 - \gamma L^2(1 + \gamma t)}
\]
Lemma 9 Suppose that Assumption 1(e) holds. The discount factor of the non-asymptotic bound in Theorem 8 will be bounded $0 < \cdot < 1$ for all $\gamma > 0$, and thus the mean squared error $\mathbb{E}(\|\theta_n - \theta^*\|^2)$ will contract for all possible values of $\gamma$. In addition the stationary term will be $> 0$ for all $\gamma > 0$.

Proof 9 The discount factor is bounded below by

$$
1 - \frac{2\gamma \lambda}{1+\gamma b} + \frac{2\gamma^2 L^2}{(1+\gamma b)^2}
$$

because $b \leq t$. We will show that this term is bounded below by 0.

A quick manipulation of the algebra gives us

(lower bound) \[ 2\gamma \lambda (1 + \gamma b) - 2\gamma^2 L^2 < (1 + \gamma b)^2 \tag{33} \]

(upper bound) \[ \gamma L^2 (1 + \gamma t) < \lambda (1 + \gamma b)^2 \tag{34} \]

(stationary bound) \[ \gamma L^2 (1 + \gamma t) < \lambda (1 + \gamma b)^2 \tag{35} \]

Both the upper bound and stationary bound are satisfied by Assumption 1(e). Further manipulating the lower bound, from Eq. (33),

$$
2\gamma \lambda + 2\gamma^2 \lambda b - 2\gamma^2 L^2 < 1 + 2\gamma b + \gamma^2 b^2
$$

$$
\gamma^2 (b^2 - 2\lambda b + 2L^2) + \gamma (2b - 2\lambda) + 1 > 0 \tag{36}
$$

Solving the equality of Eq. (36) (with the quadratic equation) gives us

$$
\frac{(2\lambda - 2b) \pm \sqrt{(2b - 2\lambda)^2 - 4(2\lambda^2 - 2\lambda b + 2L^2)}}{2(b^2 - 2\lambda b + 2L^2)} = (2\lambda - 2b) \pm \frac{\sqrt{4\lambda^2 - 8L^2}}{2(b^2 - 2\lambda b + 2L^2)}
$$

$$
= (\lambda - b) \pm \frac{\sqrt{\lambda^2 - 2L^2}}{b^2 - 2\lambda b + 2L^2}
$$

35
Recall that for a second-degree polynomial of the form \(a_2x^2 + a_1x + 1\), the convexity is determined by \(a_2\). Because \(L \geq \lambda\) (a standard assumption), the discriminant \((\lambda^2 - 2L^2) < 0\) and thus there are no real roots. Looking at the convexity,

\[
(b^2 - 2\lambda b + 2L^2) > (b^2 - 2\lambda b + \lambda^2) = (b - \lambda)^2 > 0
\]

The strict inequality is because of the following. For all observed Fisher information matrices, (with \(p\) the dimension)

\[
\text{trace}(\hat{I}_n(\theta)) \geq b \Rightarrow \mathbb{E}\text{trace}(\hat{I}_n(\theta)) \geq b \Rightarrow \lambda \cdot p \geq b
\]

Thus for all \(\gamma \in \mathbb{R}\) the lower bound represented by Eq. (33) is satisfied. We have zero real roots and a convex function.

C Computation of ISGD

Here, we show that the ISGD procedure can be computed efficiently. Most of the ideas here have been presented in earlier work (Kivinen et al., 2006; Kulis and Bartlett, 2010; Toulis et al., 2014), but we present them here as well for clarity and completeness.

Consider the ISGD procedure:

\[
\theta_n = \theta_{n-1} - \gamma \nabla \ell(y_n, x_n^\top \theta_n).
\]

Note that \(\nabla \ell(y, x^\top \theta) = h(y, x^\top \theta)x\), where \(h\) is scalar and is defined as \(h(y, \eta) = \partial \ell(y, \eta)/\partial \eta\). Therefore we can write, for some \(\xi \in \mathbb{R}\),

\[
\theta_n = \theta_{n-1} - \gamma \xi h(y_n, x_n^\top \theta_{n-1})x_n = \theta_{n-1} - \gamma \xi h_{n-1}x_n, \tag{37}
\]
\[ \theta_n = \theta_{n-1} - \gamma h(y_n, x_n^\top \theta_{n-1}) x_n, \]  

(38)

Substituting Eq. (37) into Eq. (38) we get

\[ \theta_n = \theta_{n-1} - \gamma h(y_n, x_n^\top \theta_{n-1} - \gamma \xi h_{n-1} |x_n||^2) x_n, \]  

(39)

Equating Eq. (39) and Eq. (37) we conclude that

\[ \xi h_{n-1} = \gamma h(y_n, x_n^\top \theta_{n-1} - \gamma \xi h_{n-1} |x_n||^2), \]

which is a one-dimensional fixed-point equation for \( \xi \). We can also see that \( \xi \in [h_{n-1}, 0] \) if \( h_{n-1} < 0 \), or \( \xi \in [0, h_{n-1}] \) if \( h_{n-1} > 0 \). Thus, search bounds are available for \( \xi \) and solving the fixed-point equation is very fast. Given \( \xi \), the implicit update can be readily computed through Eq. (37).