Neural Optimization Kernel: Towards Robust Deep Learning

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Abstract

Deep neural networks (NN) have achieved great success in many applications. However, why do deep neural networks obtain good generalization at an over-parameterization regime is still unclear. To better understand deep NN, we establish the connection between deep NN and a novel kernel family, i.e., Neural Optimization Kernel (NOK). The architecture of structured approximation of NOK performs monotonic descent updates of implicit regularization problems. We can implicitly choose the regularization problems by employing different activation functions, e.g., ReLU, max pooling, and soft-thresholding. We further establish a new generalization bound of our deep structured approximated NOK architecture. Our unsupervised structured approximated NOK block can serve as a simple plug-in of popular backbones for a good generalization against input noise.

1 Introduction

Deep neural networks (DNNs) have obtained great success in many applications, including computer vision [19], reinforcement learning [31] and natural language processing [27], etc. However, the theory of deep learning is much less explored compared with its great empirical success. A key challenge of deep learning theory is that deep neural networks are heavily over-parameterized. Namely, the number of parameters is much larger than training samples. In practice, as the depth and width increasing, the performance of deep NN also becomes better [36] [41], which is far beyond the traditional learning theory regime.

In the traditional neural networks and kernel methods literature, it is well known the connection between the infinite width neural networks and Gaussian process [21], and the universal approximation power of NN [24]. However, these theories cannot explain why the success of deep neural networks. A recent work, Neural Tangent Kernel [23] (NTK), shows the connection between training an infinite-width NN and performing functional gradient descent in a Reproducing Kernel Hilbert Space (RKHS) associated with the NTK. Because of the convexity of the functional optimization problem, Jacot et al. show the global convergence for infinite-width NN under the NTK regime. Along this direction, Hanin et al. [17] analyze the NTK with finite width and depth. Shankar et al. [35] empirically investigate the performance of some simple compositional kernels, NTKs, and deep neural networks. Nitanda et al. [32] further show the minimax optimal convergence rate of average stochastic gradient descent in a two-layer NTK regime.

Despite the success of NTK [23] on showing the global convergence of NN, its expressive power is limited. Zhu et al. [1] provide an example that shallow kernel methods (including NTK) need a much larger number of training samples to achieve the same small population risk compared with a three-layer ResNet. They further point out the importance of hierarchical learning in deep neural networks [2]. In [2], they give the theoretical analysis of learning a target network family with square activation function under deep NN regime. Besides, there are quite a few works focus on the analysis of two-layer networks [3] [6] [24] [28] [34] [39] and shallow kernel methods without hierarchical learning [6] [13] [44] [8] [26].

Although some particular examples show deep models have more powerful expressive power than shallow ones [1] [12] [2], how and why deep neural networks benefit from the depth remain unclear. Zhu et al. [2] highlight the importance of a backward feature correction. To better understand deep neural networks, we investigate the deep NN from a different kernel method perspective.
Our contributions are summarized as follows:

- We propose a novel Neural Optimization Kernel (NOK) family that broadens the connection between kernel methods and deep neural networks.

- Theoretically, we show that the architecture of NOK performs optimization of implicit regularization problems. We prove the monotonic descent property for a wide range of both convex and non-convex regularized problems. Moreover, we prove a $O(1/T)$ convergence rate for convex regularized problems. Namely, our NOK family performs an optimization through model architecture. A $T$-layer model performs $T$-step monotonic descent updates.

- We propose a novel data-dependent structured approximation method, which establishes the connection between training deep neural networks and kernel methods associated with NOKs. The resultant computation graph is a ResNet-type finite width NN. The activation function of NN specifies the regularization problem explicitly or implicitly. Our structured approximation preserved the monotonic descent property and $O(1/T)$ convergence rate. Furthermore, we propose both supervised and unsupervised learning schemes. Moreover, we prove a new Rademacher complexity bound and generalization bound of our structured approximated NOK architecture.

- Empirically, we show that our unsupervised data-dependent structured approximation block can serve as a simple plug-in of popular backbones for a good generalization against input noise. Extensive experiments on CIFAR10 and CIFAR100 with ResNet and DenseNet backbones show the good generalization of our structured approximated NOK against the Gaussian noise, Laplace noise, and FGSM adversarial attack [10].

2 Neural Optimization Kernel

Denote $\mathcal{L}_2$ as the Gaussian square-integrable function space, i.e., $\mathcal{L}_2 := \{f|\mathbb{E}_{w \sim \mathcal{N}(0, I_d)} [f(w)^2] < \infty\}$, and denote $\mathcal{L}_2$ as the spherically square-integrable function space, i.e., $\mathcal{L} \mathcal{L}_2 := \{f|\mathbb{E}_{w \sim \mathcal{N}(0, \sqrt{d-1})} [f(w)^2] < \infty\}$.

Denote $\mathcal{F} = \mathcal{L}_2$ or $\mathcal{F} = \mathcal{L}_2$, $f(\cdot, x) \in \mathcal{F}$ is a function indexed by $x$. We simplify the notation $f(w, x)$ as $f(w)$ when the dependence of $x$ is clear from the context.

For $\forall f(\cdot, x), f(\cdot, y) \in \mathcal{F}$, where $\mathcal{F} = \mathcal{L}_2$ or $\mathcal{F} = \mathcal{L}_2$, define function $k(\cdot, \cdot) : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ as

$$k(x, y) = \mathbb{E}_w [f(w, x)f(w, y)].$$  \hspace{1cm} (1)

Then, we know $k(\cdot, \cdot)$ is a bounded kernel, which is shown in Proposition [1]. All detailed proofs are given in Appendix.

**Proposition 1.** For $\forall f(\cdot, x), f(\cdot, y) \in \mathcal{F}$ ($\mathcal{F} = \mathcal{L}_2$ or $\mathcal{F} = \mathcal{L}_2$), define function $k(x, y) = \mathbb{E}_w [f(w, x)f(w, y)] : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$, then $k(x, y)$ is a bounded kernel, i.e., $k(x, y) = k(y, x) < \infty$ and $k(x, y)$ is positive definite.

For $\forall f \in \mathcal{F}$, where $\mathcal{F} = \mathcal{L}_2$ or $\mathcal{F} = \mathcal{L}_2$, define operator $A(\cdot) : \mathcal{F} \to \mathbb{R}^d$ as $A(f) := \mathbb{E}_w [fw(w)]$. Define operator $A^* : \mathcal{R}^d \to \mathcal{F}$ as $A^*(x) = w^\top x$, $w \sim \mathcal{N}(0, I_d)$ or $w \sim \mathcal{U}ni[\sqrt{d-1}].$ We know $A \circ A^*(\cdot) = \mathbb{E}_w [\phi_\lambda(f(w))]$, where $\phi_\lambda(\cdot)$ is a function with parameter $\lambda$ and bounded from below, and $\mathbb{E}_w [\phi_\lambda(f(w))]$ exists for some $f \in \mathcal{F}$. Several examples of $\phi_\lambda$ and the corresponding proximal operators are shown in Table 1. It is worth noting that $\phi_\lambda(\cdot)$ can be either convex or non-convex.

Our Neural Optimization Kernel (NOK) is defined upon the solution of optimization problems. Before giving our Neural Optimization Kernel (NOK) definition, we first introduce a family of functional optimization problems. The $\Phi_\lambda$-regularized optimization problem is defined as

$$\min_{f \in \mathcal{F}} \frac{1}{2} \|x - A(f)\|_2^2 + \Phi_\lambda(f) = \frac{1}{2} \|x - \mathbb{E}_w [wf(w)]\|_2^2 + \mathbb{E}_w [\phi_\lambda(f(w))],$$ \hspace{1cm} (2)

where $\mathcal{F} = \mathcal{L}_2$ or $\mathcal{F} = \mathcal{L}_2$, $f(\cdot) := f(\cdot, x)$ is a function indexed by $x$. We simplify the notation $f(w, x)$ as $f(w)$ as the dependence of $x$ is clear from the context.

**Intuition:** The reconstruction problem in Eq. (2) can be viewed as an autoencoder. We find a function embedding $f(\cdot, x)$ to represent the input data $x$. In contrast, the standard autoencoders usually extract finite-dimensional vector features to represent the input data for downstream tasks [15, 18]. Function representation may encode richer information than finite-dimensional vector features.

For $\phi_\lambda(\cdot)$ with efficient proximal operators $h(\cdot)$ defined as $h(z) = \arg \min_w \frac{1}{2} (w - z)^2 + \phi_\lambda(z)$, we can optimize the problem [2] by iterative updating with Eq. (3):

$$f_{t+1}(\cdot) = h(A^*(x) + f_t(\cdot) - A^* \circ A(f_t(\cdot))).$$ \hspace{1cm} (3)

The initialization is $f_0(\cdot) = 0$.

**Remark:** In the update rule (3), the term $-A^* \circ A(f_t(\cdot))$ can be viewed as a two-layer transformed residual modular of $f_t(\cdot)$. Then adding a skip connection $f_t(\cdot)$ and a biased term $A^*(x)$. As shown
in [1, 2], a ResNet-type architecture (residual modular with skip connections) is crucial for obtaining a small error with sample and time efficiency.

For both convex and non-convex function \( \phi \), our update rule in Eq. (3) leads to a monotonic descent.

**Theorem 1. (Monotonic Descent) For a function \( \phi(\cdot) \), denote \( h(\cdot) \) as the proximal operator of \( \phi(\cdot) \). Suppose \( |h(x)| \leq c|x| \) (or \(|h(x)| \leq c\), \( 0 < c < \infty \) (e.g., hard thresholding function). Given a bounded \( x \in \mathbb{R}^d \), set function \( f_{t+1}(\cdot) = h(A^*(x) + f_t(\cdot) - A^* \circ f_t(\cdot)) \) and \( f_0 \in \mathcal{F} \) (e.g., \( f_0 = 0 \)). Denote \( Q(f) = \frac{1}{2}||x - A(f)||^2 \). For all \( t \geq 0 \), we have

\[
Q(f_{t+1}) \leq Q(f_t)
\]

Remark: Assumption \(|h(x)| \leq c|x| \) (or \(|h(x)| \leq c\), \( 0 < c < \infty \)) is used to ensure that each \( f_t \in \mathcal{F} \). Neural networks with a activation function \( h(\cdot) \), e.g., sigmoid, tanh, and ReLU, as long as \( h(\cdot) \) satisfies the above assumption, it corresponds to a (implicit) \( \phi(\cdot) \)-regularized problem. Theorem 1 shows that a T-layer network performs T-steps monotonic updates of the \( \phi(\cdot) \)-regularized objective \( Q(\cdot) \).

For a convex \( \phi \), we can achieve a \( O(\frac{1}{T}) \) convergence rate, which is formally shown in Theorem 2.

**Theorem 2. For a convex function \( \phi(\cdot) \), denote \( h(\cdot) \) as the proximal operator of \( \phi(\cdot) \). Suppose \(|h(x)| \leq c|x| \) (or \(|h(x)| \leq c\), \( 0 < c < \infty \)). Given a bounded \( x \in \mathbb{R}^d \), set function \( f_{t+1}(\cdot) = h(A^*(x) + f_t(\cdot) - A^* \circ f_t(\cdot)) \) and \( f_0 \in \mathcal{F} \) (e.g., \( f_0 = 0 \)). Denote \( Q(f) = \frac{1}{2}||x - A(f)||^2 + \Phi_A(f) \) and \( f_t \in \mathcal{F} \) as an optimal of \( Q(\cdot) \). For all \( T \geq 1 \), we have

\[
T(Q(f_T) - Q(f_*)) \
\leq \frac{1}{2} \mathbb{E}_w[(f_0(w) - f_*(w))^2] - \frac{1}{2} \mathbb{E}_w[(f_T(w) - f_*(w))^2] \\
- \frac{1}{2} \sum_{t=0}^{T-1} \mathbb{E}_w[(f_{t+1}(w) - f_t(w))^2] \\
- \frac{1}{2} \sum_{t=0}^{T-1} (t+1) \mathbb{E}_w[(f_{t+1}(w) - f_t(w))^2].
\]

Remark: A ReLU \( h(x) = \max(z, 0) \) corresponds to \( \phi(z) = \begin{cases} 0, & z \geq 0 \\ +\infty, & z < 0 \end{cases} \) (a lower semi-continuous convex function), which results in a convex regularization problem. A T-layer NN obtains \( O(1/T) \) convergence rate, which is faster than non-convex cases. This explains the success of ReLU on training deep NN from a NN architecture optimization perspective.

3 Structured Approximation

The orthogonal sampling [30] and spherically structured sampling [29, 31] have been successfully used for Gaussian and spherical integral approximation. In the QMC area, randomization of structured points set is standard and widely used to achieve an unbiased estimator (the same marginal distribution \( p(w) \)). In the hypercube domain \([0, 1]^d\), a uniformly distributed vector shift is employed. In the hypersphere domain \( S^{d-1} \), a uniformly random rotation is used. For the purpose of acceleration, [29] employs a diagonal random rotation matrix to approximate the full matrix rotation, which results in a \( O(d) \) rotation time complexity instead of \( O(d^3) \) complexity in computing SVM of random Gaussian matrix (full rotation). When the goal is to reduce approximation error, we can use the standard full matrix random orthogonal rotation of the structured points [29] as an unbiased estimator of
Define operator 

\[ W = \sqrt{d} R^T B \in \mathbb{R}^{d \times N}, \]

where \( R^T R = RR^T = I_d \) is a trainable orthogonal matrix parameter, \( N \) denotes the number of samples, and \( WW^T/N = I_d \). The structured matrix \( B \) can either be a concatenation of random orthogonal matrices \( \mathbb{R} \), or be the structured matrix in \([29,30]\) to satisfy \( WW^T/N = I_d \).

Remark: The orthogonal property of the operator \( A \circ A^* = I_d \) is vitally important to achieve \( O(\frac{1}{T}) \) convergence rate with our update rule. It leads to a ResNet-type network architecture, which enables a stable gradient flow for training. When approximated with finite samples, standard Monte Carlo sampling does not maintain the orthogonal property, which degenerates the convergence. In contrast, our structured approximation preserves the second order moment \( \mathbb{E}[ww^T] = I_d \). Namely, our approximation maintains the orthogonal property, i.e., \( \widehat{A} \circ \widehat{A}^* = I_d \).

With the orthogonal property, we can obtain the same convergence rate (w.r.t. the approximation objective) with our update rule. Moreover, for a k-sparse constrained problem, we prove the strictly monotonic descent property of our structured approximation when using \( B \) in \([29,30]\).

### 3.1 Convergence Rate for Finite Dimensional Approximation Problem

The finite approximation of problem \((2)\) is given as

\[ \hat{Q}(y) := \frac{1}{2}\|x - \hat{A}(y)\|^2 + \frac{1}{d}\phi_L(y) = \frac{1}{2}\|x - \frac{1}{N}Wy\|^2 + \frac{1}{d}\phi_L(y), \]

where \( y \in \mathbb{R}^N \) and \( \phi_L(y) := \sum_{i=1}^{N} \phi_L(y_i) \).

The finite dimension update rule is given as:

\[ y_{t+1} = h(W^Tx + (I - \frac{1}{N}W^TW)y_t). \]

Thanks to the structured \( W = \sqrt{d} R^T B \), we show the monotonic descent property, convergence rate for convex \( \phi_L \), and a strictly monotonic descent for a k-sparse constrained problem.

For both convex and non-convex \( \phi_L \), our update rule in Eq. \((8)\) leads to a monotonic descent.

**Theorem 3.** (Monotonic Descent) For a function \( \phi_L(y) \), denote \( h(\cdot) \) as the proximal operator of \( \phi_L(y) \). Given a bounded \( x \in \mathbb{R}^d \), set \( y_{t+1} = h(W^Tx + (I - \frac{1}{N}W^TW)y_t) \) with \( \frac{1}{N}WW^T = I_d \). Define \( \hat{Q}(y) := \frac{1}{2}\|x - \hat{A}(y)\|^2 + \frac{1}{d}\phi_L(y) \). For \( t \geq 0 \), we have

\[
\hat{Q}(y_{t+1}) \leq \hat{Q}(y_t) - \frac{1}{2N}\|y_{t+1} - y_t\|^2 + \frac{1}{2}\|W(y_{t+1} - y_t)\|^2 \\
= \hat{Q}(y_t) - \frac{1}{2N}\|(I_d - \frac{1}{N}W^TW)(y_{t+1} - y_t)\|^2 \\
\leq \hat{Q}(y_t) - \frac{1}{2N}\|y_{t+1} - y_t\|^2. \tag{10}
\]

**Remark:** For the finite dimensional case, the monotonic descent property is preserved. For popular activation functions, e.g., sigmoid, tanh and ReLU, it corresponds to a finite dimensional (implicit) \( \phi_\cdot \)-regularized problem. A T-layer NN performs T-steps monotonic descent of the \( \phi_\cdot \)-regularized problem \( \hat{Q}(\cdot) \) despite the non-convexity of the activation function \( h(\cdot) \). Interestingly, by choosing different activation functions, we implicitly choose the regularizations of the optimization problem. Our network structure can perform monotonic descent for a wide range of implicit optimization problems.

For convex \( \phi_L \), we can achieve an \( O(\frac{1}{T}) \) convergence rate, which is formally shown in Theorem 4.

**Theorem 4.** For a convex function \( \phi_L(y) \), denote \( h(\cdot) \) as the proximal operator of \( \phi_L(y) \). Given a bounded \( x \in \mathbb{R}^d \), set \( y_{t+1} = h(W^Tx + (I - \frac{1}{N}W^TW)y_t) \) with \( \frac{1}{N}WW^T = I_d \). Define \( \hat{Q}(y) := \frac{1}{2}\|x - \hat{A}(y)\|^2 + \frac{1}{d}\phi_L(y) \) and \( y^* \) as an optimal of \( \hat{Q}(\cdot) \). For \( T \geq 1 \), we have

\[
T(\hat{Q}(y_T) - \hat{Q}(y^*)) \\
\leq \frac{1}{2N}\|y_0 - y^*\|^2 - \frac{1}{2N}\|y_T - y^*\|^2 - \frac{1}{2}\sum_{t=0}^{T-1} \|W(y_t - y^*)\|^2 \\
- \frac{1}{2}\sum_{t=0}^{T-1} \frac{t + 1}{N}\|y_{t+1} - y_t\|^2. \tag{11}
\]

**Remark:** Term \(-\frac{1}{2}\sum_{t=0}^{T-1} \frac{t + 1}{N}\|y_{t+1} - y_t\|^2, \) and term \(-\frac{1}{2}\sum_{t=0}^{T-1} \frac{1}{N}\|W(y_t - y^*)\|^2, \) are always non-positive. Thus, we know \( \hat{Q}(y_T) - \hat{Q}(y^*) \leq O(\frac{1}{T}) \).

**Theorem 5.** (Strictly Monotonic Descent of k-sparse problem) Let \( L(y) = \frac{1}{2}\|x - Dy\|^2 \), s.t. \( \|y\|_0 \leq k \) with \( D = \frac{\sqrt{k}}{\sqrt{N}}R^T B \), where \( B \) is constructed as in [30] with...
\[ N = 2n, d = 2m. \] Set \( y_{t+1} = h(a_{t+1}) \) with sparsity \( k \)
and \( a_{t+1} = D^\top x + (I - D^\top D)y_t \). For \( \forall t \geq 1 \), we have
\[
L(y_{t+1}) \leq L(y_t) + \frac{1}{2}\|y_{t+1} - a_{t+1}\|^2 - \frac{1}{2}\|y_t - a_{t+1}\|^2 \nonumber
- \frac{n - (2k - 1)\sqrt{n} - m}{2n}\|y_{t+1} - y_t\|^2 \leq L(y_t),
\]
where \( h(\cdot) \) is defined as
\[
h(z_j) = \begin{cases} z_j & \text{if } |z_j| \text{ is one of the } k\text{-highest values of } |z| \\ 0 & \text{otherwise} \end{cases}
\]
Remark: When sparsity \( k < \frac{n - m + \sqrt{n}}{2\sqrt{n}} \), we have
\( L(y_{t+1}) < L(y_t) \) unless \( y_{t+1} = y_t \). Our update with
the structured \( D \) makes a strictly monotonic descent process each step.

### 3.2 Learning Parameter \( R \)

**Supervised Learning:** For the each \( i \text{-th} \) layer, we can maintain an orthogonal matrix \( R_i \). The orthogonal matrix \( R_i \) can be parameterized by exponential mapping or Cayley mapping [20] of a skew-symmetric matrix. We can employ the Cayley mapping to enable gradient update w.r.t. a loss function \( \ell(\cdot) \) in an end-to-end training. Specifically, the orthogonal matrix \( R_i \) can be obtained by the Cayley mapping of a skew-symmetric matrix as
\[
R_i = (I + M_i)(I - M_i)^{-1},
\]
where \( M_i \) is a skew-symmetric matrix, i.e., \( M_i = -M_i^\top \in \mathbb{R}^{d \times d} \). For a skew-symmetric matrix \( M_i \), only the upper triangular matrix (without main diagonal) are free parameters. Thus, total the number of free parameters of \( T \)-Layer is \( Td(d-1)/2 \). Particularly, when sharing the orthogonal matrix parameter, i.e., \( R_1 = \cdots = R_T = R \), the monotonic descent property and the convergence rate of the regularized optimization problems are well maintained. In this case, it is a recurrent neural network architecture.

**Unsupervised Learning:** The parameter \( R \) can also be learned in an unsupervised manner. Specifically, for a finite dataset \( X \), the finite dimensional approximation problem with the structured \( W = \sqrt{d}R^\top B \) is given as
\[
\min_{Y, R} \frac{1}{N}\|X - \frac{\sqrt{d}}{N}R^\top BY\|^2_F + \frac{1}{N}\phi_{\lambda}(Y) \nonumber
\]
subject to \( R^\top R = RR^\top = I_d \),
\]
where \( \phi_{\lambda}(\cdot) \) is a separable non-convex or convex regularization function with parameter \( \lambda \), i.e., \( \phi_{\lambda}(Y) = \sum_i \phi_{\lambda}(y^{(i)}) \).

The problem \([15]\) can be solved by the alternative descent method. For a fixed \( R \), we perform an iterative update of \( Y \) a few steps to decrease the objective. For the fixed \( Y \), parameter \( R \) has a closed-form solution.

**Fix \( R \), Optimize \( Y \):** The problem \([15]\) can be rewritten as:
\[
\frac{1}{N}\|X - \frac{\sqrt{d}}{N}R^\top BY\|^2_F + \frac{1}{N}\phi_{\lambda}(Y) = \sum_i \tilde{Q}(y^{(i)}).
\]
Thus, with fixed \( R \), we can update each \( y^{(i)} \) by Eq. \([9]\) in parallel. We can perform \( T_1 \) steps update with initialization as the output of previous alternative phase, i.e., \( Y_0^{T_1} = Y_0 \) (and initialization \( Y_0^0 = 0 \) and \( R_0 = I_d \)).

**Fix \( Y \), Optimize \( R \):** This is the nearest orthogonal matrix problem, which has a closed-form solution as shown in [34]. Let \( \frac{\sqrt{d}}{N}BY^\top = UTV^\top \) obtained by singular value decomposition (SVD), where \( U, V \) are orthogonal matrix. Then, Eq. \([15]\) is minimized by \( R = UV^\top \).

Remark: A \( T_2 \)-step alternative descent computation graph of \( R \) and \( Y \) can be viewed as a \( T_1T_2 \)-layer NN block, which can be used as a plug-in of popular backbones for a good generalization against input noise.

### 3.3 Kernel Approximation

Define \( k_{T, N}(x, x') = \frac{1}{N} < y_T(W, x), y_T(W, x') > \), where \( y_T(W, x) : \mathcal{R}^d \rightarrow \mathcal{R}^N \) is a finite approximation of \( f_T(\cdot, x) \in \mathcal{H}_{k_T} \). We know \( k_{T, N}(x, x') \) is bounded kernel, and it is an approximation of kernel \( k_{T, \infty} = \mathbb{E}_{w}[f(w, x)f_T(w, x')] \).

Remark: Let \( B \) be a points set that marginally uniformly distributed on the surface of sphere \( S^{d-1} \) (e.g., block-wise random orthogonal rotation of structured samples [29]). Employing our structured approximation \( W = R^\top B \), we know \( \forall R \in SO(d) \) and \( \forall f \in Z_2 \),
\[
\lim_{N \rightarrow \infty} \frac{\sum_{i=1}^N f(w)}{N} = \mathbb{E}_{w \sim \text{Unif}[S^{d-1}]}[f(w)].
\]
It means that although the orthogonal rotation parameter \( R \) is learned, we still maintain an unbiased estimator of \( \mathbb{E}_{w}[f(w)] \).

**First-Layer Kernel:** Set \( y = 0 \) and \( f_0 = 0 \), we know \( y_i(x) = h(w_i^\top x) \) and \( f_1(w, x) = h(w^\top x) \). Suppose \( |h(x)| \leq c|x| \) (or \( |h(x)| \leq c \), \( 0 < c < \infty \)), it follows that
\[
\lim_{N \rightarrow \infty} k_{1, N}(x, x') = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1}^N h(w_i^\top x)h(w_i^\top x') = \mathbb{E}_{w}[h(w^\top Rx)h(w^\top Rx')] = \mathbb{E}_{w}[h(w^\top x')h(w^\top x')] = k_{1, \infty}(x, x')
\]
In Eq. (17), we use the fact that a rotation does not change the uniform surface measure on $S^{d-1}$. The first layer kernel $k_{1,N}$ uniformly converge to $k_{1,\infty}$ over a bounded domain $\mathcal{X} \times \mathcal{X}$.

### Higher-Layer Kernel:
For both the shared $\mathbf{R}$ case and the unsupervised updating $\mathbf{R}$ case, the monotonic descent property and convergence rate is well preserved for any bounded $x \in \mathcal{X}$. With the same assumption of $h(\cdot)$ and $y = 0$, as $N \to \infty$, we know $\mathbf{y}_t \to \mathbf{f}_t \in \mathcal{U}_2$, where $\mathbf{f}_t$ is a countable-infinite dimensional function. And inequality (10) and inequality (11) uniformly converges to inequality (18) and inequality (19) over a bounded domain $\mathcal{X}$, respectively.

$$Q(\hat{f}_t) \leq Q(f_t) - \frac{\lambda}{2} \mathbb{E}_w[(\hat{f}_t(w) - f_t(w))^2] + \frac{1}{2} \mathbb{E}_w[\mathbb{E}_w(\hat{f}_t(w) - f_t(w))^2] \leq Q(f_t).$$

(18)

$$T(Q(\hat{f}_t) - Q(f_t)) \leq \frac{1}{2} \mathbb{E}_w[(\hat{f}_t(w) - f_t(w))^2] - \frac{1}{2} \mathbb{E}_w[(f_T(w) - f_T(w))^2] - \frac{1}{2} \sum_{t=0}^{T-1} \mathbb{E}_w[\mathbb{E}_w(\hat{f}_t(w) - f_T(w))^2] \leq \frac{1}{2} \sum_{t=0}^{T-1} (t+1) \mathbb{E}_w[\mathbb{E}_w(\hat{f}_t(w) - f_T(w))^2]$$

(19)

It is worth noting that $\lim_{N \to \infty} k_{T,N}$ converge to a $\hat{k}_{T,\infty}$ that is determined by the initialization $\mathbf{R}_0$ and dataset $\mathbf{X}$. Specifically, for both the unsupervised learning case and the shared parameter case, the approximated kernel converge to a fixed kernel as the width tends to infinity. As $N \to \infty$, training a finite structured NN with GD tends to perform a functional gradient descent with a fixed kernel. For a strongly convex regularized regression problem, functional gradient descent leads to global convergence.

For the case of updating $T$-layer parameter $\mathbf{R}_t, t \in \{1, \cdots, T\}$ in a supervised manner, the sequence $\{\mathbf{R}_t\}$ determines the kernel. When the data distribution is isotropic, e.g., $\mathcal{U} / n! [S^{d-1}]$, the monotonic descent property is preserved for the expectation $\mathbb{E}_X[Q(\hat{f}_t, X)]$ (at least one step descent). Actually, when parameters of each layer are learned in a supervised manner, the model is adjusted to fit the supervised signal. When the prior regularization $\mathbb{E}_w[\phi_\lambda(\mathbf{f}(\mathbf{w}, X))]$ is consistent with learning the supervised signal, the monotonic descent property is well preserved. When the prior regularization contradicts the supervised signal, the monotonic descent property for prior is weakened.

### Functional Optimization
We can minimize a regularized expected risk given as

$$J(f) := \mathbb{E}_X, Y \left[ \ell(g(X), Y) + \frac{\lambda}{2} \|g\|_{\mathcal{H}_k}^2 \right]$$

$$+ \beta \mathbb{E}_X \left[ \frac{1}{2} \|X - \mathbb{E}_w[w \mathbf{f}(\mathbf{w}, X)]\|_2^2 + \mathbb{E}_w[\phi_\lambda(f(\mathbf{w}, X))] \right]$$

(20)

where the function space $\mathcal{H}_k \ni g$ is determined by the kernel $k(x, y) = \mathbb{E}_w[f(\mathbf{w}, x) f(\mathbf{w}, y)]$. $J_2$ can be viewed as an implicit regularization to determine the candidate function family for supervised learning. Our NOK enables us to implicitly optimize the objective $J_2$ through neural network architecture. Namely, the function space $\mathcal{H}_{k_T} \ni g$ is determined by the kernel associated with the $T$-step update $f_T$. With our NOK, $J_2$ with convex regularization $\phi_\lambda(\cdot)$ can be optimized with a convergence rate $O(\frac{1}{T})$ by the $T$-layer network architecture. When $\phi_\lambda(\cdot)$ is an indicator function, the optimal $J_2$ actually is the $l_2$-norm optimal transport between $p(X)$ and a probability measure induced by the transform of random variable $X$ (i.e., $\mathbb{E}_w[w f_X(w, X)]$). By employing different activation function $h(\cdot)$, we implicitly choose the regularization term $J_2$ to be optimized.

For a convex function $\ell(\cdot)$, $J_1(g)$ is strongly convex w.r.t. the function $g \in \mathcal{H}_k$. Functional gradient descent can converge to a minimizer of $J_1$. For regression problems, $\ell(z, y) = \frac{1}{2}(z - y)^2$, the functional gradient of $J_1$ is

$$\partial J_1(g) = \mathbb{E}_{X,Y}[\partial z = g(X) \ell(g(X), Y) k(., X)] + \lambda g = (\Sigma + \lambda I)g - \mathbb{E}_{X,Y}[Y k(., X)],$$

(21)

where $\Sigma := \mathbb{E}_{X \sim p_X}[k(., X) \otimes k(., X)]$ denotes the covariance operator.

We can perform the average stochastic gradient descent using a stochastic unbiased estimator of Eq. (21). Since it is a strongly convex problem, we can achieve $O(\frac{1}{T})$ convergence rate (Theorem A in [22]). It means that training deep NN (with our structured approximated NOK architecture) at the infinity width regime converges to a global minimum.

### 5 Rademacher Complexity and Generalization Bound
We show the Rademacher complexity bound and the generalization bound of our structured approximated NOK (SNOK).

#### Neural Network Structure:
For structured approximated NOK networks (SNOK), the $1$-$T$ layers are given as

$$y_{t+1} = h(D^T R_t x + (I - D^T D) y_t),$$

(22)

where $\mathbf{R}_t$ are free parameters such that $\mathbf{R}_t^T \mathbf{R}_t = \mathbf{R}_t$; $\mathbf{R}_t = \mathbf{I}_d$. And $\mathbf{D}$ is a scaled structured spherical samples such that $\mathbf{D} \mathbf{D}^T = \mathbf{I}_d$ [29], and $y_0 = 0$.

The last layer $(T+1)^{th}$ layer is given by $z = w^T y_{T+1}$. Consider a $L$-Lipschitz continuous loss func-
tion $\ell(z, y) : Z \times Y \to [0, 1]$ with Lipschitz constant $L$ w.r.t. the input $z$.

**Rademacher Complexity** [5]: Rademacher complexity of a function class $G$ is defined as

$$\mathcal{R}_N(G) := \frac{1}{N} \mathbb{E} \left[ \sup_{g \in G} \sum_{i=1}^N \epsilon_i g(x_i) \right],$$  \hspace{1cm} (23)

where $\epsilon_i, i \in \{1, \cdots, N\}$ are i.i.d. samples drawn uniformly from $\{+1, -1\}$ with probability $P[\epsilon_i = +1] = P[\epsilon_i = -1] = 1/2$. And $x_i, i \in \{1, \cdots, N\}$ are i.i.d. samples from $X$.

**Theorem 6.** (Rademacher Complexity Bound) Consider a Lipschitz continuous loss function $\ell(z, y) : Z \times Y \to [0, 1]$ with Lipschitz constant $L$ w.r.t. the input $z$. Let $\ell(z, y) := \ell(z, y) - \ell(0, y)$. Let $\tilde{G}$ be the function class of our $(T+1)$-layer SNOK mapping from $X$ to $Z$. Suppose the activation function $h(y) \leq |y|$ (element-wise), and the $l_2$-norm of last layer weight is bounded, i.e. $\|w\|_2 \leq B_w$. Let $(x_i, y_i)_{i=1}^N$ be i.i.d. samples drawn from $X \times Y$. Let $Y_{T+1} = [y_{T+1}^{(1)}, \cdots, y_{T+1}^{(N)}]$ be the $T$th layer output with input $X$. Denote the mutual coherence of $Y_{T+1}$ as $\mu^*$, i.e. $\mu^* = \mu(Y_{T+1}) \leq 1$. Then, we have

$$\mathcal{R}_N(\tilde{\ell} \circ \tilde{G}) = \frac{1}{N} \mathbb{E} \left[ \sup_{g \in \tilde{G}} \sum_{i=1}^N \epsilon_i \tilde{\ell}(g(x_i), y_i) \right] \leq \frac{LB_w \sqrt{((N-1)\mu^* + 1)T}}{N} \|X\|_F, \hspace{1cm} (24)$$

where $X = [x_1, \cdots, x_N]$, and $\| \cdot \|_F$ and $\| \cdot \|_2$ denote the matrix Frobenius norm and matrix spectral norm, respectively.

**Remark:** A small mutual coherence $\mu(Y_{T+1})$ leads to a small Rademacher complexity bound. Moreover, the Rademacher complexity bound has a complexity $O(\sqrt{T})$ w.r.t. the depth of NN (SNOK).

**Theorem 7.** (Generalization Bound) Consider a Lipschitz continuous loss function $\ell(z, y) : Z \times Y \to [0, 1]$ with Lipschitz constant $L$ w.r.t. the input $z$. Let $\ell(z, y) := \ell(z, y) - \ell(0, y)$. Let $G$ be the function class of our $(T+1)$-layer SNOK mapping from $X$ to $Z$. Suppose the activation function $h(y) \leq |y|$ (element-wise), and the $l_2$-norm of last layer weight is bounded, i.e., $\|w\|_2 \leq B_w$. Let $(x_i, y_i)_{i=1}^N$ be i.i.d. samples drawn from $X \times Y$. Let $Y_{T+1} = [y_{T+1}^{(1)}, \cdots, y_{T+1}^{(N)}]$ be the $T$th layer output with input $X$. Denote the mutual coherence of $Y_{T+1}$ as $\mu^*$, i.e. $\mu^* = \mu(Y_{T+1}) \leq 1$. Then, for $\forall N$ and $\forall \delta, 0 < \delta < 1$, with a probability at least $1 - \delta$, $\forall g \in \tilde{G}$, we have

$$\mathbb{E} [\ell(g(X), Y)] \leq \frac{1}{N} \sum_{i=1}^N \ell(g(x_i), y_i) + \frac{LB_w \sqrt{((N-1)\mu^* + 1)T}}{N} \|X\|_F + \frac{8\ln(2/\delta)}{N},$$  \hspace{1cm} (25)

where $X = [x_1, \cdots, x_N]$, and $\| \cdot \|_F$ and $\| \cdot \|_2$ denote the matrix Frobenius norm and matrix spectral norm, respectively.

**Remark:** The mutual coherence $\mu(Y_{T+1})$ (or $\|Y_{T+1}^T Y_{T+1}^T - \mathcal{I}\|^2_F$, etc.) of the last layer representation can serve as a good regularization to reduce Rademacher complexity and generalization bound. A small mutual coherence means that the direction feature vectors $\{y_{T+1}^{(1)}, \cdots, y_{T+1}^{(N)}\}$ are well spaced on the hypersphere. Namely, encouraging the last-layer embedding direction feature vectors $\{y_{T+1}^{(1)}, \cdots, y_{T+1}^{(N)}\}$ well spaced on the hypersphere leads to small Rademacher complexity and generalization bounds. When the width of SNOK ($N_D$) is large enough, specifically, when $N_D > N$, it is possible to obtain $\mu(Y_{T+1}) = 0$ (orthogonal representation), which significantly reduces the generalization bound. Namely, overparameterized deep NNs can increase the expressive power to reduce empirical risk [1] [2] [3] and reduce the generalization bound at the same time.

### 6 Experiments

We evaluate the performance of our unsupervised SNOK blocks on classification tasks with input noise (Gaussian noise or Laplace noise), and under FGSM adversarial attack [13]. In all the experiments, the input noise is added after input normalization. The standard deviation of input noise is set to $\{0, 0.1, 0.2, 0.3\}$, respectively. We employ both DenseNet-100 [22] and ResNet-34 [19] as backbone. We test the performance of four methods in comparison: (1) Vanilla Backbone, (2) Backbone + Mean Filter, (3) Backbone + Median Filter, (4) Backbone + SNOK. For both Mean Filter and Median Filter cases, we set the filter neighborhood size as $3 \times 3$ same as in [25]. For our SNOK case, we plug two SNOK blocks before and after the first learnable Corev2D layer. In all the experiments, CIFAR10 and CIFAR100 datasets [25] are employed for evaluation. All the methods are evaluated over five independent runs with seeds $\{1, 2, 3, 4, 5\}$. During training, we stored the model every five epochs, and reported all evaluation results over all the stored mod-
Figure 1: Mean test accuracy ± std over 5 independent runs on CIFAR10/CIFAR100 dataset under FGSM adversarial attack for DenseNet and ResNet backbone.

Figure 2: Mean test accuracy ± std over 5 independent runs on DenseNet with Gaussian noise.

The experimental results of different models under the FGSM attack are shown in Fig. 1. Our SNOK plug-in achieves a significantly higher test accuracy than baselines. The results of classification with Gaussian input noise on DenseNet backbone are shown in Fig. 2. Our SNOK obtains competitive performance on the clean case and increasingly better performance as the std increases. More detailed experimental results are presented in Appendix K.

7 Conclusion and Future Work

We proposed a novel kernel family NOK that broadens the connection between deep neural networks and kernel methods. The architecture of our structured approximated NOK performs monotonic descent updates of implicit regularization problems. We can implicitly choose the regularization problems by employing different activation functions, e.g., ReLU, max pooling, and soft-thresholding. Moreover, by taking advantage of the connection to kernel methods, we show that training regularized NOK at an infinite width regime with functional gradient descent converges to a global minimizer. Furthermore, we establish generalization bounds of our SNOK. We show that increasing the width of SNOK can increase the expressive power to reduce the empirical risk and potentially reduce the generalization bound simultaneously through last-layer feature mutual coherence regularization (i.e., $\mu(Y_{T+1})$). In particular, when the width of SNOK is larger than the number of training data, last-layer orthogonal representation can significantly reduce the generalization bound. Our unsupervised structured approximated NOK block can serve as a simple plug-in of popular backbones for a good generalization against input noise. Extensive experiments on CIFAR10 and CIFAR100 with ResNet and DenseNet backbones show the good generalization of our structured approximated NOK against the Gaussian noise, Laplace noise, and FGSM adversarial attack.

In the future, we will investigate the convergence behavior of training the supervised SNOK with SGD at a finite width regime. More interestingly, we will investigate our SNOK with shared parameter $R$ as recurrent neural network architectures.
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A Proof of Proposition

Kernel Property:

**Proposition.** For \( \forall f(\cdot, x), f(\cdot, y) \in \mathcal{F} \) (\( \mathcal{F} = \mathcal{L}_2 \) or \( \mathcal{F} = \mathcal{L}_2 \)), define function \( k(x, y) = E_w[f(w, x)f(w, y)] \) : \( \mathcal{X} \times \mathcal{X} \to \mathcal{R} \), then \( k(x, y) \) is a bounded kernel, i.e., \( k(x, y) = k(y, x) < \infty \) and \( k(x, y) \) is positive definite.

**Proof.** (i) Symmetric property is straightforward by definition.

(ii) From Cauchy–Schwarz inequality,

\[
\begin{align*}
    k(x, y) &= E_w[f(w, x)f(w, y)] \\
    &\leq \sqrt{E_w[f(w, x)^2]E_w[f(w, y)^2]} < \infty \\
    &\quad (26)
\end{align*}
\]

(iii) Positive definite property. For \( \forall n \in \mathbb{N}, \forall \alpha_1 \cdots, \alpha_n \in \mathcal{R} \) and \( \forall x_1, \cdots, x_n \in \mathcal{X} \), we have

\[
\sum_i \sum_j \alpha_i \alpha_j k(x_i, x_j) = E_w[(\sum_i \alpha_i f(w, x_i))^2] \geq 0
\]

B Proof of Theorem

Convex \( \phi \)-regularization:

\[
\min_{f \in \mathcal{F}} \frac{1}{2} \|x - E_w[w f(w)]\|^2 + E_w[\phi(f(w))]
\]

where \( \mathcal{F} = \mathcal{L}_2 \) or \( \mathcal{F} = \mathcal{L}_2 \). And \( \mathcal{L}_2 \) denotes the Gaussian square integrable functional space, i.e., \( \mathcal{L}_2 := \{ f | E_w[N(0, I_d) \| f(w) \|^2] < \infty \} \), \( \mathcal{L}_2 \) denotes the sphere square integrable functional space, i.e., \( \mathcal{L}_2 := \{ f | E_w[U_{n(\sqrt{\alpha}d-1)} \| f(w) \|^2] < \infty \} \) and \( \phi(\cdot) \) denotes a convex function bounded from below.

**Lemma 1.** \( E_{w \sim U_{n(\sqrt{\alpha}d-1)}}[ww^\top] = I_d \).

**Proof.**

\[
I_d = E_{x \sim N(0, I_d)}[xx^\top]
\]

\[
= \int \frac{1}{(2\pi)^{D/2}} e^{-\frac{\|x\|^2}{2}} xx^\top \, dx
\]

\[
= \int_0^{\infty} \frac{2\pi^{D/2}}{\Gamma(D/2)} r^{D-1} e^{-\frac{r^2}{2}} \frac{1}{(2\pi)^{D/2}} vv^\top \, d\sigma(v) \, dr
\]

\[
= \int_0^{\infty} \frac{2\pi^{D/2}}{\Gamma(D/2)} r^{D-1} e^{-\frac{r^2}{2}} \frac{1}{(2\pi)^{D/2}} vv^\top \, d\sigma(v)
\]

\[
= \int_0^{\infty} \frac{2\pi^{D/2}}{\Gamma(D/2)} r^{D-1} e^{-\frac{r^2}{2}} \frac{1}{(2\pi)^{D/2}} vv^\top \, d\sigma(v)
\]

\[
= \int_{S^{D-1}} vv^\top \, d\sigma(v)
\]

\[
= \int_{S^{D-1}} vv^\top \, d\sigma(v)
\]

\[
= E_{w \sim U_{n(\sqrt{\alpha}d-1)}}[ww^\top]
\]

where \( \sigma(\cdot) \) denotes the normalized surface measure, \( \chi(d) \) denotes the Chi distribution with degree \( d \), \( \Gamma(\cdot) \) denotes the gamma function.

**Lemma 2.** Let \( f \in \mathcal{F} \) with \( \mathcal{F} = \mathcal{L}_2 \) or \( \mathcal{F} = \mathcal{L}_2 \), then we have

\[
E_w[f(w)^2] - \|E_w[w f(w)]\|^2_2 = E_w[(f(w) - w^\top E_w[w f(w)])^2] \geq 0
\]

(34)
Proof. Let \( w_i \) denote the \( i \)th component of \( w \), from Cauchy–Schwarz inequality, we know that
\[
(E_w[w_i f(w)])^2 \leq E_w[w_i^2]E_w[f(w)^2] = E_w[f(w)^2] < \infty \tag{35}
\]
Thus the expectation \( E_w[w f(w)] \) exits.

Since \( E_w[w w^\top] = I_d \), we have
\[
\|E_w[w f(w)]\|^2_2 = (E_w[w f(w)])^\top (E_w[w f(w)])
\]
\[
= (E_w[w f(w)])^\top E_w[w w^\top] (E_w[w f(w)])
\]
\[
= E_w[(w^\top E_w[w f(w)])^2] \tag{37}
\]
It follows that
\[
E_w[f(w)^2] - \|E_w[w f(w)]\|^2_2
\]
\[
= E_w[f(w)^2] - 2\|E_w[w f(w)]\|^2_2 + \|E_w[w f(w)]\|^2_2 \tag{39}
\]
\[
= E_w[f(w)^2] - 2(E_w[w f(w)])^\top (E_w[w f(w)]) + E_w[(w^\top E_w[w f(w)])^2] \tag{40}
\]
\[
= E_w[f(w)^2] - 2E_w[(w^\top w) E_w[w f(w)] + E_w[(w^\top E_w[w f(w)])^2] \tag{41}
\]
\[
= E_w[(f(w) - w^\top E_w[w f(w)])^2] \geq 0 \tag{42}
\]

Lemma 3. Let \( f \in \mathcal{F} \) with \( \mathcal{F} = \mathcal{L}_2 \) or \( \mathcal{F} = \mathcal{L}_2 \), we have
\[
\|x - E_w[w f(w)]\|^2_2 = E_w[(w^\top (x - E_w[w f(w)]))^2] \tag{43}
\]
Proof. Since \( E_w[w w^\top] = I_d \), we have
\[
\|x - E_w[w f(w)]\|^2_2 = (x - E_w[w f(w)])^\top (x - E_w[w f(w)]) \tag{44}
\]
\[
= (x - E_w[w f(w)])^\top E_w[w w^\top] (x - E_w[w f(w)]) \tag{45}
\]
\[
= E_w[(w^\top (x - E_w[w f(w)]))^2] \tag{46}
\]

Lemma 4. Denote \( L(f) := \frac{1}{2}\|x - E_w[w f(w)]\|^2_2 \). For \( f, g \in \mathcal{F} \) with \( \mathcal{F} = \mathcal{L}_2 \) or \( \mathcal{F} = \mathcal{L}_2 \), we have \( L(f) = L(g) + E_w[w^\top (E_w[w g(w)] - x)(f(w) - g(w))] + \frac{1}{2}\|E_w[w (f(w) - g(w))]\|^2_2 \).

Proof.
\[
\frac{1}{2}\|x - E_w[w f(w)]\|^2_2 = \frac{1}{2}\|x - E_w[w g(w)] + E_w[w g(w)] - E_w[w f(w)]\|^2_2 \tag{47}
\]
\[
= \frac{1}{2}\|x - E_w[w g(w)]\|^2_2 + \frac{1}{2}\|E_w[w g(w)] - E_w[w f(w)]\|^2_2 + (x - E_w[w g(w)], E_w[w g(w)] - E_w[w f(w)]) \tag{48}
\]
The inner product term can be rewritten as
\[
\langle x - E_w[w g(w)], E_w[w g(w)] - E_w[w f(w)] \rangle = (x - E_w[w g(w)])^\top E_w[w (g(w) - f(w))] \tag{49}
\]
\[
= E_w[(x - E_w[w g(w)])^\top w (g(w) - f(w))] \tag{50}
\]
It follows that
\[
\frac{1}{2}\|x - E_w[w f(w)]\|^2_2 = \frac{1}{2}\|x - E_w[w g(w)]\|^2_2 + \frac{1}{2}\|E_w[w (g(w) - f(w))]\|^2_2 + E_w[w^\top (E_w[w g(w)] - x)(f(w) - g(w))] \tag{51}
\]
\]
Lemma 5. For \( \forall f_t, f_{t+1}, f^* \in \mathcal{F} \) with \( \mathcal{F} = \mathcal{L}_2 \) or \( \mathcal{F} = \mathcal{L}_2^c \), we have

\[
L(f_{t+1}) = L(f^*) + \mathbb{E}_w[w^\top (\mathbb{E}_w[w f_t(w)] - x) (f_{t+1}(w) - f^*(w))] + \frac{1}{2} \| \mathbb{E}_w[w (f_{t+1}(w) - f_t(w))] \|_2^2 \\
- \frac{1}{2} \| \mathbb{E}_w[w (f_t(w) - f^*(w))] \|_2^2
\]

(52)

Proof. From Lemma [4] we know that

\[
L(f_{t+1}) = L(f_t) + \mathbb{E}_w[w^\top (\mathbb{E}_w[w f_t(w)] - x) (f_{t+1}(w) - f_t(w))] + \frac{1}{2} \| \mathbb{E}_w[w (f_{t+1}(w) - f_t(w))] \|_2^2
\]

(53)

\[
L(f^*) = L(f_t) + \mathbb{E}_w[w^\top (\mathbb{E}_w[w f_t(w)] - x) (f^*(w) - f_t(w))] + \frac{1}{2} \| \mathbb{E}_w[w (f^*(w) - f_t(w))] \|_2^2
\]

(54)

Plug \( L(f_t) \) into Eq. (53), we can obtain that

\[
L(f_{t+1}) = L(f^*) + \mathbb{E}_w[w^\top (\mathbb{E}_w[w f_t(w)] - x) (f^*(w) - f_t(w))] - \frac{1}{2} \| \mathbb{E}_w[w (f^*(w) - f_t(w))] \|_2^2
\\
+ \mathbb{E}_w[w^\top (\mathbb{E}_w[w f_t(w)] - x) (f_{t+1}(w) - f_t(w))] + \frac{1}{2} \| \mathbb{E}_w[w (f_{t+1}(w) - f_t(w))] \|_2^2
\]

(55)

\[
= L(f^*) + \mathbb{E}_w[w^\top (\mathbb{E}_w[w f_t(w)] - x) (f_{t+1}(w) - f^*(w))] + \frac{1}{2} \| \mathbb{E}_w[w (f_{t+1}(w) - f_t(w))] \|_2^2
\\
- \frac{1}{2} \| \mathbb{E}_w[w (f_t(w) - f^*(w))] \|_2^2
\]

(56)

Lemma 6. For a convex function \( \phi_\lambda(\cdot) \), denote \( h(\cdot) \) as the proximal operator of \( \phi_\lambda(\cdot) \), i.e., \( h(z) = \arg\min_x \frac{1}{2} (x - z)^2 + \phi_\lambda(x) \), let \( f_{t+1} = h \circ g_{t+1} \in \mathcal{F} \) with \( \mathcal{F} = \mathcal{L}_2 \) or \( \mathcal{F} = \mathcal{L}_2^c \), then for \( \forall f^* \in \mathcal{F} \), we have

\[
\mathbb{E}_w[\phi_\lambda(f_{t+1}(w))] \leq \mathbb{E}_w[\phi_\lambda(f^*(w))] - \mathbb{E}_w[(g_{t+1}(w) - f_{t+1}(w))(f^*(w) - f_{t+1}(w))]
\]

(57)

Proof. Since \( \phi_\lambda(\cdot) \) is convex function and \( f_{t+1}(w) = \arg\min_x \phi_\lambda(x) + \frac{1}{2} \| x - g_{t+1}(w) \|_2^2 \), we have

\[
0 \in \partial \phi_\lambda(f_{t+1}(w)) + (f_{t+1}(w) - g_{t+1}(w)) \implies (g_{t+1}(w) - f_{t+1}(w)) \in \partial \phi_\lambda(f_{t+1}(w))
\]

(58)

From the definition of subgradient and convex function \( \phi_\lambda(\cdot) \), we have

\[
\phi_\lambda(f_{t+1}(w)) \leq \phi_\lambda(f^*(w)) - (g_{t+1}(w) - f_{t+1}(w))(f^*(w) - f_{t+1}(w))
\]

(59)

It follows that

\[
\mathbb{E}_w[\phi_\lambda(f_{t+1}(w))] \leq \mathbb{E}_w[\phi_\lambda(f^*(w))] - \mathbb{E}_w[(g_{t+1}(w) - f_{t+1}(w))(f^*(w) - f_{t+1}(w))]
\]

(60)

Lemma 7. Denote \( h(\cdot) \) as the proximal operator of \( \phi_\lambda(\cdot) \). Suppose \( |h(x)| \leq c|x| \) (or \( |h(x)| \leq c \)), \( 0 < c < \infty \). Given a bounded \( x \in \mathbb{R}^d \), set function \( g_{t+1}(w) = w^\top x + f_t(w) - w^\top \mathbb{E}_w[w f_t(w)] \) with \( f_t \in \mathcal{L}_2 \) and \( w \sim \mathcal{N}(0, I_d) \) (or \( f_t \in \mathcal{L}_2^c \) and \( w \sim \mathcal{U}\left[\sqrt{dS^{d-1}}\right] \)). Set \( f_{t+1} = h \circ g_{t+1} \), then, we know \( f_{t+1} \in \mathcal{F} \) with \( \mathcal{F} = \mathcal{L}_2 \) or \( \mathcal{F} = \mathcal{L}_2^c \), respectively.

Proof. Case \( |h(x)| \leq c|x| \), \( 0 < c < \infty \): It is straightforward to know \( \mathbb{E}_w[h(g_{t+1}(w))^2] \leq c^2 < \infty \), thus \( f_{t+1} \in \mathcal{F} \).

Case \( |h(x)| \leq c|x| \), \( 0 < c < \infty \): Since \( |h(x)| \leq c|x| \), we know that

\[
h(g_{t+1}(w))^2 \leq c^2 g_{t+1}(w)^2 = c^2 (w^\top x + f_t(w) - w^\top \mathbb{E}_w[w f_t(w)])^2
\]

(61)

\[
\leq 2c^2 (w^\top (x - \mathbb{E}_w[w f_t(w)]))^2 + 2c^2 f_t(w)^2
\]

(62)
It follows that
\[
E_w[h(g_{t+1}(w))^2] \leq c^2 E_w[(w^\top x + f_t(w) - w^\top E_w[w f_t(w)])^2]
\]
\[
\leq 2c^2 E_w[(w^\top (x - E_w[w f_t(w)])^2)] + 2c^2 E_w[f_t(w)^2]
\]
\[
= 2c^2 \|x - E_w[w f_t(w)]\|^2 + 2c^2 E_w[f_t(w)^2]
\]
\[
\leq 4c^2 \|x\|^2 + 4c^2 \|E_w[w f_t(w)]\|^2 + 2c^2 E_w[f_t(w)^2]
\]
(63)
(64)
(65)
(66)

From Lemma 2, we know \(\|E_w[w f_t(w)]\|^2 \leq E_w[f_t(w)^2]\) is bounded, together with \(\|x\|_2 < \infty\), it follows that \(E_w[f_{t+1}(w)^2] = E_w[h(g_{t+1}(w))^2] < \infty\). Thus, \(f_{t+1} \in F\).

**Lemma 8.** For a convex function \(\phi_\lambda(\cdot)\), denote \(h(\cdot)\) as the proximal operator of \(\phi_\lambda(\cdot)\), i.e., \(h(z) = \arg \min_x \frac{1}{2} (x - z)^2 + \phi_\lambda(x)\). Suppose \(|h(x)| \leq c|x|\) (or \(h(x) \leq c\)), \(0 < c < \infty\) (e.g., soft thresholding function). Given a bounded \(x \in \mathbb{R}^d\), set function \(g_{t+1}(w) = w^\top x + f_t(w) - w^\top E_w[w f_t(w)]\) with \(f_t \in \mathcal{L}_2\) and \(w \sim N(0, I_d)\) (or \(f_t \in \mathcal{L}_2\) and \(w \sim \text{Unif} [\sqrt{d}^{-1}]\)). Set \(f_{t+1} = h \circ g_{t+1}\). Denote \(Q(f) = L(f) + E_w[\phi_\lambda(f(w))]\) with \(L(f) := \frac{1}{2} \|x - E_w[w f(w)]\|^2\), for \(\forall f^* \in F\) with \(F = \mathcal{L}_2\) or \(F = \mathcal{L}_2\), we have
\[
Q(f_{t+1}) \leq Q(f^*) + \frac{1}{2} E_w[(f_t(w) - f^*(w))^2] - \frac{1}{2} E_w[(f_{t+1}(w) - f^*(w))^2]
\]
\[
- \frac{1}{2} \|E_w[w(f_t(w) - f^*(w))]\|^2
\]
(67)

**Proof.** From Lemma 5, we know that
\[
L(f_{t+1}) = L(f^*) + E_w[w^\top (E_w[w f_t(w)] - x)(f_{t+1}(w) - f^*(w))] + \frac{1}{2} \|E_w[w(f_{t+1}(w) - f_t(w))]\|^2
\]
\[
- \frac{1}{2} \|E_w[w(f_t(w) - f^*(w))]\|^2
\]
(68)

Together with Lemma 6, it follows that
\[
Q(f_{t+1})
\]
\[
\leq Q(f^*) - E_w[(g_{t+1}(w) - f_{t+1}(w))(f^*(w) - f_{t+1}(w))] + E_w[w^\top (E_w[w f_t(w)] - x)(f_{t+1}(w) - f^*(w))]
\]
\[
+ \frac{1}{2} \|E_w[w(f_{t+1}(w) - f_t(w))]\|^2 - \frac{1}{2} \|E_w[w(f_t(w) - f^*(w))]\|^2
\]
(69)
(70)

\[
= Q(f^*) + E_w[(g_{t+1}(w) - f_{t+1}(w) + w^\top (E_w[w f_t(w)] - x))(f_{t+1}(w) - f^*(w))]
\]
\[
+ \frac{1}{2} \|E_w[w(f_{t+1}(w) - f_t(w))]\|^2 - \frac{1}{2} \|E_w[w(f_t(w) - f^*(w))]\|^2
\]
\[
= Q(f^*) + E_w[(f_t(w) - f_{t+1}(w))(f_{t+1}(w) - f^*(w))]
\]
\[
+ \frac{1}{2} \|E_w[w(f_{t+1}(w) - f_t(w))]\|^2 - \frac{1}{2} \|E_w[w(f_t(w) - f^*(w))]\|^2
\]
(71)
(72)

Note that
\[
E_w[(f_t(w) - f_{t+1}(w))(f_{t+1}(w) - f^*(w))]
\]
\[
= E_w[(f_t(w) - f_{t+1}(w))(f_{t+1}(w) - f_{t+1}(w) + f_{t+1}(w) - f^*(w))]
\]
\[
= E_w[(f_t(w) - f_{t+1}(w))(f_t(w) - f^*(w))] - E_w[(f_t(w) - f_{t+1}(w))^2]
\]
(73)
(74)

Also note that \(ab = \frac{a^2 + b^2 - (a - b)^2}{2}\), it follows that
\[
(f_t(w) - f_{t+1}(w))(f_t(w) - f^*(w)) = \frac{(f_t(w) - f_{t+1}(w))^2 + (f_t(w) - f^*(w))^2 - (f_{t+1}(w) - f^*(w))^2}{2}
\]
(75)

It follows that
\[
E_w[(f_t(w) - f_{t+1}(w))(f_{t+1}(w) - f^*(w))]
\]
\[
= \frac{1}{2} E_w[(f_t(w) - f^*(w))^2] - \frac{1}{2} E_w[(f_{t+1}(w) - f^*(w))^2] - \frac{1}{2} E_w[(f_{t+1}(w) - f_t(w))^2]
\]
(76)
Plug Eq.(76) into Eq.(72), we can obtain that
\[
Q(f_{t+1}) \leq Q(f^*) + \frac{1}{2} \mathbb{E}_w[(f_t(w) - f^*(w))^2] - \frac{1}{2} \mathbb{E}_w[|f_{t+1}(w) - f_t(w)|^2] + \frac{1}{2} \mathbb{E}_w[(f_{t+1}(w) - f_t(w))^2]
\]
\[
+ \frac{1}{2} \mathbb{E}_w[(f_{t+1}(w) - f_t(w))^2] - \frac{1}{2} \mathbb{E}_w[(f_{t+1}(w) - f_t(w))^2] - \frac{1}{2} \mathbb{E}_w[(f_{t+1}(w) - f_t(w))^2]
\]
\[
(77)
\]
From Lemma 3 we know \(\mathbb{E}_w[w(f_{t+1}(w) - f_t(w))]_2 \leq \mathbb{E}_w[(f_{t+1}(w) - f_t(w))^2].\) It follows that
\[
Q(f_{t+1}) \leq Q(f^*) + \frac{1}{2} \mathbb{E}_w[(f_t(w) - f^*(w))^2] - \frac{1}{2} \mathbb{E}_w[(f_{t+1}(w) - f^*(w))^2]
\]
\[
- \frac{1}{2} \mathbb{E}_w[(f_{t+1}(w) - f^*(w))^2]
\]
(78)

**Lemma 9. (Strictly Monotonic Descent (a.s.))** Following the same condition of Lemma 3, we have
\[
Q(f_{t+1}) \leq Q(f_t) - \frac{1}{2} \mathbb{E}_w[(f_{t+1}(w) - f_t(w))^2]
\]
(79)

**Proof.** It follows directly from Lemma 3 by setting \(f^* = f_t.\)

**Theorem.** For a convex function \(\phi_L(\cdot),\) denote \(h(\cdot)\) as the proximal operator of \(\phi_L(\cdot),\) i.e., \(h(z) = \arg\min_x \frac{1}{2} \langle x - z \rangle^2 + \phi_L(x).\) Suppose \(|h(x)| \leq c|x|\) (or \(|h(x)| \leq c),\) \(0 < c < \infty.\) Given a bounded \(x \in \mathbb{R}^d,\) set function \(g_{t+1}(w) = w^\top x + f_t(w) - w^\top \mathbb{E}_w[w f_t(w)]\) with \(w \sim \mathcal{N}(0, I_d)\) (or \(w \sim \text{Unif}[\sqrt{d}S^{d-1}]\)). Set \(f_{t+1} = h \circ g_{t+1}\) and \(f_0 = f\) in \(\mathcal{F}\) with \(\mathcal{F} = \mathbb{L}_2\) or \(\mathcal{F} = \mathbb{E}_2\) (e.g., \(f_0 = 0).\) Denote \(Q(f) = L(f) + \mathbb{E}_w[\phi_L(f(w))]\) with \(L(f) := \frac{1}{2} \|x - \mathbb{E}_w[w f(w)]\|_2^2.\) Denote \(f_0, f_1, \ldots\) as an optimal of \(Q(\cdot)\), we have
\[
T \left( Q(f_T) - Q(f_0) \right) \leq \frac{1}{2} \mathbb{E}_w[(f_0(w) - f_0(w))^2] - \frac{1}{2} \mathbb{E}_w[(f_T(w) - f_0(w))^2]
\]
\[
- \frac{1}{2} \sum_{t=0}^{T-1} \mathbb{E}_w[w(f_t(w) - f_0(w))]_2 - \frac{1}{2} \sum_{t=0}^{T-1} (t + 1) \mathbb{E}_w[(f_{t+1}(w) - f_t(w))^2]
\]
(80)

**Proof.** From Lemma 3 by setting \(f^* = f_t,\) we can obtain that
\[
Q(f_{t+1}) \leq Q(f_t) + \frac{1}{2} \mathbb{E}_w[(f_t(w) - f_0(w))^2] - \frac{1}{2} \mathbb{E}_w[(f_{t+1}(w) - f_t(w))^2]
\]
\[
- \frac{1}{2} \mathbb{E}_w[w(f_t(w) - f_0(w))]_2
\]
(81)

Telescope the inequality (81) from \(t = 0\) to \(t = T - 1,\) we can obtain that
\[
\sum_{t=0}^{T-1} Q(f_{t+1}) - TQ(f_0) \leq \frac{1}{2} \mathbb{E}_w[(f_0(w) - f_0(w))^2] - \frac{1}{2} \mathbb{E}_w[(f_T(w) - f_0(w))^2]
\]
\[
- \frac{1}{2} \sum_{t=0}^{T-1} \mathbb{E}_w[w(f_t(w) - f_0(w))]_2
\]
(82)

In addition, from Lemma 3 we can obtain that
\[
Q(f_T) \leq Q(f_t) - \frac{1}{2} \sum_{t=0}^{T-1} \mathbb{E}_w[(f_{t+1}(w) - f_t(w))^2]
\]
(83)

It follows that
\[
TQ(f_T) - TQ(f_0) \leq \sum_{t=0}^{T-1} Q(f_{t+1}) - TQ(f_0) - \frac{1}{2} \sum_{t=0}^{T-1} \sum_{t=0}^{T-1} \mathbb{E}_w[(f_{t+1}(w) - f_t(w))^2]
\]
\[
= \sum_{t=0}^{T-1} Q(f_{t+1}) - TQ(f_0) - \frac{1}{2} \sum_{t=0}^{T-1} (t + 1) \mathbb{E}_w[(f_{t+1}(w) - f_t(w))^2]
\]
(84)
Plug inequality \[82\] into inequality \[85\], we can obtain that
\[
TQ(f_T) - TQ(f_s) \leq \frac{1}{2} E_w[(f_0(w) - f_s(w))^2] - \frac{1}{2} E_w[(f_T(w) - f_s(w))^2]
\]
\[
= \frac{1}{2} T \sum_{t=0}^{T-1} \|E_w[w(f_t(w) - f_s(w))\|^2 - \frac{1}{2} (t+1) E_w[(f_{t+1}(w) - f_t(w))^2]
\]
\[86\]

C Proof of Theorem 1

Non-convex \(\phi\)-regularization:

**Theorem.** For a (non-convex) regularization function \(\phi_\lambda(\cdot)\), denote \(h(\cdot)\) as the proximal operator of \(\phi_\lambda(\cdot)\), i.e.,
\[
h(z) = \arg\min_x \frac{1}{2} \|x - z\|^2 + \phi_\lambda(x).
\]
Suppose \(\|h(x)\| \leq c \|x\|\) (or \(\|h(x)\| \leq c\)), \(0 < c < \infty\) (e.g., hard thresholding function). Given a bounded \(x \in \mathbb{R}^d\), set function \(g_{t+1}(w) = w^\top x + f_t(w) - w^\top E_w[w f_t(w)]\) with \(f_t \in \mathcal{L}_2\) and \(w \sim \mathcal{N}(0, I_d)\) (or \(f_t \in \mathcal{L}_2\), \(w \sim \text{Unif}([\sqrt{d}^{-1}], 1)\)). Set \(f_{t+1} = h \circ g_{t+1}\. Denote Q(f) = L(f) + E_w[\phi_\lambda(f(w))]\) with \(L(f) := \frac{1}{2} \|x - E_w[w f(w)]\|^2\), we have
\[
Q(f_{t+1}) \leq Q(f_t) - \frac{1}{2} E_w[(f_{t+1}(w) - f_t(w) - w^\top E_w[w(f_{t+1}(w) - f_t(w))])^2] \leq Q(f_t)
\]
\[87\]

**Proof.** From Lemma 4, we know that
\[
L(f_{t+1}) = L(f_t) + E_w[w^\top (E_w[w f_t(w)] - x)(f_{t+1}(w) - f_t(w))] + \frac{1}{2} \|E_w[w(f_{t+1}(w) - f_t(w))\|^2
\]
\[88\]
Let \(g_{t+1}(w) = w^\top x + f_t(w) - w^\top E_w[w f_t(w)]\), together with Eq. \[88\], we can obtain that
\[
L(f_{t+1}) = L(f_t) + E_w[(f_t(w) - g_{t+1}(w))(f_{t+1}(w) - f_t(w))] + \frac{1}{2} \|E_w[w(f_{t+1}(w) - f_t(w))\|^2
\]
\[89\]
Note that \(ab = \frac{(a+b)^2-a^2-b^2}{2}\), it follows that
\[
(f_t(w) - g_{t+1}(w))(f_{t+1}(w) - f_t(w)) = \left(\frac{f_{t+1}(w) - g_{t+1}(w)}{2}\right)^2 - \left(\frac{f_t(w) - g_{t+1}(w)}{2}\right)^2 - \left(\frac{f_{t+1}(w) - f_t(w)}{2}\right)^2
\]
\[90\]
Since \(f_{t+1} = h \circ g_{t+1}\) is the solution of the proximal problem, i.e.,
\(f_{t+1}(w) = \arg\min_x (x - g_{t+1}(w))^2 + \phi_\lambda(x)\), we know that
\[
\left(\frac{f_{t+1}(w) - g_{t+1}(w)}{2}\right)^2 - \left(\frac{f_t(w) - g_{t+1}(w)}{2}\right)^2 \leq \phi_\lambda(f_t(w)) - \phi_\lambda(f_{t+1}(w))
\]
\[91\]
It follows that
\[
E_w[(f_t(w) - g_{t+1}(w))(f_{t+1}(w) - f_t(w))] = E_w\left[\left(\frac{f_{t+1}(w) - g_{t+1}(w)}{2}\right)^2 - \left(\frac{f_t(w) - g_{t+1}(w)}{2}\right)^2 - \left(\frac{f_{t+1}(w) - f_t(w)}{2}\right)^2\right]
\]
\[92\]
\[
\leq E_w[\phi_\lambda(f_t(w))] - E_w[\phi_\lambda(f_{t+1}(w))] + \frac{1}{2} E_w[(f_{t+1}(w) - f_t(w))^2]
\]
\[93\]
Plug inequality \[93\] into Eq. \[89\], we can achieve that
\[
L(f_{t+1}) + E_w[\phi_\lambda(f_{t+1}(w))] \leq L(f_t) + E_w[\phi_\lambda(f_t(w))] - \frac{1}{2} E_w[(f_{t+1}(w) - f_t(w))^2]
\]
\[94\]
From Lemma 2 we know that
\[
E_w[(f_{t+1}(w) - f_t(w))^2] - \frac{1}{2}E_w[w(f_{t+1}(w) - f_t(w))]^2
= E_w[(f_{t+1}(w) - f_t(w) - w^T E_w[w(f_{t+1}(w) - f_t(w))])^2]
\]
(95)

It follows that
\[
Q(f_{t+1}) \leq Q(f_t) - \frac{1}{2}E_w[(f_{t+1}(w) - f_t(w) - w^T E_w[w(f_{t+1}(w) - f_t(w))])^2] \leq Q(f_t)
\]
(96)

\[ \square \]

D Proof of Theorem 3

To prove the Theorem 3, we first show some useful Lemmas.

Lemma 10. Suppose \( \frac{1}{N} WW^T = I_d \), for any bounded \( y \in \mathbb{R}^N \), we have \( \frac{1}{N} \|y\|^2_2 - \frac{1}{N} \|Wy\|^2_2 = \frac{1}{N} \|y - \frac{1}{N} W^T Wy\|^2_2 \geq 0 \).

Proof.
\[
\frac{1}{N} \|y\|^2_2 - \frac{1}{N} \|Wy\|^2_2 = \|y\|^2_2 - \frac{1}{N} \|Wy\|^2_2 + \frac{1}{N} \|Wy\|^2_2
= \frac{1}{N} \|y\|^2_2 - \frac{2}{N^2} y^TW^TWy + \frac{1}{N^2} y^TW^TWy
= \frac{1}{N} \|y\|^2_2 - \frac{2}{N^2} y^TW^TWy + \frac{1}{N^2} y^TW^TWy
= \frac{1}{N} \|y - \frac{1}{N} W^T Wy\|^2_2 \geq 0
\]
(97)

Lemma 11. Denote \( L(y) := \frac{1}{2} \|x - \frac{1}{N} Wy\|^2_2 \). For \( \forall y, z \in \mathbb{R}^N \), we have \( L(z) = L(y) + < \frac{1}{N} W^T Wy - \frac{1}{N} W^T x, z - y > + \frac{1}{2} \|\frac{1}{N} W(z - y)\|^2_2 \).

Proof.
\[
\frac{1}{2} \|x - \frac{1}{N} Wz\|^2_2 = \frac{1}{2} \|x - \frac{1}{N} Wy + \frac{1}{N} Wy - \frac{1}{N} Wz\|^2_2
= L(y) + < \frac{1}{N} Wy - x, \frac{1}{N} W(z - y) > + \frac{1}{2} \|\frac{1}{N} W(z - y)\|^2_2
= L(y) + < \frac{1}{N^2} W^T Wy - \frac{1}{N} W^T x, z - y > + \frac{1}{2} \|\frac{1}{N} W(z - y)\|^2_2
\]
(101)

Theorem. (Monotonic Descent) For a function \( \phi_\lambda(\cdot) \), denote \( h(\cdot) \) as the proximal operator of \( \phi_\lambda(\cdot) \). Given a bounded \( x \in \mathbb{R}^d \), set \( y_{t+1} = h(W^T x + (I - \frac{1}{N} W^T W)y_t) \) with \( \frac{1}{N} WW^T = I_d \). Denote \( \hat{Q}(y) := \frac{1}{2} \|x - \frac{1}{N} Wy\|^2_2 + \frac{1}{N} \phi_\lambda(y) \). For \( t \geq 0 \), we have
\[
\hat{Q}(y_{t+1}) \leq \hat{Q}(y_t) - \frac{1}{2N} \|I_d - \frac{1}{N} W^T W\| (y_{t+1} - y_t)\| \leq \hat{Q}(y_t)
\]
(104)

Proof. Denote \( L(y) := \frac{1}{2} \|x - \frac{1}{N} Wy\|^2_2 \), from Lemma 10, we know that
\[
L(y_{t+1}) = L(y_t) + < \frac{1}{N^2} W^T Wy_{t+1} - \frac{1}{N} W^T x, y_{t+1} - y_t > + \frac{1}{2} \|\frac{1}{N} W(y_{t+1} - y_t)\|^2_2
\]
(105)
Let \( a_{t+1} = W^T x + (I - \frac{1}{N} W^T W)y_t \). Together with Eq. (107), we can obtain that
\[
L(y_{t+1}) = L(y_t) + \frac{1}{N} W^T W y_t - \frac{1}{N} W^T x, y_{t+1} - y_t > + \frac{1}{2} \| \frac{1}{N} W (y_{t+1} - y_t) \|_2^2
\]
(106)
\[
= \frac{1}{N} L(y_t) + \frac{1}{N} < y_t - a_{t+1}, y_{t+1} - y_t > + \frac{1}{2} \| \frac{1}{N} W (y_{t+1} - y_t) \|_2^2
\]
(107)
Note that \( a^T b = \frac{\|a+b\|_2^2 - \|a\|_2^2 - \|b\|_2^2}{2} \), it follows that
\[
< y_t - a_{t+1}, y_{t+1} - y_t > = \frac{\|y_{t+1} - a_{t+1}\|_2^2 - \|y_t - a_{t+1}\|_2^2 - \|y_{t+1} - y_t\|_2^2}{2}
\]
(108)
Since \( y_{t+1} = h(a_{t+1}) \) is the solution of the proximal problem, i.e., \( y_{t+1} = \arg \min_y \frac{1}{2} \|y - a_{t+1}\|_2^2 + \phi_\lambda(y) \), we can achieve that
\[
\frac{1}{2} \|y_{t+1} - a_{t+1}\|_2^2 + \phi_\lambda(y_{t+1}) \leq \frac{1}{2} \|y_t - a_{t+1}\|_2^2 + \phi_\lambda(y_t)
\]
(109)
It can be rewritten as
\[
\frac{1}{2} \|y_{t+1} - a_{t+1}\|_2^2 - \frac{1}{2} \|y_t - a_{t+1}\|_2^2 \leq \phi_\lambda(y_t) - \phi_\lambda(y_{t+1})
\]
(110)
Together with Eq. (107), Eq. (108) and inequality (110), it follows that
\[
L(y_{t+1}) + \frac{1}{N} \phi_\lambda(y_{t+1}) \leq L(y_t) + \frac{1}{N} \phi_\lambda(y_t) - \frac{1}{2N} \|y_{t+1} - y_t\|_2^2 + \frac{1}{2} \| \frac{1}{N} W (y_{t+1} - y_t) \|_2^2
\]
(111)
Together with Lemma 10 we can achieve that
\[
\hat{Q}(y_{t+1}) \leq \hat{Q}(y_t) - \frac{1}{2N} \|(I_d - \frac{1}{N} W^T W)(y_{t+1} - y_t)\|_2^2 \leq \hat{Q}(y_t)
\]
(112)

E Proof of Theorem 4

Before proving Theorem 4, we first show some useful Lemmas.

Lemma 12. Denote \( L(y) := \frac{1}{2} \|x - \frac{1}{N} W y\|_2^2 \). For any bounded \( y_t, y_{t+1}, z \in \mathbb{R}^N \), we have
\[
L(y_{t+1}) = L(z) + \left\langle \frac{1}{N} W^T W y_t - \frac{1}{N} W^T x, y_{t+1} - z \right\rangle + \frac{1}{2} \| \frac{1}{N} W (y_{t+1} - y_t) \|_2^2
\]
(113)

Proof. Denote \( L(y) := \frac{1}{2} \|x - \frac{1}{N} W y\|_2^2 \). From Lemma 11 we can achieve that
\[
L(z) = L(y_t) + \frac{1}{N^2} W^T W y_t - \frac{1}{N} W^T x, z - y_t > + \frac{1}{2} \| \frac{1}{N} W (z - y_t) \|_2^2
\]
(114)
\[
L(y_{t+1}) = L(y_t) + \frac{1}{N^2} W^T W y_t - \frac{1}{N} W^T x, y_{t+1} - y_t > + \frac{1}{2} \| \frac{1}{N} W (y_{t+1} - y_t) \|_2^2
\]
(115)
It follows that
\[
L(y_{t+1}) = L(z) - \left\langle \frac{1}{N^2} W^T W y_t - \frac{1}{N} W^T x, z - y_t \right\rangle + \left\langle \frac{1}{N^2} W^T W y_t - \frac{1}{N} W^T x, y_{t+1} - y_t \right\rangle
+ \frac{1}{2} \| \frac{1}{N} W (y_{t+1} - y_t) \|_2^2 - \frac{1}{2} \| \frac{1}{N} W (z - y_t) \|_2^2
\]
(116)
\[
= L(z) + \left\langle \frac{1}{N^2} W^T W y_t - \frac{1}{N} W^T x, y_{t+1} - z \right\rangle + \frac{1}{2} \| \frac{1}{N} W (y_{t+1} - y_t) \|_2^2
- \frac{1}{2} \| \frac{1}{N} W (z - y_t) \|_2^2
\]
(117)
Lemma 13. For a convex function \( \phi_L(\cdot) \), let \( h(\cdot) \) be the proximal operator w.r.t. \( \phi_L(\cdot) \). Denote \( \tilde{Q}(y) := \frac{1}{2} ||x - \frac{1}{N} W y||_2^2 + \frac{1}{N} \phi_L(y) \), for any bounded \( y_t, z \in \mathbb{R}^N \), set \( a_{t+1} = W^\top x + (I - \frac{1}{N} W^\top W)y_t \) and \( y_{t+1} = h(a_{t+1}) \), then we have

\[
\hat{Q}(y_{t+1}) \leq \hat{Q}(z) + \frac{1}{2N} (||y_t - z||_2^2 - ||y_{t+1} - z||_2^2) - \frac{1}{2} \frac{1}{N} W(z - y_t)||_2^2
\]

(118)

Proof. Since \( y_{t+1} = \text{arg min}_y \phi_L(y) + \frac{1}{2} ||y - a_{t+1}||_2^2 \), we have

\[
0 \in \partial \phi_L(y_{t+1}) + (y_{t+1} - a_{t+1}) \implies (a_{t+1} - y_{t+1}) \in \partial \phi_L(y_{t+1})
\]

(119)

For a convex function \( \phi_L(y) \) and subgradient \( g \in \partial \phi_L(y) \), we know \( \phi_L(z) \geq \phi_L(y) + \langle g, z - y \rangle \), it follows that

\[
\phi_L(z) \geq \phi_L(y_{t+1}) + \langle a_{t+1} - y_{t+1}, z - y_{t+1} \rangle
\]

(120)

Together with Lemma 12, we can obtain that

\[
L(y_{t+1}) + \frac{1}{N} \phi_L(y_{t+1}) \leq L(z) + \frac{1}{N} \phi_L(z) - \frac{1}{N} \langle a_{t+1} - y_{t+1}, z - y_{t+1} \rangle
\]

\[
+ \left( \frac{1}{N^2} W^\top W y_t - \frac{1}{N} W^\top x, y_{t+1} - z \right) + \frac{1}{2} \frac{1}{N} W(y_{t+1} - y_t)||_2^2
\]

\[
- \frac{1}{2} \frac{1}{N} W(z - y_t)||_2^2
\]

(121)

It follows that

\[
\hat{Q}(y_{t+1}) \leq \hat{Q}(z) + \frac{1}{N} \langle y_t - y_{t+1}, y_{t+1} - z \rangle + \frac{1}{2} \frac{1}{N} W(y_{t+1} - y_t)||_2^2 - \frac{1}{2} \frac{1}{N} W(z - y_t)||_2^2
\]

(122)

Note that \( a^\top b = \frac{|a + b||b| - |a||b|^2}{2} \), it follows that

\[
\langle y_t - y_{t+1}, y_{t+1} - z \rangle = \frac{1}{2} ||y_t - z||_2^2 - \frac{1}{2} ||y_t - y_{t+1}||_2^2 - \frac{1}{2} ||y_t - y_{t+1}||_2^2
\]

(123)

Together with inequality (122), we can achieve that

\[
\hat{Q}(y_{t+1}) \leq \hat{Q}(z) + \frac{1}{2N} (||y_t - z||_2^2 - ||y_{t+1} - z||_2^2 - ||y_t - y_{t+1}||_2^2) + \frac{1}{2} \frac{1}{N} W(y_{t+1} - y_t)||_2^2
\]

\[
- \frac{1}{2} \frac{1}{N} W(z - y_t)||_2^2
\]

(124)

From Lemma 10, we know \( \frac{1}{N} ||y_t - y_{t+1}||_2^2 \geq \frac{1}{N} W(y_{t+1} - y_t)||_2^2 \), it follows that

\[
\hat{Q}(y_{t+1}) \leq \hat{Q}(z) + \frac{1}{2N} (||y_t - z||_2^2 - ||y_{t+1} - z||_2^2) - \frac{1}{2} \frac{1}{N} W(z - y_t)||_2^2
\]

(125)

Lemma 14. (Strictly Monotonic Descent) For a convex function \( \phi_L(\cdot) \), let \( h(\cdot) \) be the proximal operator w.r.t \( \phi_L(\cdot) \). Denote \( \tilde{Q}(y) := \frac{1}{2} ||x - \frac{1}{N} W y||_2^2 + \frac{1}{N} \phi_L(y) \), for any bounded \( y_t \in \mathbb{R}^N \), set \( a_{t+1} = W^\top x + (I - \frac{1}{N} W^\top W)y_t \) and \( y_{t+1} = h(a_{t+1}) \), then we have

\[
\hat{Q}(y_{t+1}) \leq \hat{Q}(y_t) - \frac{1}{2N} ||y_{t+1} - y_t||_2^2
\]

(126)

Proof. From Lemma 13, setting \( z = y_t \), we can directly get the result.

Theorem. For a convex function \( \phi_L(\cdot) \), denote \( h(\cdot) \) as the proximal operator of \( \phi_L(\cdot) \). Given a bounded \( x \in \mathbb{R}^d \), set \( y_{t+1} = h(W^\top x + (I - \frac{1}{N} W^\top W)y_t) \) with \( \frac{1}{N} WW^\top = I_d \). Denote \( \bar{Q}(y) := \frac{1}{2} ||x - \bar{A}(y)||_2^2 + \frac{1}{N} \phi_L(y) \) and \( \bar{y} \) as an optimal of \( \bar{Q}(\cdot) \), for \( T \geq 1 \), we have

\[
T(\hat{Q}(y_T) - \hat{Q}(\bar{y})) \leq \frac{1}{2N} ||y_0 - \bar{y}||_2^2 - \frac{1}{2N} ||y_T - \bar{y}||_2^2 - \frac{1}{2} \sum_{t=0}^{T-1} \frac{1}{N} W(y_t - \bar{y})||_2^2
\]

\[
- \frac{1}{2} \sum_{t=0}^{T-1} \frac{T + 1}{N} ||y_{t+1} - y_t||_2^2
\]

(127)
Proof. From Lemma 14, setting $z = y^*$, we can achieve that

$$
\hat{Q}(y_{t+1}) \leq \hat{Q}(y^*) + \frac{1}{2N} \left( \|y_t - y^*\|^2 - \|y_{t+1} - y^*\|^2 \right) - \frac{1}{2} \left\| \frac{1}{N} W(y^* - y_t) \right\|^2 \tag{128}
$$

Telescope the inequality (128) from $t = 0$ to $t = T - 1$, we can obtain that

$$
\sum_{t=0}^{T-1} \hat{Q}(y_{t+1}) - T\hat{Q}(y^*) \leq \frac{1}{2N} \|y_0 - y^*\|^2 - \frac{1}{2N} \|y_T - y^*\|^2 - \frac{1}{2} \sum_{t=0}^{T-1} \left\| \frac{1}{N} W(y_t - y^*) \right\|^2 \tag{129}
$$

From Lemma 14 we know that

$$
\hat{Q}(y_{t+1}) \leq \hat{Q}(y_t) - \frac{1}{2N} \|y_{t+1} - y_t\|^2 \tag{130}
$$

It follows that

$$
\hat{Q}(y_T) \leq \hat{Q}(y_t) - \frac{1}{2N} \sum_{i=t}^{T-1} \|y_{i+1} - y_i\|^2 \tag{131}
$$

Then, we can achieve that

$$
T\hat{Q}(y_T) - T\hat{Q}(y^*) \leq \sum_{t=0}^{T-1} \hat{Q}(y_{t+1}) - T\hat{Q}(y^*) - \frac{1}{2N} \sum_{t=0}^{T-1} \sum_{i=t}^{T-1} \|y_{i+1} - y_i\|^2 \\
= \sum_{t=0}^{T-1} \hat{Q}(y_{t+1}) - T\hat{Q}(y^*) - \frac{1}{2N} \sum_{t=0}^{T-1} (t + 1) \|y_{t+1} - y_t\|^2 \tag{132}
$$

Plug inequality (129) into inequality (133), we obtain that

$$
T(\hat{Q}(y_T) - \hat{Q}(y^*)) \leq \frac{1}{2N} \|y_0 - y^*\|^2 - \frac{1}{2N} \|y_T - y^*\|^2 - \frac{1}{2} \sum_{t=0}^{T-1} \left\| \frac{1}{N} W(y_t - y^*) \right\|^2 \\
- \frac{1}{2} \sum_{t=0}^{T-1} \frac{t + 1}{N} \|y_{t+1} - y_t\|^2 \tag{134}
$$

$\square$

F Proof of Theorem 5

We first show the structured samples $B$ constructed in [29][30].

Without loss of generality, we assume that $d = 2m$, $N = 2n$. Let $F \in \mathbb{C}^{n \times n}$ be an $n \times n$ discrete Fourier matrix. $F_{k,j} = e^{\frac{2\pi i k j}{2n}}$ is the $(k,j)^{th}$ entry of $F$, where $i = \sqrt{-1}$. Let $\Lambda = \{k_1, k_2, ..., k_m\} \subset \{1, ..., n-1\}$ be a subset of indexes.

The structured matrix $B$ can be constructed as Eq. (135).

$$
B = \frac{\sqrt{n}}{\sqrt{m}} \begin{bmatrix} 
\text{Re} F_\Lambda & -\text{Im} F_\Lambda \\
\text{Im} F_\Lambda & \text{Re} F_\Lambda 
\end{bmatrix} \in \mathbb{R}^{d \times N} \tag{135}
$$

where Re and Im denote the real and imaginary parts of a complex number, and $F_\Lambda$ in Eq. (136) is the matrix constructed by $m$ rows of $F$

$$
F_\Lambda = \frac{1}{\sqrt{m}} \begin{bmatrix}
e^{\frac{2\pi i k_1}{n}} & \cdots & e^{\frac{2\pi i k_1}{n}} \\
\vdots & \ddots & \vdots \\
e^{\frac{2\pi i k_m}{n}} & \cdots & e^{\frac{2\pi i k_m}{n}}
\end{bmatrix} \in \mathbb{C}^{m \times n}. \tag{136}
$$
The index set can be constructed by a closed-form solution [30] or by a coordinate descent method [29].
Specifically, for a prime number $n$ such that $m$ divides $n-1$, i.e., $m|(n-1)$, we can employ a closed-form construction as in [30]. Let $g$ denote a primitive root modulo $n$. We can construct the index $\Lambda = \{k_1, k_2, ..., k_m\}$ as

$$\Lambda = \{g^0, g^{\frac{n-1}{m}}, g^{\frac{2(n-1)}{m}}, ..., g^{\frac{(m-1)(n-1)}{m}}\} \mod n.$$  \hspace{1cm} (137)

The resulted structured matrix $B$ has a bounded mutual coherence, which is shown in Theorem 8.

**Theorem 8.** [30] Suppose $d = 2m, N = 2n$, and $n$ is a prime such that $m|(n-1)$. Construct matrix $B$ as in Eq. (135) with index set $\Lambda$ as Eq. (137). Let mutual coherence $\mu(B) := \max_{i \neq j} |\frac{b_i^*b_j}{\|b_i\|_2\|b_j\|_2}|$. Then $\mu(B) \leq \frac{\sqrt{m}}{m}$.

**Remark:** The bound of mutual coherence in Theorem 8 is non-trivial when $n < m^2$. For the case $n \geq m^2$, we can use the coordinate descent method in [29] to minimize the mutual coherence.

We now show the orthogonal property of our data-dependent structured samples $D = \frac{\sqrt{2}}{\sqrt{N}}R^\top B$

**Proposition 2.** Suppose $d = 2m, N = 2n$. Let $D = \frac{\sqrt{2}}{\sqrt{N}}R^\top B$ with $B$ constructed as in Eq. (135). Then $DD^\top = I_d$ and column vector has constant norm, i.e., $\|d_j\|_2 = \sqrt{\frac{m}{n}}, \forall j \in \{1, \cdots, N\}$.

**Proof.** Since $DD^\top = \frac{d}{N}BB^\top = \frac{m}{n}BB^\top = \frac{m}{n}BB^\top$, where $B = \frac{\sqrt{m}}{\sqrt{N}}B$. It follows that

$$\bar{B} = \begin{bmatrix} \text{Re}F_{\Lambda} & -\text{Im}F_{\Lambda} \\ \text{Im}F_{\Lambda} & \text{Re}F_{\Lambda} \end{bmatrix} \in \mathbb{R}^{d \times N}$$  \hspace{1cm} (138)

Let $c_i \in \mathbb{C}^{1 \times n}$ be the $i^{th}$ row of matrix $F_{\Lambda} \in \mathbb{C}^{m \times n}$ in Eq. (136). Let $v_i \in \mathbb{R}^{1 \times 2n}$ be the $i^{th}$ row of matrix $\bar{B} \in \mathbb{R}^{2m \times 2n}$ in Eq. (138). For $1 \leq i, j \leq m, i \neq j$, we know that

$$v_i^\top v_{i+m} = 0,$$  \hspace{1cm} (139)

$$v_i^\top v_{j+m} = v_i^\top v_j = \text{Re}(c_i^*c_j),$$  \hspace{1cm} (140)

$$v_i^\top v_{j+m} = -v_i^\top v_j = \text{Im}(c_i^*c_j),$$  \hspace{1cm} (141)

where $*$ denotes the complex conjugate, $\text{Re}(-)$ and $\text{Im}(-)$ denote the real and imaginary parts of the input complex number.

For a discrete Fourier matrix $F$, we know that

$$c_i^*c_j = \frac{1}{n} \sum_{k=0}^{n-1} e^{2\pi i(-i-j)k/n} = \begin{cases} 1, & \text{if } i = j \\ 0, & \text{otherwise} \end{cases}$$  \hspace{1cm} (142)

When $i \neq j$, from Eq. (142), we know $c_i^*c_j = 0$. Thus, we have

$$v_i^\top v_{i+m} = v_i^\top v_j = \text{Re}(c_i^*c_j) = 0, \hspace{1cm} (143)$$

$$v_i^\top v_{j+m} = -v_i^\top v_j = \text{Im}(c_i^*c_j) = 0, \hspace{1cm} (144)$$

When $i = j$, we know that $v_i^\top v_{i+m} = v_i^\top v_i = c_i^*c_i = 1$.

Put two cases together, also note that $d = 2m$, we have $DD^\top = \frac{m}{n}BB^\top = I_d$.

The $l_2$-norm of the column vector of $\bar{B}$ is given as

$$\|\bar{b}_j\|_2 = \frac{1}{n} \sum_{i=1}^{m} \left( \sin^2 \frac{2\pi k_i j}{n} + \cos^2 \frac{2\pi k_i j}{n} \right) = \frac{m}{n}$$  \hspace{1cm} (145)

Thus, we have $\|d_j\|_2 = \|\bar{b}_j\|_2 = \sqrt{\frac{m}{n}}$ for $j \in \{1, \cdots, M\}$.
Lemma 15. Let $D = \frac{\sqrt{d}}{\sqrt{N}}R^T B$, where $B$ is constructed as in Eq. (135) with index set $\Lambda$ as Eq. (137) with $N = 2n, d = 2m$. \[ \forall y \in \mathbb{R}^N, ||y||_0 \leq 2k, \text{ we have } ||Dy||_2 - ||y||_2 \leq -\frac{n-(2k-1)\sqrt{n}+m}{n}||y||_2 \]

Proof. Denote $M = D^T D$. Since the column vector of $D$ has constant norm, i.e., $||d_j||_2 = \frac{n}{m}$, it follows that

\[ ||Dy||_2^2 = y^T My = ||d_j||_2^2 \left( \sum_{i=1}^{N} y_i^2 - \sum_{i=1}^{N} \sum_{j=1, j \neq i}^{N} y_i y_j M_{ij} \right) \]

(146)

\[ = \frac{m}{n} ||y||_2^2 + \frac{m}{n} \sum_{i=1}^{N} \sum_{j=1, j \neq i}^{N} y_i y_j M_{ij} \]

(147)

\[ \leq \frac{m}{n} ||y||_2^2 + \frac{m}{n} \mu(D) \left( \sum_{i=1}^{N} \sum_{j=1, j \neq i}^{N} |y_i||y_j| \right) \]

(148)

\[ = \frac{m}{n} ||y||_2^2 + \frac{m}{n} \mu(D) \left( \sum_{i=1}^{N} |y_i|^2 - \sum_{i=1}^{N} y_i^2 \right) \]

(149)

Since $||y||_0 \leq 2k$, we know there is at most $2k$ non-zero elements among $y$. Thus, we know that

\[ ||Dy||_2^2 \leq \frac{m}{n} ||y||_2^2 + \frac{m}{n} \mu(D) \left( \sum_{i=1}^{N} |y_i|^2 - \sum_{i=1}^{N} y_i^2 \right) \]

(150)

\[ \leq \frac{m}{n} ||y||_2^2 + \frac{m}{n} \mu(D) (2k \sum_{i=1}^{N} y_i^2 - \sum_{i=1}^{N} y_i^2) \]

(151)

\[ = \frac{m}{n} ||y||_2^2 + \frac{m}{n} \mu(D) (2k - 1) ||y||_2^2 \]

(152)

Since $\mu(D) = B$, from Theorem 8, we know $\mu(D) \leq \frac{\sqrt{m}}{m}$. It follows that

\[ ||Dy||_2^2 \leq \frac{m}{n} ||y||_2^2 + \frac{m}{n} \mu(D) (2k - 1) ||y||_2^2 \]

(153)

\[ \leq \frac{m}{n} ||y||_2^2 + \frac{m}{n} (2k - 1) \sqrt{m} ||y||_2^2 \]

(154)

\[ = \frac{(2k - 1) \sqrt{m} + m}{n} ||y||_2^2 \]

(155)

It follows that $||Dy||_2^2 - ||y||_2^2 \leq \frac{(2k-1)\sqrt{m}+m-n}{n}||y||_2^2$. \[ \square \]

Theorem. (Strictly Monotonic Descent of $k$-sparse problem) Let $L(y) = \frac{1}{2}||x - Dy||_2^2$, s.t. $||y||_0 \leq k$ with $D = \frac{\sqrt{d}}{\sqrt{N}}R^T B$, where $B$ is constructed as in Eq. (135) with index set $\Lambda$ as Eq. (137) with $N = 2n, d = 2m$. Set $y_{t+1} = h(a_{t+1})$ with sparsity $k$ and $a_{t+1} = D^T x + (I - D^T D)y_t$, we have

\[ L(y_{t+1}) \leq L(y_t) + \frac{1}{2}||y_{t+1} - a_{t+1}||_2^2 - \frac{1}{2}||y_t - a_{t+1}||_2^2 - \frac{n-(2k-1)\sqrt{m}-m}{2n}||y_{t+1} - y_t||_2^2 \leq L(y_t) \]

(156)

where $h(\cdot)$ is defined as

\[ h(z_j) = \begin{cases} 
 z_j & \text{if } |z_j| \text{ is one of the $k$-highest values of } |z| \in \mathbb{R}^N \\
 0 & \text{otherwise} 
\end{cases} \]

(157)

Proof. Denote $L(y) := \frac{1}{2}||x - Dy||_2^2$. It follows that

\[ L(y_{t+1}) = \frac{1}{2}||x - Dy_{t+1}||_2^2 = \frac{1}{2}||x - Dy_t + Dy_t - Dy_{t+1}||_2^2 \]

(158)

\[ = L(y_t) + \langle x - Dy_t, D(y_t - y_{t+1}) \rangle + ||D(y_t - y_{t+1})||_2^2 \]

(159)

\[ = L(y_t) + \langle D^T x - D^T Dy_t, y_t - y_{t+1} \rangle + ||D(y_t - y_{t+1})||_2^2 \]

(160)

\[ = L(y_t) + \langle D^T Dy_t - D^T x, y_{t+1} - y_t \rangle + ||D(y_t - y_{t+1})||_2^2 \]

(161)
Let \( a_{t+1} = D^\top x + (I - D^\top D)y_t \), together with Eq. (161), we can obtain that

\[
L(y_{t+1}) = L(y_t) + \langle y_t - a_{t+1}, y_{t+1} - y_t \rangle + \frac{1}{2} \| D(y_{t+1} - y_t) \|^2_2 \tag{162}
\]

and

\[
= L(y_t) + \frac{\| y_{t+1} - a_{t+1} \|^2_2 - \| y_t - a_{t+1} \|^2_2}{2} - \frac{\| y_{t+1} - y_t \|^2_2}{2} + \frac{1}{2} \| D(y_{t+1} - y_t) \|^2_2 \tag{163}
\]

From Lemma [15], we know that

\[
\frac{1}{2} \| D(y_{t+1} - y_t) \|^2_2 - \frac{1}{2} \| y_{t+1} - y_t \|^2_2 \leq -\frac{n - (2k - 1)\sqrt{n} - m}{2n} \| y_{t+1} - y_t \|^2_2
\]

It follows that

\[
L(y_{t+1}) \leq L(y_t) + \frac{1}{2} \| y_{t+1} - a_{t+1} \|^2_2 - \frac{1}{2} \| y_t - a_{t+1} \|^2_2 - \frac{n - (2k - 1)\sqrt{n} - m}{2n} \| y_{t+1} - y_t \|^2_2 \tag{165}
\]

Note that \( y_{t+1} := \arg \min_{y \| y \|_2 \leq 1} \| y - a_{t+1} \|^2_2 \), we know \( \| y_{t+1} - a_{t+1} \|^2_2 \leq \| y_t - a_{t+1} \|^2_2 \). It follows that \( L(y_{t+1}) \leq L(y_t) \), in which the equality holds true when \( \| y_{t+1} - a_{t+1} \|^2_2 = \| y_t - a_{t+1} \|^2_2 \) and \( \| y_{t+1} - y_t \|^2_2 = 0 \).

\[\square\]

G A Better Diagonal Random Rotation for SSF [29]

In [29], a diagonal rotation matrix \( D \) is constructed by sampling its diagonal elements uniformly from \( \{-1, +1\}\). In this section, we propose a better diagonal random rotation. Without loss of generality, we assume that \( d = 2m, N = 2n \).

We first generate a diagonal complex matrix \( D \in \mathbb{C}^{m \times m} \), in which the diagonal elements are constructed as

\[
D_{jj} = \cos \theta_j + i \sin \theta_j, \forall j \in \{1, \cdots, m\}
\]  

where \( \theta_j, \forall j \in \{1, \cdots, m\} \) are i.i.d. samples from the uniform distribution \( Un(0, 2\pi) \), and \( i = \sqrt{-1} \).

We then generate a uniformly random permutation \( \Pi : \{1, \cdots, d\} \rightarrow \{1, \cdots, d\} \). The SSF samples can be constructed as \( H = \Pi \circ B \) with \( B \):

\[
\bar{B} = \frac{\sqrt{n}}{\sqrt{m}} \begin{bmatrix} \text{Re} \bar{F}_A & -\text{Im} \bar{F}_A \\ \text{Im} \bar{F}_A & \text{Re} \bar{F}_A \end{bmatrix} \in \mathbb{R}^{d \times N}
\]  

where \( \bar{F}_A = DF_A \).

It is worth noting that \( H^\top H = B^\top B \), which means that the proposed diagonal rotation scheme preserved the pairwise inner product of SSF [29]. Moreover, the SSF with the proposed random rotation maintains \( O(d) \) space complexity and \( O(n \log n) \) (matrix-vector product) time complexity by FFT.

H Rademacher Complexity

Neural Network Structure: For structured approximated NOK networks (SNOK), the 1-\( T \) layers are given as

\[
y_{t+1} = h(D^\top R_t x + (I - D^\top D)y_t)
\]  

where \( R_t \) are free parameters such that \( R_t^\top R_t = R_t^\top R_t = I_d \). And \( D \) is the scaled structured spherical samples such that \( DD^\top = I_d \), and \( y_0 = 0 \).

The last layer ( \((T+1)\)th layer) is given by \( z = w^\top y_{T+1} \). Consider a \( L \)-Lipschitz continuous loss function \( \ell(z, y) : \mathcal{Z} \times \mathcal{Y} \rightarrow [0, 1] \) with Lipschitz constant \( L \) w.r.t the input \( z \).
Rademacher Complexity: Rademacher complexity of a function class $G$ is defined as

$$\mathcal{R}_N(G) := \frac{1}{N} \mathbb{E} \left[ \sup_{g \in G} \sum_{i=1}^{N} \epsilon_i g(x_i) \right]$$  \hspace{1cm} (169)$$

where $\epsilon_i, i \in \{1, \cdots, N\}$ are i.i.d. samples drawn uniformly from $\{+1, -1\}$ with probability $P[\epsilon_i = +1] = P[\epsilon_i = -1] = 1/2$. And $x_i, i \in \{1, \cdots, N\}$ are i.i.d. samples from $X$.

**Theorem. (Rademacher Complexity Bound)** Consider a Lipschitz continuous loss function $\ell(z, y) : Z \times Y \to [0, 1]$ with Lipschitz constant $L$ w.r.t the input $z$. Let $\bar{\ell}(z, y) := \ell(z, y) - \ell(0, y)$. Let $\hat{G}$ be the function class of our $(T+1)$-layer SNOK mapping from $X$ to $Z$. Suppose the activation function $|h(y)| \leq |y|$ (element-wise), and the $l_2$-norm of last layer weight is bounded, i.e., $\|w\|_2 \leq B_w$. Let $(x_i, y_i)_{i=1}^N$ be i.i.d. samples drawn from $X \times Y$. Let $Y_{T+1} = [y_{T+1}^{(1)}, \cdots, y_{T+1}^{(N)}]$ be the $T^{th}$ layer output with input $X$. Denote the mutual coherence of $Y_{T+1}$ as $\mu^*$, i.e., $\mu^* = \mu(Y_{T+1}) = \max_{i \neq j} \frac{y_{T+1}^{(1)} \cdot y_{T+1}^{(j)}}{\|y_{T+1}^{(1)}\|_2 \|y_{T+1}^{(j)}\|_2} \leq 1$. Then, we have

$$\mathcal{R}_N(\bar{\ell} \circ \hat{G}) = \frac{1}{N} \mathbb{E} \left[ \sup_{g \in \hat{G}} \sum_{i=1}^{N} \epsilon_i \bar{\ell}(g(x_i), y_i) \right] \leq \frac{LB_w \sqrt{((N-1)\mu^* + 1)T}}{N} \|X\|_F$$  \hspace{1cm} (170)$$

where $X = [x_1, \cdots, x_N]$. $\| \cdot \|_2$ and $\| \cdot \|_F$ denote the spectral norm and the Frobenius norm of input matrix, respectively.

**Remark:** The Rademacher complexity bound has a complexity $O(\sqrt{T})$ w.r.t. the depth of NN (SNOK).

**Proof.** Since $\bar{\ell}$ is $L$-Lipschitz continuous function, from the composition rule of Rademacher complexity, we know that

$$\mathcal{R}_N(\bar{\ell} \circ \hat{G}) \leq L \mathcal{R}_N(\hat{G})$$  \hspace{1cm} (171)$$
It follows that

$$
\mathcal{R}_N(\tilde{G}) = \frac{1}{N} \mathbb{E} \left[ \sup_{\theta \in \Theta} \sum_{i=1}^{N} \epsilon_i f(x_i) \right]
$$  \hspace{1cm} (172)

$$
= \frac{1}{N} \mathbb{E} \left[ \sup_{w, \{R_t \in SO(d)\}_{t=1}^{T}} \sum_{i=1}^{N} \epsilon_i \langle w, y^{(i)}_{T+1} \rangle \right]
$$  \hspace{1cm} (173)

$$
= \frac{1}{N} \mathbb{E} \left[ \sup_{w, \{R_t \in SO(d)\}_{t=1}^{T}} \left( w, \sum_{i=1}^{N} \epsilon_i y^{(i)}_{T+1} \right) \right]
$$  \hspace{1cm} (174)

$$
\leq \frac{1}{N} \mathbb{E} \left[ \sup_{w, \{R_t \in SO(d)\}_{t=1}^{T}} \|w\|_2 \left( \sum_{i=1}^{N} \epsilon_i y^{(i)}_{T+1} \right) \right] \quad \text{(Cauchy-Schwarz inequality)} \hspace{1cm} (175)

\leq \frac{B_w}{N} \mathbb{E} \left[ \sup_{\{R_t \in SO(d)\}_{t=1}^{T}} \left( \sum_{i=1}^{N} \epsilon_i y^{(i)}_{T+1} \right) \right]
$$  \hspace{1cm} (176)

$$
= \frac{B_w}{N} \mathbb{E} \left[ \sup_{\{R_t \in SO(d)\}_{t=1}^{T}} \left( \sum_{i=1}^{N} \epsilon_i y^{(i)}_{T+1} \right) \right]
$$  \hspace{1cm} (177)

$$
= \frac{B_w}{N} \mathbb{E} \left[ \sup_{\{R_t \in SO(d)\}_{t=1}^{T}} \left( \sum_{i=1}^{N} \epsilon_i y^{(i)}_{T+1} \right) \right]
$$  \hspace{1cm} (178)

$$
\leq \frac{B_w}{N} \mathbb{E} \left[ \sup_{\{R_t \in SO(d)\}_{t=1}^{T}} \left( \sum_{i=1}^{N} \epsilon_i y^{(i)}_{T+1} \right) \right]
$$  \hspace{1cm} (179)

$$
\leq \frac{B_w}{N} \mathbb{E} \left[ \sup_{\{R_t \in SO(d)\}_{t=1}^{T}} \left( \sum_{i=1}^{N} \epsilon_i y^{(i)}_{T+1} \right) \right]
$$  \hspace{1cm} (180)

Inequality \[180\] is because of the Jensen inequality and concavity of the square root function.

Note that \( |\epsilon_i| = 1, \forall i \in \{1, \cdots, N\} \), and the mutual coherence of \( Y_{T+1} \) is \( \mu^* \), i.e., \( \mu^* = \mu(Y_{T+1}) \leq 1 \), it follows that

$$
\mathcal{R}_N(\tilde{F}) \leq \frac{B_w}{N} \mathbb{E} \left[ \sup_{\{R_t \in SO(d)\}_{t=1}^{T}} \left( \sum_{i=1}^{N} \epsilon_i y^{(i)}_{T+1} \right) \right]
$$  \hspace{1cm} (181)

$$
\leq \frac{B_w}{N} \mathbb{E} \left[ \sup_{\{R_t \in SO(d)\}_{t=1}^{T}} \left( \sum_{i=1}^{N} \epsilon_i y^{(i)}_{T+1} \right) \right]
$$  \hspace{1cm} (182)

$$
= \frac{B_w}{N} \mathbb{E} \left[ \sup_{\{R_t \in SO(d)\}_{t=1}^{T}} \left( \sum_{i=1}^{N} \epsilon_i y^{(i)}_{T+1} \right) \right]
$$  \hspace{1cm} (183)

$$
\leq \frac{B_w}{N} \mathbb{E} \left[ \sup_{\{R_t \in SO(d)\}_{t=1}^{T}} \left( \sum_{i=1}^{N} \epsilon_i y^{(i)}_{T+1} \right) \right]
$$  \hspace{1cm} (184)

where \( Y_{T+1} = [y^{(1)}_{T+1}, \cdots, y^{(N)}_{T+1}] \) and \( \| \cdot \|_F \) denotes the Frobenius norm.

Since \( |h(Y)| \leq |Y| \) (element-wise), (e.g., ReLU, max-pooling, soft-thresholding), it follows that

$$
\|Y_{T+1}\|_F^2 = \|h(D^T R_T X + (I - D^T D) Y_T)\|_F^2
$$  \hspace{1cm} (186)

$$
\leq \|D^T R_T X + (I - D^T D) Y_T\|_F^2
$$  \hspace{1cm} (187)
In addition, we have
\[
\| D^\top R_T X + (I - D^\top D) Y_T \|_F^2 = \| D^\top R_T X \|_F^2 + \| (I - D^\top D) Y_T \|_F^2 \\
+ 2 \langle D^\top R_T X, (I - D^\top D) Y_T \rangle \tag{188}
\]

Note that \( DD^\top = I_d \) and \( R_T^\top R_T = R_T R_T^\top = I_d \), we have
\[
\| D^\top R_T X \|_F^2 = \| X \|_F^2 \tag{189}
\]
\[
\langle D^\top R_T X, (I - D^\top D) Y_T \rangle = \text{tr} \left( X^\top R_T^\top D(I - D^\top D) Y_T \right) = 0 \tag{190}
\]

Denote \( \beta = \|I - D^\top D\|_2^2 \), it follows that
\[
\| D^\top R_T X + (I - D^\top D) Y_T \|_F^2 = \| D^\top R_T X \|_F^2 + \| (I - D^\top D) Y_T \|_F^2 \\
+ 2 \langle D^\top R_T X, (I - D^\top D) Y_T \rangle \tag{191}
\]
\[
= \| X \|_F^2 + \| (I - D^\top D) Y_T \|_F^2 \tag{192}
\]
\[
\leq \| X \|_F^2 + \| I - D^\top D \|_2^2 \| Y_T \|_F^2 = \| X \|_F^2 + \beta \| y_T \|_F^2 \tag{193}
\]

Recursively apply the above procedure from \( t = T \) to \( t = 1 \), together with \( Y_0 = 0 \), we can achieve that
\[
\| Y_{T+1} \|_F^2 \leq \| X \|_F^2 \left( \sum_{i=0}^{T-1} \beta^i \right) \tag{194}
\]

Together with inequality \( \| y_T \|_F \), it follows that
\[
\mathcal{R}_N(\hat{G}) \leq \frac{B_w}{N} \sqrt{\sup_{\{R_i \in SO(d)\}_{i=1}^T} ((N-1)\mu^* + 1) \| Y_{T+1} \|_F^2} \tag{195}
\]
\[
\leq \frac{B_w}{N} \sqrt{\left( (N-1)\mu^* + 1 \right) \sum_{i=0}^{T-1} \beta^i \| X \|_F} \tag{196}
\]

Finally, we obtain that
\[
\mathcal{R}_N(\ell \circ \hat{G}) = \frac{1}{N} \mathbb{E} \left[ \sup_{g \in \mathcal{B}} \sum_{i=1}^{N} \epsilon_i g(x_i, y_i) \right] \leq \frac{LB_w \sqrt{\left( (N-1)\mu^* + 1 \right) \sum_{i=0}^{T-1} \beta^i \| X \|_F}}{N} \tag{197}
\]

Now, we show that \( \beta = \|I - D^\top D\|_2^2 \leq 1 \). From the definition of spectral norm, we have that
\[
\beta = \|I - D^\top D\|_2^2 = \sup_{\| y \|_2 = 1} \| (I - D^\top D) y \|_2^2 \tag{198}
\]
\[
= \sup_{\| y \|_2 = 1} y^\top (I - D^\top D)^\top (I - D^\top D) y \tag{199}
\]
\[
= \sup_{\| y \|_2 = 1} y^\top (I - 2D^\top D + D^\top DD^\top D) y \tag{200}
\]
\[
= \sup_{\| y \|_2 = 1} y^\top (I - D^\top D) y \tag{201}
\]
\[
= 1 - \min_{\| y \|_2 = 1} \| Dy \|_2 \leq 1 \tag{202}
\]

Since matrix \( D \) is not full rank, we know \( \beta = 1 \).
I Generalization Bound

Theorem. Consider a Lipschitz continuous loss function $\ell(z, y) : \mathcal{Z} \times \mathcal{Y} \to [0, 1]$ with Lipschitz constant $L$ w.r.t the input $z$. Let $\tilde{\ell}(z, y) := \ell(z, y) - \ell(0, y)$. Let $\tilde{G}$ be the function class of our $(T+1)$-layer SNOK mapping from $\mathcal{X}$ to $\mathcal{Z}$. Suppose the activation function $|h(y)| \leq |y|$ (element-wise), and the $L_2$-norm of last layer weight is bounded, i.e., $\|w\|_2 \leq B_w$. Let $\{(x_i, y_i)\}_{i=1}^N$ be i.i.d. samples drawn from $\mathcal{X} \times \mathcal{Y}$. Let $Y_{T+1}$ be the $T^{th}$ layer output with input $X$. Denote the mutual coherence of $Y_{T+1}$ as $\mu^*$, i.e., $\mu^* = \mu(Y_{T+1}) \leq 1$. Then, for $\forall N$ and $\forall \delta, 0 < \delta < 1$, with a probability at least $1 - \delta$, $\forall y \in \tilde{G}$, we have

$$
\mathbb{E}[\ell(g(X), Y)] \leq \frac{1}{N} \sum_{i=1}^N \ell(g(x_i), y_i) + \frac{LB_w \sqrt{(N-1)\mu^* + 1}}{N} \|X\|_F + \sqrt{\frac{8\ln(2/\delta)}{N}}
$$

where $X = [x_1, \cdots, x_N]$, and $\| \cdot \|_F$ denotes the Frobenius norm.

Proof. Plug the Rademacher complexity bound of SNOK (our Theorem 6) into the Theorem 8 in [5], we can obtain the bound.

J Rademacher Complexity and Generalization Bound for A More General Structured Neural Network Family

Neural Network Structure: For a more general structured neural network family that includes SNOK, the 1-$T$ layers are given as

$$
y_{t+1} = h(D_t x + (I - D_t^\top D_t) y_t)
$$

where $D_t \in \mathbb{R}^{d_t \times d}$ are free parameters such that $D_tD_t^\top = I_d$ and $d_d > d$, and $y_0 = 0$.

The last layer $(T+1)^{th}$ layer is given by $z = w^\top y_{T+1}$. Consider a $L$-Lipschitz continuous loss function $\ell(z, y) : \mathcal{Z} \times \mathcal{Y} \to [0, 1]$ with Lipschitz constant $L$ w.r.t. the input $z$.

Theorem 9. (Rademacher Complexity Bound) Consider a Lipschitz continuous loss function $\ell(z, y) : \mathcal{Z} \times \mathcal{Y} \to [0, 1]$ with Lipschitz constant $L$ w.r.t. the input $z$. Let $\tilde{\ell}(z, y) := \ell(z, y) - \ell(0, y)$. Let $\tilde{G}$ be the function class of the above $(T+1)$-layer structured NN mapping from $\mathcal{X}$ to $\mathcal{Z}$. Suppose the activation function $|h(y)| \leq |y|$ (element-wise), and the $L_2$-norm of last layer weight is bounded, i.e., $\|w\|_2 \leq B_w$. Let $\{(x_i, y_i)\}_{i=1}^N$ be i.i.d. samples drawn from $\mathcal{X} \times \mathcal{Y}$. Let $Y_{T+1} = [y_{T+1}^{(1)}, \cdots, y_{T+1}^{(N)}]$ be the $T^{th}$ layer output with input $X$. Denote the mutual coherence of $Y_{T+1}$ as $\mu^*$, i.e., $\mu^* = \mu(Y_{T+1}) = \max_{i \neq j} \frac{\|y_{T+1}^{(i)} - y_{T+1}^{(j)}\|_2}{\|y_{T+1}^{(i)}\|_2 \|y_{T+1}^{(j)}\|_2} \leq 1$. Then, we have

$$
\mathfrak{R}_N(\tilde{\ell} \circ \tilde{G}) = \frac{1}{N} \mathbb{E} \left[ \sup_{g \in \tilde{G}} \sum_{i=1}^N \epsilon_i \tilde{\ell}(g(x_i), y_i) \right] \leq \frac{LB_w \sqrt{T((N-1)\mu^* + 1)}}{N} \|X\|_F
$$

where $X = [x_1, \cdots, x_N]$. $\| \cdot \|_2$ and $\| \cdot \|_F$ denote the spectral norm and the Frobenius norm of input matrix, respectively.

Remark: The Rademacher complexity bound has a complexity $O(\sqrt{T})$ w.r.t. the depth of NN.

Proof. Since $\tilde{\ell}$ is $L$-Lipschitz continuous function, from the composition rule of Rademacher complexity, we know that

$$
\mathfrak{R}_N(\tilde{\ell} \circ \tilde{G}) \leq L \mathfrak{R}_N(\tilde{G})
$$
It follows that
\[
\mathcal{R}_N(\hat{G}) = \frac{1}{N} \mathbb{E} \left[ \sup_{g \in \hat{G}} \sum_{i=1}^{N} \epsilon_i g(x_i) \right] 
\]  
(207)
\[
= \frac{1}{N} \mathbb{E} \left[ \sup_{\mathbf{w}, \{D_t \in \mathcal{M}\}_{t=1}^{T}} \sum_{i=1}^{N} \epsilon_i \langle \mathbf{w}, y_{T+1}^{(i)} \rangle \right] 
\]  
(208)
\[
= \frac{1}{N} \mathbb{E} \left[ \sup_{\mathbf{w}, \{D_t \in \mathcal{M}\}_{t=1}^{T}} \langle \mathbf{w}, \sum_{i=1}^{N} \epsilon_i y_{T+1}^{(i)} \rangle \right] 
\]  
(209)
\[
\leq \frac{1}{N} \mathbb{E} \left[ \sup_{\mathbf{w}, \{D_t \in \mathcal{M}\}_{t=1}^{T}} \| \mathbf{w} \|_2 \left\| \sum_{i=1}^{N} \epsilon_i y_{T+1}^{(i)} \right\|_2 \right] 
\]  
(Cauchy-Schwarz inequality)  
(210)
\[
\leq \frac{B_{\mathcal{E}}}{N} \mathbb{E} \left[ \sup_{\{D_t \in \mathcal{M}\}_{t=1}^{T}} \left\| \sum_{i=1}^{N} \epsilon_i y_{T+1}^{(i)} \right\|_2 \right] 
\]  
(211)
\[
= \frac{B_{\mathcal{E}}}{N} \mathbb{E} \left[ \sup_{\{D_t \in \mathcal{M}\}_{t=1}^{T}} \left\| \sum_{i=1}^{N} \epsilon_i y_{T+1}^{(i)} \right\|_2 \right] \sum_{i=1}^{N} \| y_{T+1}^{(i)} \|_2 + \sum_{i=1}^{N} \sum_{j=1, j \neq i}^{N} \epsilon_i \epsilon_j y_{T+1}^{(i)\top} y_{T+1}^{(j)} 
\]  
(212)
\[
= \frac{B_{\mathcal{E}}}{N} \mathbb{E} \left[ \sup_{\{D_t \in \mathcal{M}\}_{t=1}^{T}} \left\| y_{T+1} \right\|_2 + \sum_{i=1}^{N} \sum_{j=1, j \neq i}^{N} \epsilon_i \epsilon_j y_{T+1}^{(i)\top} y_{T+1}^{(j)} \right] 
\]  
(213)
\[
= \frac{B_{\mathcal{E}}}{N} \mathbb{E} \left[ \sup_{\{D_t \in \mathcal{M}\}_{t=1}^{T}} \left\| y_{T+1} \right\|_2 + \sum_{i=1}^{N} \sum_{j=1, j \neq i}^{N} \epsilon_i \epsilon_j y_{T+1}^{(i)\top} y_{T+1}^{(j)} \right] 
\]  
(214)
\[
\leq \frac{B_{\mathcal{E}}}{N} \mathbb{E} \left[ \sup_{\{D_t \in \mathcal{M}\}_{t=1}^{T}} \left\| y_{T+1} \right\|_2 + \sum_{i=1}^{N} \sum_{j=1, j \neq i}^{N} \epsilon_i \epsilon_j y_{T+1}^{(i)\top} y_{T+1}^{(j)} \right] 
\]  
(215)

Inequality (215) is because of the Jensen inequality and concavity of the square root function.

Note that $|\epsilon_i| = 1, \forall i \in \{1, \cdots, N\}$, and the mutual coherence of $Y_{T+1}$ is $\mu^*$, i.e., $\mu^* = \mu(Y_{T+1}) \leq 1$, it follows that
\[
\mathcal{R}_N(\hat{G}) \leq \frac{B_{\mathcal{E}}}{N} \mathbb{E} \left[ \sup_{\{D_t \in \mathcal{M}\}_{t=1}^{T}} \left\| y_{T+1} \right\|_2 + \sum_{i=1}^{N} \sum_{j=1, j \neq i}^{N} \epsilon_i \epsilon_j y_{T+1}^{(i)\top} y_{T+1}^{(j)} \right] 
\]  
(216)
\[
\leq \frac{B_{\mathcal{E}}}{N} \mathbb{E} \left[ \sup_{\{D_t \in \mathcal{M}\}_{t=1}^{T}} \sum_{i=1}^{N} \left\| y_{T+1}^{(i)} \right\|_2^2 + \sum_{i=1}^{N} \sum_{j=1, j \neq i}^{N} \epsilon_i \epsilon_j y_{T+1}^{(i)\top} y_{T+1}^{(j)} \right] \mu^* 
\]  
(217)
\[
\leq \frac{B_{\mathcal{E}}}{N} \mathbb{E} \left[ \sup_{\{D_t \in \mathcal{M}\}_{t=1}^{T}} \sum_{i=1}^{N} \left(1 - \mu^* \right) \left\| y_{T+1}^{(i)} \right\|_2^2 + \mu^* \left( \sum_{i=1}^{N} \left\| y_{T+1}^{(i)} \right\|_2^2 \right)^2 \right] 
\]  
(218)
\[
\leq \frac{B_{\mathcal{E}}}{N} \mathbb{E} \left[ \left(1 - \mu^* \right) \left\| Y_{T+1} \right\|_F^2 + N \mu^* \left\| Y_{T+1} \right\|_F^2 \right] 
\]  
(Cauchy-Schwarz)  
(219)
\[
\leq \frac{B_{\mathcal{E}}}{N} \mathbb{E} \left[ \left( (N-1) \mu^* + 1 \right) \left\| Y_{T+1} \right\|_F^2 \right] 
\]  
(220)

where $Y_{T+1} = [y_{T+1}^{(1)}, \cdots, y_{T+1}^{(N)}]$ and $\| \cdot \|_F$ denotes the Frobenius norm.

Since $|h(Y)| \leq |Y|$ (element-wise), (e.g., ReLU, max-pooling, soft-thresholding), it follows that
\[
\left\| Y_{T+1} \right\|_F^2 = \left\| h(D_T \mathbf{X} + (I - D_T)Y_T) \right\|_F^2 \leq \left\| D_T \mathbf{X} + (I - D_T)Y_T \right\|_F^2 
\]  
(221)
\[
\leq \left\| D_T \mathbf{X} \right\|_F^2 + \left\| I - D_T \right\|_F^2 Y_T \right\|_F^2 
\]  
(222)
In addition, we have
\[
\|D_T^T X + (I - D_T^T D_T)Y_T\|^2_F = \|D_T^T X\|^2_F + \|(I - D_T^T D_T)Y_T\|^2_F + 2\langle D_T^T X, (I - D_T^T D_T)Y_T \rangle
\] (223)

Note that \(D_T^T D_T = I_d\), we have
\[
\|D_T^T X\|^2_F = \|X\|^2_F
\] (224)
\[
\langle D_T^T X, (I - D_T^T D_T)Y_T \rangle = \text{tr} \left( X_T^T D_T(I - D_T^T D_T)Y_T \right) = 0
\] (225)

It follows that
\[
\|D_T^T X + (I - D_T^T D_T)Y_T\|^2_F = \|D_T^T X\|^2_F + \|(I - D_T^T D_T)Y_T\|^2_F + 2\langle D_T^T X, (I - D_T^T D_T)Y_T \rangle
\] (226)
\[
= \|X\|^2_F + \|(I - D_T^T D_T)Y\|^2_F
\] (227)
\[
\leq \|X\|^2_F + \|I - D_T^T D_T\|^2_F \|Y\|^2_F = \|X\|^2_F + \|Y\|^2_F
\] (228)

Recursively apply the above procedure from \(t = T\) to \(t = 1\), together with \(Y_0 = 0\), we can achieve that
\[
\|Y_{T+1}\|^2_F \leq T\|X\|^2_F
\] (229)

Together with inequality (220), it follows that
\[
\mathcal{R}_N(\tilde{G}) \leq \frac{B_w}{N} \sqrt{\sup_{\{D_t \in \mathcal{M}\}_{t=1}^T} (\|(N-1)\mu^* + 1\|Y_{T+1}\|^2_F)}
\]
\[
\leq \frac{B_w \sqrt{T((N-1)\mu^* + 1)}}{N} \|X\|_F
\] (230)

Finally, we obtain that
\[
\mathcal{R}_N(\tilde{G} \circ \tilde{G}) = \frac{1}{N} \mathbb{E} \left[ \sup_{g \in \tilde{G}} \sum_{i=1}^N \varepsilon_i \tilde{\ell}(g(x_i), y_i) \right] \leq \frac{L B_w \sqrt{T((N-1)\mu^* + 1)}}{N} \|X\|_F
\] (232)

\[\square\]

**Theorem 10.** Consider a Lipschitz continuous loss function \(\ell(z, y) : \mathcal{Z} \times \mathcal{Y} \to [0, 1]\) with Lipschitz constant \(L\) w.r.t the input \(z\). Let \(\hat{\ell}(z, y) := \ell(z, y) - \ell(0, 0)\). Let \(\tilde{G}\) be the function class of our general \((T+1)\)-layer structured NN mapping from \(\mathcal{X}\) to \(\mathcal{Z}\). Suppose the activation function \(h(y)\) is \(\|y\|_2 \leq B_w\) (element-wise), and the \(l_2\)-norm of last layer weight is bounded, i.e., \(\|w\|_2 \leq B_w\). Let \((x_i, y_i)_{i=1}^N\) be i.i.d. samples drawn from \(\mathcal{X} \times \mathcal{Y}\). Let \(Y_{T+1}\) be the \(T^{th}\) layer output with input \(X\). Denote the mutual coherence of \(Y_{T+1}\) as \(\mu^*\), i.e., \(\mu^* = \mu(Y_{T+1}) \leq 1\). Then, for \(\forall N\) and \(\forall \delta, 0 < \delta < 1\), with a probability at least \(1 - \delta\), \(\forall g \in \tilde{G}\), we have
\[
\mathbb{E}[\hat{\ell}(g(X), Y)] \leq \frac{1}{N} \sum_{i=1}^N \hat{\ell}(g(x_i), y_i) + \frac{L B_w \sqrt{T((N-1)\mu^* + 1)}}{N} \|X\|_F + \sqrt{\frac{8 \ln(2/\delta)}{N}}
\] (233)

where \(X = [x_1, \cdots, x_N]\), and \(\|\cdot\|_F\) denotes the Frobenius norm.

**Proof.** Plug the Rademacher complexity bound of general structured NN (our Theorem 9) into the Theorem 8 in [5], we can obtain the bound. \(\square\)

**K** Experimental Results on Classification with Gaussian Input Noise and Laplace Input Noise
Figure 3: Mean test accuracy ± std over 5 independent runs on CIFAR10 dataset with Gaussian noise for DenseNet and ResNet backbone.

Figure 4: Mean test accuracy ± std over 5 independent runs on CIFAR100 dataset with Gaussian noise for DenseNet and ResNet backbone.
Figure 5: Mean test accuracy ± std over 5 independent runs on CIFAR10 dataset with Laplace noise for DenseNet and ResNet backbone.

Figure 6: Mean test accuracy ± std over 5 independent runs on CIFAR100 dataset with Laplace noise for DenseNet and ResNet backbone.