Invexifying Regularization of Non-Linear Least-Squares Problems

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Abstract

We consider regularization of non-convex optimization problems involving a non-linear least-squares objective. By adding an auxiliary set of variables, we introduce a novel regularization framework whose corresponding objective function is not only provably invex, but it also satisfies the highly desirable Polyak–Lojasiewicz inequality for any choice of the regularization parameter. Although our novel framework is entirely different from the classical \( \ell_2 \)-regularization, an interesting connection is established for the special case of under-determined linear least-squares. In particular, we show that gradient descent applied to our novel regularized formulation converges to the same solution as the linear ridge-regression problem. Numerical experiments corroborate our theoretical results and demonstrate the method’s performance in practical situations as compared to the typical \( \ell_2 \)-regularization.

1 Introduction

Consider the non-linear regression problem

\[
\min_x \left\{ f(x) \triangleq \frac{1}{2} \|g(x)\|^2 \right\}, \tag{1}
\]

where \( g : \mathbb{R}^d \to \mathbb{R}^n \) is a non-linear sufficiently smooth mapping. Problems of this form are very common in the field of machine learning, where \( g \) and \( x \), respectively, represent the model to train/fit and its parameters. For example, a nonlinear regression task involving a neural-network model \( g \) with weights parameters \( x \) and a least-squares loss (Goodfellow et al., 2016). Here, each component of the vector valued function \( g \) can correspond to an individual input from a training dataset of size \( n \). Beyond machine learning, such problems arise frequently across many areas of science and engineering, e.g., PDE-constrained inverse problems (Roosta et al., 2014a,b). Historically, low-dimensional models \( (d \leq n) \) have been used to great effect over a diverse range of practical settings (Bates and Watts, 2007). In recent years, driven by modern machine-learning applications, more attention has been given to problems (1) in which \( f \) is high-dimensional \( (d \gg 1) \) and even over-parameterized \( (d \gg n) \). Notable examples include generative models like auto-encoders, (Chen et al., 2019), and generative adversarial networks, (Mao et al., 2017). In all these cases, the training/fitting often involves some form of regularization of (1). In principle, there are two, often complementary, perspectives on regularization: one from the viewpoint of improving generalization and predictive performance, and the other with regards to improving the optimization landscape as a way to facilitate the training procedure.

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Regularization to Improve Generalization. In all machine learning problems, avoiding the pitfalls of over-fitting and improving generalization performance constitute a major challenge in the training procedure (Mohri et al., 2018; Shalev-Shwartz and Ben-David, 2014). This is particularly important in over-parameterized settings or small-data learning tasks, where over-fitting can be a major hindrance in obtaining good out-of-sample predictive performance.

In this light, various regularization techniques have been proposed to mitigate over-fitting in a variety of settings. These techniques range from the traditional ridge-type $\ell_2$-regularization, to more recent techniques such as weight decay (Krogh and Hertz, 1992; Loshchilov and Hutter, 2017), dropout (Hinton et al., 2012; Baldi and Sadowski, 2013), and various data augmentation techniques (Shorten and Khoshgoftaar, 2019). One can broadly, and perhaps loosely, categorize these regularization techniques into two main groups: those that directly regularize the model to reduce its representational capacity, e.g., $\ell_2$-regularization, weight decay, and dropout, and those that instead aim to enhance the size and quality of training datasets, e.g., data augmentation. It is also typical to see these regularization techniques used in conjunction with one another.

Regularization to Facilitate Optimization. Unless $g$ is a linear map, the problem (1) amounts to a non-convex optimization problem. In this light, the vast majority of optimization research has typically focused on developing (general purpose) optimization algorithms that, in the face of such non-convexity, come equipped with strong convergence guarantees, e.g., Cutkosky and Orabona (2019); Basu et al. (2019); Vogels et al. (2019); Muecke et al. (2019); Yu and Jin (2019); Haddadpour et al. (2019); Xu et al. (2020); Tripuraneni et al. (2018); Bellavia et al. (2020); Wang et al. (2019); Blanchet et al. (2019); Gupta et al. (2018); Anil et al. (2020); Yao et al. (2020); Liu and Roosta (2021). However, most of these methods involve subtleties and disadvantages that can make their use far less straightforward in many training procedures. For example, complex, computationally intensive, and non-trivial steps in the algorithm and/or difficulty in fine-tuning the underlying hyper-parameters.

As a result, to improve the optimization landscape of (1) and lessen the challenges faced by the optimization procedure, and hence to facilitate the training procedure, one can “perturb” the original problem (1) to a nearby problem, which exhibits more favorable structural properties, e.g., better condition number, “rounder” level-sets, better smoothness properties, etc. Perhaps, the simplest and the most well-known strategy for this purpose is the traditional $\ell_2$-regularization, which instead of (1) considers the alternative objective $f(x) + \lambda \|x\|^2$ for some constant $\lambda > 0$. This technique attempts to improve upon the conditioning of the problem (1) by “smoothing out” the highly non-convex regions of its landscape.

Complementary in Spirit, but Conflicting in Reality. Although, these two viewpoints on regularization are complementary in spirit, the underlying techniques employed can at times be at odds with each other. For example, to smooth out the optimization landscape, consider the $\ell_2$ regularization of (1) as $f(x) + \lambda \|x\|^2$. Although this new objective might have better structural properties than the original non-regularized problem, e.g., better conditioning and “rounder” level-sets, it can still be non-convex and challenging to optimize. In fact, it will only be convex for sufficiently large values of $\lambda$, and the lower-bound of such values relies on practically unknowable constants related to the spectrum of the Hessian of $f$. However, for such large values, the benefits offered by the convexity of the regularized function comes at a great cost: the obtained solution will most likely be far too biased to be relevant to the original problem or any out-of-sample
generalizations (Golatkar et al., 2019). In this light, a regularization technique that can offer the best of both worlds is highly desirable. Our aim in this paper is to propose one such regularization method that not only can greatly improve generalization performance, but it also provably offers a structurally easier model to train/fit.

1.1 Our Approach and Contributions

Our novel regularization framework involves adding an auxiliary set of variables, and in essence “lifting” the original optimization problem to higher dimensions. The additional set of variables are directly coupled with the output of the non-linear mapping $g$. In this light, not only does our framework regularize the model itself, but it also non-trivially and adaptively interacts with the input training data throughout training. We show that the new regularized problem, though still non-convex, will enjoy several highly-desirable properties, which can greatly facilitate the training procedure. Remarkably, these properties hold regardless of the non-linear mapping, $g$, and the regularization parameter.

Assuming $g$ is differentiable, we recall that analyzing the Jacobian of $g$, denoted by $J_g$, gives insights to the optimization landscape of (1), e.g., Zhang et al. (2018); Golatkar et al. (2019); Li et al. (2018). In general, this Jacobian may be rank-deficient over sets of points in $\mathbb{R}^d$. In such situations, the optimization landscape may exhibit a high degree of non-convexity. The key insight is that when $J_g$ has full row-rank, the structure of (1) guarantees valuable properties of $f$, which we shall soon detail. To enforce this situation, we introduce an auxiliary variable $p \in \mathbb{R}^n$ and consider the new optimization problem

$$\min_{x,p} \left\{ \hat{f}(x,p) = \frac{1}{2} \|g(x) + \lambda p\|^2 \right\}, \tag{2}$$

where $\lambda > 0$ is a pre-selected constant. Clearly, the the Jacobian of $g(x) + \lambda p$, which is $[J_g(x) \quad \lambda I]$, is guaranteed to have full row-rank for any value of $\lambda > 0$. This will have profound, and highly desirable, implications on the loss landscape of $\hat{f}$. Specifically, we show that (2) induces the following properties, which are formalized in Section 2.

Contributions. Let us briefly highlight our contributions.

(i) We first show that our novel regularization framework coincides, in an intriguing manner, with the classical $\ell_2$-regularization, for the special case when $g$ is an affine mapping.

(ii) For arbitrarily non-linear $g$, we then show that the function $\hat{f}$, in (2), is invex for any value of $\lambda$ (Theorem 2-(i)), which is a pleasant “middle ground” between convexity and non-convexity.

(iii) More importantly, we show the function $\hat{f}$ satisfies the highly desirable Polyak–Lojasiewicz (PL) inequality for any value of $\lambda$ (Theorem 2-(ii)), which allows for exponentially fast convergence of many optimization algorithms.

(iv) We finally study the empirical performance of our novel regularization framework on several challenging ML problems.
Remark 1. Note that \( \min_{x,p} \hat{f}(x, p) = 0 \), i.e., the new regularization amounts to an interpolating model. In sharp contrast to the classical \( \ell_2 \)-regularization whose optimal value is almost always non-trivial, the interpolation property of (2) provides a significantly useful feature in practice. Namely, it allows for monitoring convergence by simply inspecting the training loss.

To our knowledge, the reformulation (2) and the addition of auxiliary variable \( p \) is novel. However, our approach here, in some sense, can be loosely connected with those presented by Liang et al. (2018); Kawaguchi and Kaelbling (2020) in which by adding one special neuron per output unit, the loss landscape is modified in a way that all sub-optimal local minima of the original problem are eliminated, i.e., one can recover the global optima of the original problem from the local minima of the modified problem. However, although the approach by Kawaguchi and Kaelbling (2020) applies more generally beyond non-linear least squares, the loss landscape remains highly non-convex with potentially many local minima, saddle points, and local maxima. Whereas, the invexity of (2) implies that all its stationary points are global optima.

One may also see some similarities between our approach and that of Hamiltonian Monte Carlo methods (HMC), where the original sample space involving “position” variables, is lifted to include auxiliary “momentum” variables (Neal et al., 2011; Betancourt, 2017). In this light, the sampling from the position-momentum phase-space in HMC resembles optimization of \( \hat{f} \) over the augmented space \((x, p) \in \mathbb{R}^{d+n}\).

2 Theoretical Analysis

Comparing (2) to the usual \( \ell_2 \)-regularization, one could suggest that in the reformulation (2), the data is being regularized instead of the parameters. This introduces highly non-trivial and adaptive interactions between the data and the variable \( p \) throughout the training procedure. In this section, we aim to develop some theoretical insights into structural properties of the proposed regularization method (2) and on the consequential effects to the training procedure.

2.1 Connection to \( \ell_2 \)-regularization

To study properties of (2), it might be more insightful to start with the simplest possible case where \( g \) is just an affine map. Clearly, this setting amounts to (1) being simply an ordinary least-squares problem. Although the reformulation (2) is completely different than the classical \( \ell_2 \)-regularization, surprisingly, it turns out that when \( g \) is affine these two regularization methods coincide. More specifically, in Theorem 1, we show that gradient descent (GD) applied to (2) converges to the unique solution of the classical ridge-regression problem.
Theorem 1 (Linear Least-Squares). Consider (1) with \( g(x) = Ax - b \), such that \( A \in \mathbb{R}^{n \times d} \) has full row-rank and \( b \in \mathbb{R}^n \), and then consider applying GD to (2), using a sufficiently small fixed step-size and starting from the origin \((x_0, p_0) = (0, 0)\). We have

(i) The iterates \( x_t \) converge to the unique solution of the ridge-regression problem. Namely,

\[
\lim_{t \to \infty} x_t = x^*(\lambda) \triangleq \arg \min_x \{ \|Ax - b\|^2 + \lambda\|x\|^2 \} = (A^T A + \lambda^2 I)^{-1} A^T b.
\]

(ii) Furthermore, \( x^*(\lambda) \) behaves consistently with the ridge-regression solution in the limiting cases of \( \lambda \). That is,

\[
\lim_{\lambda \to 0} x^*(\lambda) = \lambda^{\dagger} b, \quad \lim_{\lambda \to \infty} x^*(\lambda) = 0, \quad \lim_{\lambda \to 0} f(x^*(\lambda)) = 0, \quad \lim_{\lambda \to \infty} f(x^*(\lambda)) = \|b\|^2,
\]

where \( \lambda^{\dagger} \) denotes the Moore–Penrose inverse of \( A \) and \( f \) is as in (1).

Proof. Here, our regularized function (2) is given by

\[
\hat{f}(x, p) = \frac{1}{2}\|Ax - b + \lambda p\|^2 = \frac{1}{2}\left\| \begin{bmatrix} A & \lambda I \end{bmatrix} \begin{bmatrix} x \\ p \end{bmatrix} - b \right\|_2^2.
\]

This involves a full row-rank coefficient matrix. Therefore, using a sufficiently small fixed step-size and starting from the origin \((x_0, p_0) = (0, 0)\), it is a well known result that the iterates from GD applied to this function will converge to the minimum-norm solution; for example, refer to Soudry et al. (2018). The minimum-norm solution is

\[
\begin{bmatrix} x^*(\lambda) \\ p^*(\lambda) \end{bmatrix} = \begin{bmatrix} A & \lambda I \end{bmatrix}^{\dagger} b = \begin{bmatrix} A^T \\ \lambda I \end{bmatrix} (AA^T + \lambda^2 I)^{-1} b = \frac{(A^T A + \lambda^2 I)^{-1} A^T b}{\lambda (AA^T + \lambda^2 I)^{-1} b}
\]

Clearly, \( \lim_{\lambda \to 0} x^*(\lambda) = A^{\dagger} b \) and \( \lim_{\lambda \to \infty} x^*(\lambda) = 0 \).

Since GD will converge to a global optimum of \( \hat{f} \), we have \( p^*(\lambda) = (b - Ax^*(\lambda))/\lambda \). Together with the property that all iterates \( x_t \) are in the range of \( A^T \) by definition of GD, we have

\[
x^*(\lambda) = A^T(AA^T)^{-1}(b - \lambda p^*(\lambda)).
\]

Therefore,

\[
f(x^*(\lambda)) = \frac{1}{2}\|AA^T(AA^T)^{-1}(b - \lambda p^*(\lambda)) - b\|^2 = \frac{1}{2}\|\lambda p^*(\lambda)\|^2 = \frac{1}{2}\|\lambda^2 (AA^T + \lambda^2 I)^{-1} b\|^2,
\]

with \( \lim_{\lambda \to 0} f(x^*(\lambda)) = 0, \lim_{\lambda \to \infty} f(x^*(\lambda)) = \|b\|^2 \). ■

2.2 General Non-linear Mapping \( g \)

As mentioned in Section 1, a fundamental distinction between our proposed formulation and \( \ell_2 \)-regularization becomes apparent when moving beyond the simple linear least-squares case of Theorem 1. This difference mainly lies in the fact that our new objective function retains fundamental aspects of its structure, regardless of the choice of \( \lambda > 0 \) or the function \( g \). In particular, the optimization landscape of the typical \( \ell_2 \)-regularized function, given by \( f(x) + \lambda \|x\|^2 \), can range from convex to highly non-convex, all depending on the non-trivial, and often unknown, interplay
between curvature of $f$ and the choice of $\lambda$. Whereas, the optimization landscape induced from our regularization in (2) retains its highly desirable structural properties of invexity and PL property, for any $\lambda > 0$.

Invexity was introduced to extend the sufficiency of the first-order optimality condition beyond simple convex programming (Mishra and Giorgi, 2008; Cambini and Martein, 2008). As a result, a differentiable function, for example, is invex if and only if all its critical points are global minima. PL inequality (Karimi et al., 2016), in fact, characterizes a special class of invex functions for which many optimization algorithms can be shown to converge exponentially fast. In its introductory paper, Polyak (1963) showed that GD enjoys a global linear convergence-rate under this condition. In recent years, it has garnered increased attention from the machine-learning community. For example, it has been at the heart of many convergence-proofs outside the limitations of strong-convexity, e.g., (Karimi et al., 2016; Bassily et al., 2018; Vaswani et al., 2019; Gower et al., 2021; Yuan et al., 2018; Ajalloeian and Stich, 2020). This inequality also has connections to other topics of interest, including over-parametrization and interpolation (Vaswani et al., 2019). For example, it has been shown that sufficiently-wide and over-parameterized neural networks, under certain assumptions, induce the PL inequality (Liu et al., 2020).

**Theorem 2 (Invexity and PL Inequality).** Suppose $g$ is differentiable and let $\lambda > 0$. The function $\hat{f}$ in (2) has the following properties.

(i) **(Invexity)** All stationary points are global minima. In particular, for all $x, y \in \mathbb{R}^d$ and $p, q \in \mathbb{R}^n$, we have

$$\hat{f}(x, p) - \hat{f}(y, q) \geq \langle \eta(x, p, y, q), \nabla \hat{f}(y, q) \rangle,$$

where

$$\eta(x, p, y, q) = [J_g(y)\lambda I]^\dagger \left( (g(x) + \lambda p) - (g(y) + \lambda q) \right).$$

(ii) **(Polyak–Lojasiewicz Inequality)** For all $x \in \mathbb{R}^d$ and $p \in \mathbb{R}^n$, we have

$$\hat{f}(x, p) \leq \frac{1}{2\lambda^2} \| \nabla \hat{f}(x, p) \|^2.$$

**Proof.**

(i) **(Invexity)** Consider the Jacobian of $g(x) + \lambda p$, which is $[J_g(x) \lambda I]$. As it is guaranteed to have full row-rank, its pseudo-inverse acts as a right inverse. Together with the convexity of the $\ell_2$-norm squared, we have, for all $x, y \in \mathbb{R}^d$ and $p, q \in \mathbb{R}^n$,

$$\hat{f}(x, p) - \hat{f}(y, q) = \frac{1}{2} \| g(x) + \lambda p \|^2 - \frac{1}{2} \| g(y) + \lambda q \|^2$$

$$\geq \left\langle (g(x) + \lambda p) - (g(y) + \lambda q), (g(y) + \lambda q) \right\rangle$$

$$= \langle \eta(x, p, y, q), \nabla \hat{f}(y, q) \rangle,$$
(ii) (Polyak–Lojasiewicz Inequality) Replacing $I$ with $\left( [J_g(x) \lambda I] [J_g(x) \lambda I]^T \right)^T$, we have

$$\hat{f}(x, p) = \frac{1}{2} \|I(g(x) + \lambda p)\|^2 = \frac{1}{2} \left\| \left( [J_g(x) \lambda I]^T \left[ J_g(x) \lambda I \right] \right) (g(x) + \lambda p) \right\|^2 = \frac{1}{2} \left\| \left( [J_g(x) \lambda I]^T \nabla \hat{f}(x, p) \right) \right\|^2.$$

Expanding and using that fact that the smallest non-zero eigenvalue of $[J_g(x) \lambda I]^T [J_g(x) \lambda I]$ is at least $\lambda^2$, we obtain the PL inequality.

So far, we have only made the basic assumption of $g$ being differentiable. Yet, from this alone, Theorem 2 shows that our regularized function (2) carries important structural guarantees, unlike that of $\ell_2$-regularization. It is commonplace in machine-learning literature to have assumptions on smoothness, i.e., on the Lipschitz continuity of the gradient, to obtain additional convergence guarantees for a given optimization algorithm. In this vein, by additionally making a reasonable assumption about twice continuous differentiability of $g$ on a compact ball, in Assumption 1, our regularized objective (2) is shown to be also locally Lipschitz-continuous on a compact ball. This is formalized in Theorem 3.

**Assumption 1.** Given $\lambda > 0$ and $x_0 \in \mathbb{R}^d$, assume the non-linear mapping $g$ is twice-continuously differentiable on the compact ball $D(x_0, \lambda) = \{ x \mid \|x - x_0\| \leq R(x_0, \lambda) \}$, where we have defined $R(x_0, \lambda) = 2 \sqrt{2\Delta_0 / \lambda}$ and $\Delta_0 = f(x_0) - \min_x f(x)$.

**Theorem 3 (Smoothness of $\hat{f}(x, p)$).** Under Assumption 1, let $\hat{D}(x_0, \lambda)$ denote the compact ball around $(x_0, 0)$ of radius $R(x_0, \lambda)$, i.e.,

$$\hat{D}(x_0, \lambda) = \left\{ (x, p) \mid \left\| \begin{bmatrix} x - x_0 \\ p \end{bmatrix} \right\| \leq R(x_0, \lambda) \right\},$$

where $R(x_0, \lambda)$ is as in Assumption 1. The function $\hat{f}$ in (2) is $L(x_0, \lambda)$-smooth on $\hat{D}$ for some constant $L(x_0, \lambda)$ that depends on $x_0$ and $\lambda$.

**Proof.** Consider the Hessian

$$\nabla^2 \hat{f}(x, p) = \left[ J_g^T(x) \lambda I \right] J_g(x) \lambda I + \left[ \lambda \nabla^2 \langle p, g(x) \rangle + \sum g_i(x) \nabla^2 g_i(x) \right] 0.$$ 

Therefore, $\| \nabla^2 \hat{f}(x, p) \|$ is upper bounded by

$$\lambda^2 + \| J_g(x) \|^2 + \| \nabla^2 g(x) \| \| g(x) \| + \lambda \| \nabla^2 \langle p, g(x) \rangle \|.$$ 

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Assumption 1 implies there exist constants $M(x_0, \lambda) < \infty$ and $N(x_0, \lambda) < \infty$, depending on $x_0$ and $\lambda$, such that $\|g(x) - g(y)\| \leq M(x_0, \lambda)\|x - y\|$ and $\|J_g(x) - J_g(y)\| \leq N(x_0, \lambda)\|x - y\|$, for all $x, y \in \mathcal{D}(x_0, \lambda)$ as defined in Assumption 1. Note that for any $(x, p) \in \hat{D}(x_0, \lambda)$, we have $x \in \mathcal{D}(x_0, \lambda)$. Therefore,

\[
\|\nabla^2 g(x)\| \leq N(x_0, \lambda) \\
\|g(x)\| \leq \|g(x) - g(x_0)\| + \|g(x_0)\| \\
\leq M(x_0, \lambda)\|x - x_0\| + \|g(x_0)\| \\
\leq M(x_0, \lambda) \cdot R(x_0, \lambda) + \|g(x_0)\|, \\
\|J_g(x)\| \leq \|J_g(x) - J_g(x_0)\| + \|J_g(x_0)\| \\
\leq N(x_0, \lambda)\|x - x_0\| + \|J_g(x_0)\| \\
\leq N(x_0, \lambda) \cdot R(x_0, \lambda) + \|J_g(x_0)\|, \\
\|\nabla^2(p, g(x))\| \leq N(x_0, \lambda)\|p\| \\
\leq N(x_0, \lambda) \cdot R(x_0, \lambda),
\]

for all $(x, p) \in \hat{D}$. Substituting these into the upper bound of $\|\nabla^2 \hat{f}(x, p)\|$ proves our claim. ■

Note that we have deliberately omitted the term $p_0$ from Assumption 1. Hence, our forthcoming convergence results assume that GD begins at the point $(x_0, 0)$ instead of the more general $(x_0, p_0)$. Although the generalized case is derivable without significant modifications, we find that it obfuscates the interoperability and significance of our results.

Since the introductory paper by Polyak (1963), it has become increasing well known in machine-learning literature that GD enjoys a global linear convergence-rate under the conditions of smoothness and the PL inequality. For example, Oymak and Soltanolkotabi (2019) considered that path obfuscates the interoperability and significance of our results. Corollary 1 is the immediate result of applying Theorems 2 and 3 to their findings.

For regularized loss, the problem of binary classification with squared-loss. The non-regularized function value evaluated at the iterates is also plotted. We see that a smaller choice of $\lambda$ relates to slower convergence in (2) and a lower non-regularized loss. Further study on this trade-off is left as future work. Note, the same step-size is used for all runs.
Corollary 1. Under Assumption 1, let $R(x_0, \lambda)$ and $L(x_0, \lambda)$ be as in Theorem 3. Starting from the point $(x_0, p_0) = (x_0, 0)$ and using a fixed step-size $\alpha \leq 1/L(x_0, \lambda)$, the iterates $(x_t, p_t)$ obtained via the GD updates

$$
\begin{bmatrix}
x_{t+1} \\
p_{t+1}
\end{bmatrix} = \begin{bmatrix}
x_t \\
p_t
\end{bmatrix} - \alpha \nabla \hat{f}(x_t, p_t),
$$

satisfy, for all $t \geq 0$,

$$
\hat{f}(x_t, p_t) \leq \left(1 - \frac{\lambda^2}{L(x_0, \lambda)}\right)^t \hat{f}(x_0, 0), \quad \text{and} \quad \sum_{t=0}^{\infty} \left(\begin{bmatrix}x_{t+1} \\
p_{t+1}\end{bmatrix} - \begin{bmatrix}x_t \\
p_t\end{bmatrix}\right) \leq R(x_0, \lambda).
$$

In Corollary 1, we have the global linear convergence-rate of GD on our regularized function (2), for any $\lambda > 0$. Moreover, the total length of the path taken by the iterates of GD never exceeds $R(x_0, \lambda)$, i.e., the iterates remain inside the ball $\tilde{D}(x_0, \lambda)$.

Perhaps, one might also wonder how the solution $x_t$ obtained from applying GD to the regularized problem (2) relates to the non-regularized problem (1)? For iterates of GD, we have $p_{t+1} = p_0 - \alpha \lambda \sum_{i=0}^{t}(g(x_i) + \lambda p_i)$. Using $p_0 = 0$ and $\alpha \leq 1/L(x_0, \lambda)$, Corollary 1 implies

$$
\|p_{t+1}\| = \alpha \lambda \|g(x_0)\| \sum_{i=0}^{t} \left(1 - \frac{\lambda^2}{L(x_0, \lambda)}\right)^{i/2}
\leq \frac{\alpha \lambda}{1 - \sqrt{1 - \lambda^2/L(x_0, \lambda)}} \|g(x_0)\|
= \alpha L(x_0, \lambda) \left(1 + \sqrt{1 - \lambda/L(x_0, \lambda)}\right) \|g(x_0)\|/\lambda
\leq \left(1 + \sqrt{1 - \lambda/L(x_0, \lambda)}\right) \|g(x_0)\|/\lambda.
$$

Now, it follows that

$$
\|g(x_t)\| \leq \sqrt{1 - \lambda/L(x_0, \lambda)}^t \|g(x_0)\| + \lambda \|p_t\|
\leq \sqrt{1 - \lambda/L(x_0, \lambda)}^t \|g(x_0)\| + \left(1 + \sqrt{1 - \lambda/L(x_0, \lambda)}\right) \|g(x_0)\|,
$$

for all iterations $t \geq 0$. Although worst-case and pessimistic, this bound gives a qualitative, albeit very loose, guide to the effect of $\lambda$ in training. It appears that smaller values of $\lambda$ amount to smaller regularization bias, at the cost of slower convergence for GD, and vice-versa. This observation is also supported by our numerical simulations; see Figure 1. This, in some very loose sense, is reminiscent of the classical bias-variance trade-off from statistics. Further investigation of the role of $\lambda$ in this context is left for future work.

3 Experiments

In this section, we examine the empirical performance of our proposed method in comparison to $\ell_2$-regularization. To align with our theoretical results, we initialize $p$ with zeros in all experiments,
Figure 2: Results of training a VAE model on 16 × 16 real-world handwritten digits from Buscema (1998). Here, we plot the non-regularized function value on the seen training dataset and unseen test dataset. Our method performs more consistently across all values of $\lambda$, and with $\lambda = 0.01$ it yields the best non-regularized function values. This includes the run where $\lambda = 0$, i.e., where the non-regularized function (1) is optimized directly.

Table 1: Performance of trained VAE models after 1000 epochs. This is measured by the non-regularized function value on the seen training dataset and unseen test dataset, and the FID and KID scores using model’s output images. Lower values are better, with the best value presented in boldface. Our method with $\lambda = 10^{-2}$ attained the best value in each metric.

|                        | Our Method | $\ell_2$ Regularization |
|------------------------|------------|-------------------------|
|                        | $\lambda = 0$ | $\lambda = 10^{-2}$ | $\lambda = 10^{-4}$ | $\lambda = 10^{-8}$ | $\lambda = 10^{-2}$ | $\lambda = 10^{-4}$ | $\lambda = 10^{-8}$ |
| Train Data Loss        | 38.31      | 36.42                   | 37.40                | 37.94                | 56.15               | 55.96                 | 37.02               |
| Test Data Loss         | 48.42      | 46.94                   | 48.55                | 48.16                | 57.15               | 57.24                 | 50.09               |
| FID Score              | 402.8      | 376.0                   | 391.7                | 390.2                | 414.9               | 410.2                  | 380.3               |
| KID Score              | 0.534      | 0.478                   | 0.520                | 0.512                | 0.577               | 0.627                  | 0.504               |

i.e., $p_0 = 0$. We will begin with, for illustrative purposes, a simple toy example of binary classification with squared-loss on synthetic data. Afterwards, we consider more realistic and challenging examples of generative models. All experiments are deterministic. Namely, all models, in a given experiment, are initialized from the same weights. Moreover, generated images are from the same random latent vector across regularization techniques.
For the generative models, we compute their Fréchet Inception Distance (FID) score (Heusel et al., 2017) and Kernel Inception Distance (KID) score (Bińkowski et al., 2018). These are commonly used and well regarded metrics for assessing generative models. We compute the score between the set of unseen real images from the test dataset and an equally sized set of generated fake images. Note, these fake images are generated from the same latent vectors across the training epochs and regularization techniques. Lower FID and KID scores are better.
Figure 4: Training a DCGAN on 64 × 64 images from the LFW dataset. Our method performs more consistently across all values of λ, and with λ = 0.0001 it yields the best FID and KID scores amongst all runs. This includes the run where λ = 0, i.e., where (1) is optimized directly. Note that the vertical axes are logarithmic.

Binary Classification With Squared-loss

In Figure 1, and to verify our theory, we consider (1) with \( f(x) = \| \sigma(Ax) - b \|^2 / 2 \), where \( \sigma \) denotes the element-wise sigmoid function, \( A \in \mathbb{R}^{64 \times 8} \), and \( b \) has elements from \{0, 1\}. The data \( A \) and \( b \) are synthetic. GD is used with the same step-size across all runs. Here, we observe that smaller values of λ in (2) result in convergence to points that return smaller function values of the original non-regularized objective function (1), i.e., a smaller regularization bias. However, this comes at the cost of slower convergence rate. Indeed, increasing λ amounts to a larger PL constant, which in turn results in faster convergence for GD on (2). The interpolation property of (2), to numerical accuracy, can be seen for all values of λ.

Variational Auto-encoder

In Figures 2 and 3, we train a deep variational auto-encoder (VAE) model (Kingma and Welling, 2013) on 16 × 16 real-world handwritten digits from Buscema (1998). For this class of models, we use the commonly implemented training procedure that was introduced by Radford et al. (2015). Namely, to use the Adam optimizer (Kingma and Ba, 2014) with the momentum term \( \beta_1 = 0.5 \). We also use a learning rate of 0.001 and batch size of 1. Relative to \( \ell_2 \)-regularization in Figure 2, our method is far more consistent between different values of λ. This, yet again, offers a highly desirable practical advantage. Indeed, the reduced difficulty of hyper-parameter tuning may amount to considerable cost savings over time in a practical setting. As indicated by Table 1, our method obtains the model with the lowest non-regularized function value on the seen training dataset and unseen test dataset, as well as the best final FID and KID scores. Some output images are shown in Figure 3. Our approach yields sharper and more realistic images with less artifacts, compared
No Regularization

Our Method, $\lambda = 1.0$

$\ell_2$ Regularization, $\lambda = 1.0$

Our Method, $\lambda = 0.01$

$\ell_2$ Regularization, $\lambda = 0.01$

Our Method, $\lambda = 0.0001$

$\ell_2$ Regularization, $\lambda = 0.0001$

Figure 5: DCGAN generated images after 100 epochs.

with the alternative.

**Deep Convolutional GAN**

Finally, in Figures 4 and 5, we consider the challenging problem of training a deep convolutional generative adversarial network (DCGAN) (Radford et al., 2015) on $64 \times 64$ real-world images from the Labeled Faces in the Wild (LFW) dataset (Huang et al., 2007). For this class of models, we use the commonly implemented training procedure that was introduced by Radford et al. (2015). Namely, to use the Adam optimizer (Kingma and Ba, 2014) with the momentum term $\beta_1 = 0.5$. We also use a learning rate of 0.0001 and batch size of 1. As was the case of the VAE, our method is far more consistent than $\ell_2$-regularization between different values of $\lambda$. Moreover, our approach yields more realistic and consistent images, with less artifacts, compared with the alternative in Figure 5.
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