Monte Carlo Non-Local Means: Random Sampling for Large-Scale Image Filtering

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Abstract—We propose a randomized version of the nonlocal means (NLM) algorithm for large-scale image filtering. The new algorithm, called Monte Carlo nonlocal means (MCNLM), speeds up the classical NLM by computing a small subset of image patch distances, which are randomly selected according to a designed sampling pattern. We make two contributions. First, we analyze the performance of the MCNLM algorithm and show that, for large images or large external image databases, the random outcomes of MCNLM are tightly concentrated around the deterministic full NLM result. In particular, our error probability bounds show that, at any given sampling ratio, the probability for MCNLM to have a large deviation from the original NLM solution decays exponentially as the size of the image or database grows. Second, we derive explicit formulas for optimal sampling patterns that minimize the error probability bound by exploiting partial knowledge of the pairwise similarity weights. Numerical experiments show that MCNLM is competitive with other state-of-the-art fast NLM algorithms for single-image denoising. When applied to denoising images using an external database containing ten billion patches, MCNLM returns a randomized solution that is within 0.2 dB of the full NLM solution while reducing the runtime by three orders of magnitude.

Index Terms—Non-local means, Monte Carlo, patch-based filtering, sampling, external denoising, concentration of measure.

I. INTRODUCTION

A. Background and Motivation

In recent years, the image processing community has witnessed a wave of research aimed at developing new image denoising algorithms that exploit similarities between non-local patches in natural images. Most of these can be traced back to the non-local means (NLM) denoising algorithm of Buades et al. [1], [2] proposed in 2005. Although it is no longer the state-of-the-art method (see [3], [4] for some more recent leading algorithms), NLM remains one of the most influential algorithms in the current denoising literature.

Given a noisy image, the NLM algorithm uses two sets of image patches for denoising. The first is a set of noisy patches \( \mathcal{Y} = \{y_1, \ldots, y_m\} \), where \( y_i \in \mathbb{R}^d \) is a \( d \)-dimensional image patch centered at the \( i \)th pixel of the noisy image. The second set, \( \mathcal{X} = \{x_1, \ldots, x_n\} \), contains patches that are obtained from some reference images. Conceptually, NLM simply replaces each noisy pixel with a weighted average of pixels in the reference set. Specifically, the filtered value at the \( i \)th pixel (for \( 1 \leq i \leq m \)) is given by

\[
z = \frac{\sum_{j=1}^{n} w_{i,j} x_j}{\sum_{j=1}^{n} w_{i,j}},
\]

where \( x_j \) denotes the value of the center pixel of the \( j \)th reference patch \( x_j \in \mathcal{X} \), and the weights \( \{w_{i,j}\} \) measure the similarities between the patches \( y_i \) and \( x_j \). A standard choice for the weights is

\[
w_{i,j} = e^{-\beta y_i^2 - \gamma (\mathbf{y}_2 / \mathbf{\lambda})^2},
\]

where \( h_t \) is a scalar parameter determined by the noise level, and \( \|\cdot\|_\lambda \) is the weighted \( \ell_2 \)-norm with a diagonal weight matrix \( \mathbf{\Lambda} \), i.e., \( \|y_i - x_j\|_\lambda^2 \overset{\text{def}}{=} (y_i - x_j)^T \mathbf{\Lambda} (y_i - x_j) \).

In most implementations of NLM (see [5]–[11]), the denoising process is based on a single image: the reference patches \( \mathcal{X} \) are the same as the noisy patches \( \mathcal{Y} \). We refer to this setting, when \( \mathcal{X} = \mathcal{Y} \), as internal denoising. This is in contrast to the setting in which the set of reference patches \( \mathcal{X} \) come from external image databases [12]–[14], which we refer to as external denoising. For example, 15,000 images (corresponding to a reference set of \( n \approx 10^{10} \) patches) were used in [13] and [14]. One theoretical argument for using large-scale external denoising was provided in [13]: It is shown that, in the limit of large reference sets (i.e., \( n \to \infty \)), external NLM converges to the minimum mean squared error estimator of the underlying clean images.

Despite its strong performance, NLM has a limitation of high computational complexity. It is easy to see that computing all the weights \( \{w_{i,j}\} \) requires \( O(mnd) \) arithmetic operations, where \( m, n, d \) are, respectively, the number of pixels in the noisy image, the number of reference patches used, and the patch dimension. Additionally, about \( O(mn) \) operations are needed to carry out the summations and multiplications in (1) for all pixels in the image. In the case of internal denoising, these numbers are nontrivial since current digital photographs can easily contain tens of millions of pixels (i.e., \( m \approx 10^7 \) or greater). For external denoising with large reference sets (e.g., \( n \sim 10^{10} \)), the complexity is even more of an issue, making it very challenging to fully utilize the vast number of images that are readily available online and potentially useful as external databases.
B. Related Work

The high complexity of NLM is a well-known challenge. Previous methods to speed up NLM can be roughly classified in the following categories:

1) Reducing the Reference Set $\mathcal{X}$: If searching through a large set $\mathcal{X}$ is computationally intensive, one natural solution is to pre-select a subset of $\mathcal{X}$ and perform computation only on this subset [15]–[17]. For example, for internal denoising, a spatial weight $w_{i,j}^s$ is often included so that

$$w_{i,j} = w_{i,j}^s \cdot e^{-\frac{\|y_i - x_j\|^2}{(2h^2)}}.$$  

A common choice of the spatial weight is

$$w_{i,j}^s = \exp\left(-d_{i,j}^2/(2h^2)\right) \cdot [d_{i,j}^2 \leq \rho],$$

where $d_{i,j}$ and $d_{i,j}^s$ are, respectively, the Euclidean distance and the $\ell_\infty$ distance between the spatial locations of the $i$th and $j$th pixels; $\mathbb{I}$ is the indicator function; and $\rho$ is the width of the spatial search window. By tuning $h_i$ and $\rho$, one can adjust the size of $\mathcal{X}$ according to the heuristic that nearby patches are more likely to be similar.

2) Reducing Dimension $d$: The patch dimension $d$ can be reduced by several methods. First, SVD projection [10], [18]–[20] can be used to project the $d$-dimensional patches onto a lower dimensional space spanned by the principal components computed from $\mathcal{X}$. Second, the integral image method [21]–[23] can be used to further speed up the computation of $\|y_i - x_j\|^2_A$. Third, by assuming a Gaussian model on the patch data, a probabilistic early termination scheme [24] can be used to stop computing the squared patch difference before going through all the pixels in the patches.

3) Optimizing Data Structures: The third class of methods embed the patches in $\mathcal{X}$ and $\mathcal{Y}$ in some form of optimized data structures. Some examples include the fast bilateral grid [25], the fast Gaussian transform [26], the Gaussian KD tree [27], [28], the adaptive manifold method [29], and the edge patch dictionary [30]. The data structures used in these algorithms can significantly reduce the computational complexity of the NLM algorithm. However, building these data structures often requires a lengthy pre-processing stage, or require a large amount of memory, thereby placing limits on one’s ability to use large reference patch sets $\mathcal{X}$. For example, building a Gaussian KD tree requires the storage of $O(nd)$ double precision numbers (see [28], [31].)

C. Contributions

In this paper, we propose a randomized algorithm to reduce the computational complexity of NLM for both internal and external denoising. We call the method Monte Carlo Non-Local Means (MCNLM), and the basic idea is illustrated in Fig. 1 for the case of internal denoising. For each pixel $i$ in the noisy image, we randomly select a set of $k$ reference pixels according to some sampling pattern and compute a $k$-subset of the weights $\{w_{i,j}\}_{j=1}^{n}$ to form an approximated solution to (1). The computational complexity of MCNLM is $O(mkd)$, which can be significantly lower than the original complexity $O(mnd)$ when only $k \ll n$ weights are computed. Furthermore, since there is no need to re-organize the data, the memory requirement of MCNLM is $O(m + n)$. Therefore, MCNLM is scalable to large reference patch sets $\mathcal{X}$, as we will demonstrate in Section V.

The two main contributions of this paper are as follows.

1) Performance Guarantee: MCNLM is a randomized algorithm. It would not be a useful one if its random outcomes fluctuated widely in different executions on the same input data. In Section III, we address this concern by showing that, as the size of the reference set $\mathcal{X}$ increases, the randomized MCNLM solutions become tightly concentrated around the original NLM solution. In particular, we show in Theorem 1 (and Proposition 1) that, for any given sampling pattern, the probability of having a large deviation from the original NLM solution drops exponentially as the size of $\mathcal{X}$ grows.

2) Optimal Sampling Patterns: We derive optimal sampling patterns to minimize the approximation error probabilities established in our performance analysis. We show that seeking the optimal sampling pattern is equivalent to solving a variant of the classical water-filling problem, for which a closed-form expression can be found (see Theorem 2). We also present two practical sampling pattern designs that exploit partial knowledge of the pairwise similarity weights.

The rest of the paper is organized as follows. After presenting the MCNLM algorithm and discuss its basic properties in Section II, we analyze the performance in Section III and derive the optimal sampling patterns in Section IV. Experimental results are given in Section V, and concluding remarks are given in Section VI.

II. MONTE CARLO NON-LOCAL MEANS

Notation: Throughout the paper, we use $m$ to denote the number of pixels in the noisy image, and $n$ the number patches in the reference set $\mathcal{X}$. We use upper-case letters, such as $X$, $Y$, $Z$, to represent random variables, and lower-case letters, such as $x$, $y$, $z$, to represent deterministic variables. Vectors are represented by bold letters, and $\mathbf{1}$ denotes a constant vector of which all entries are one. Finally, for notational simplicity in presenting our theoretical analysis, we assume that all pixel intensity values have been normalized to the range $[0, 1]$.

A. The Sampling Process

As discussed in Section I, computing all the weights $\{w_{i,j}\}_{1 \leq i \leq m, 1 \leq j \leq n}$ is computationally prohibitive when...
m and n are large. To reduce the complexity, the basic idea of MCNLM is to randomly select a subset of k representatives of \{w_{i,j}\} (referred to as samples) to approximate the sums in the numerator and denominator in (1). The sampling process in the proposed algorithm is applied to each of the m pixels in the noisy image independently. Since the sampling step and subsequent computations have the same form for each pixel, we shall drop the pixel index i in \{w_{i,j}\}, writing the weights as \{w_j\}$_{1 \leq j \leq n}$ for notational simplicity.

The sampling process of MCNLM is determined by a sequence of independent random variables \{I_j\}$_{j=1}^n$ that take the value 0 or 1 with the following probabilities

\[
\Pr[I_j = 1] = p_j \quad \text{and} \quad \Pr[I_j = 0] = 1 - p_j, \quad (5)
\]

The jth weight \(w_j\) is sampled if and only if \(I_j = 1\). In what follows, we assume that \(0 < p_j \leq 1\), and refer to the vector of all these probabilities \(\mathbf{p} \equiv [p_1, \ldots, p_n]^T\) as the sampling pattern of the algorithm.

The ratio between the number of samples taken and the number of reference patches in \(\mathcal{X}\) is a random variable

\[
S_n = \frac{1}{n} \sum_{j=1}^n I_j, \quad (6)
\]

of which the expected value is

\[
E[S_n] = \frac{1}{n} \sum_{j=1}^n E[I_j] = \frac{1}{n} \sum_{j=1}^n p_j \quad \text{def} = \bar{\zeta}. \quad (7)
\]

We refer to \(S_n\) and \(\bar{\zeta}\) as the empirical sampling ratio and the average sampling ratio, respectively. \(\bar{\zeta}\) is an important parameter of the MCNLM algorithm. The original (or “full”) NLM corresponds to the setting when \(\bar{\zeta} = 1\): In this case, \(\mathbf{p} = 1 \equiv [1, \ldots, 1]^T\), so that all the samples are selected with probability one.

B. The MCNLM Algorithm

Given a set of random samples from \(\mathcal{X}\), we approximate the numerator and denominator in (1) by two random variables

\[
A(\mathbf{p}) \equiv \frac{1}{n} \sum_{j=1}^n \frac{x_j w_j}{p_j} I_j \quad \text{and} \quad B(\mathbf{p}) \equiv \frac{1}{n} \sum_{j=1}^n \frac{w_j}{p_j} I_j, \quad (8)
\]

where the argument \(\mathbf{p}\) emphasizes the fact that the distributions of \(A\) and \(B\) are determined by the sampling pattern \(\mathbf{p}\).

It is easy to compute the expected values of \(A(\mathbf{p})\) and \(B(\mathbf{p})\) as

\[
\mu_A \equiv E[A(\mathbf{p})] = \frac{1}{n} \sum_{j=1}^n x_j w_j, \quad (9)
\]

\[
\mu_B \equiv E[B(\mathbf{p})] = \frac{1}{n} \sum_{j=1}^n w_j. \quad (10)
\]

Thus, up to a common multiplicative constant \(1/n\), the two random variables \(A(\mathbf{p})\) and \(B(\mathbf{p})\) are unbiased estimates of the true numerator and denominator, respectively.

Algorithm 1 Monte Carlo Non-local Means (MCNLM)

1: For each noisy pixel \(i = 1, \ldots, m\), do the followings.
2: Input: Noisy patch \(y_i \in \mathcal{Y}\), database \(\mathcal{X} = \{x_1, \ldots, x_n\}\) and sampling pattern \(\mathbf{p} = [p_1, \ldots, p_n]^T\) such that \(0 < p_j \leq 1\), and \(\sum_{j=1}^n p_j = n\).
3: Output: A randomized estimate \(Z(\mathbf{p})\).
4: for \(j = 1, \ldots, n\) do
5: Generate a random variable \(I_j \sim \text{Bernoulli}(p_j)\).
6: if \(I_j = 1\), then compute the weight \(w_j\).
7: end for
8: Compute \(A(\mathbf{p}) = \frac{1}{n} \sum_{j=1}^n \frac{w_j x_j}{p_j} I_j\).
9: Compute \(B(\mathbf{p}) = \frac{1}{n} \sum_{j=1}^n \frac{w_j}{p_j} I_j\).
10: Output \(Z(\mathbf{p}) = A(\mathbf{p})/B(\mathbf{p})\).

The full NLM result \(z\) in (1) is then approximated by

\[
Z(\mathbf{p}) \equiv \frac{A(\mathbf{p})}{B(\mathbf{p})} = \frac{\sum_{j=1}^n \frac{w_j x_j}{p_j} I_j}{\sum_{j=1}^n \frac{w_j}{p_j} I_j}. \quad (11)
\]

In general, \(E[Z(\mathbf{p})] = E\left[\frac{A(\mathbf{p})}{B(\mathbf{p})}\right] \neq E\left[\frac{A(\mathbf{p})}{B(\mathbf{p})}\right] = z\), and thus \(Z(\mathbf{p})\) is a biased estimate of \(z\). However, we will show in Section III that the probability of having a large deviation in \(|Z(\mathbf{p}) - z|\) drops exponentially as \(n \to \infty\). Thus, for a large \(n\), the MCNLM solution (11) can still form a very accurate approximation of the original NLM solution (1).

Algorithm 1 shows the pseudo-code of MCNLM for internal denoising. We note that, except for the Bernoulli sampling process, all other steps are identical to the original NLM. Therefore, MCNLM can be thought of as adding a complementary sampling process on top of the original NLM. The marginal cost of implementation is thus minimal.

Example 1: To empirically demonstrate the usefulness of the simple sampling mechanism of MCNLM, we apply the algorithm to a 1072 × 712 image shown in Fig. 2(a). Here, we use \(\mathcal{X} = \mathcal{Y}\), with \(m = n \approx 7.6 \times 10^5\). In this experiment, we let the noise be i.i.d. Gaussian with zero mean and standard deviation \(\sigma = 15/255\). The patch size is \(5 \times 5\). In computing the similarity weights in (3) and (4), we set the parameters as follows: \(h_r = 15/255\), \(h_s = \infty\), \(\rho = \infty\) (i.e., no spatial windowing) and \(\mathbf{A} = \frac{1}{n} \mathbf{I}\). We choose a uniform sampling pattern, i.e., \(\mathbf{p} = [\zeta, \ldots, \zeta]^T\), for some sampling ratio \(0 < \zeta < 1\).

The results of this experiment are shown in Fig. 2 and Fig. 3. The peak signal-to-noise ratio (PSNR) curve detailed in Fig. 3 shows that MCNLM converges to its limiting value rapidly as the sampling ratio \(\zeta\) approaches 1. For example, at \(\zeta = 0.1\) (i.e., a roughly ten-fold reduction in computational complexity), MCNLM achieves a PSNR that is only 0.2dB away from the full NLM result. More numerical experiments will be presented in Section V.

III. PERFORMANCE ANALYSIS

One fundamental question about MCNLM is whether its random estimate \(Z(\mathbf{p})\) as defined in (11) will be a good approximation of the full NLM solution \(z\), especially when
Fig. 2. Denoising an image of size 1072 \times 712 by MCNLM with uniform sampling. (a) The original image is corrupted with i.i.d. Gaussian noise with \( \sigma = \frac{15}{255} \) (top). (b) and (c) Denoised images with sampling ratio \( \xi = 0.005 \) (bottom left) and \( \xi = 0.1 \) (bottom right), respectively. Shown in parenthesis are the PSNR values (in dB) averaged over 100 trials.

Fig. 3. PSNR as a function of the average sampling ratio \( \xi \). The “circled” line indicates the result of MCNLM. The horizontal line indicates the result of the full NLM (i.e., MCNLM at \( \xi = 1 \)). Note that at \( \xi = 0.1 \), MCNLM achieves a PSNR that is only 0.2 dB below the full NLM result. Additional experiments are presented in Section V.

A. Concentration of Measure Bounds

The mathematical tool we use to analyze the proposed MCNLM algorithm comes from the probabilistic large deviations theory [32], in particular, the concentration of measure inequalities. The inequalities have been widely used to quantify the following phenomenon: A smooth function \( f(X_1, \ldots, X_n) \) of a large number of independent random variables \( X_1, \ldots, X_n \) tends to concentrate very tightly around its mean \( E[f(X_1, \ldots, X_n)] \). Roughly speaking, this concentration phenomenon happens because, while \( X_1, \ldots, X_n \) are individually random in nature, it is unlikely for many of them to work collaboratively to alter the overall system by a significant amount. Thus, for large \( n \), the randomness of these variables tends to be “canceled out” and the function \( f(X_1, \ldots, X_n) \) stays roughly constant.

To gain insights from a concrete example, we first apply the concentration inequalities to study the empirical sampling ratio \( S_n \) as defined in (6). Here, the independent random variables are the Bernoulli random variables \( \{I_j\}_{1 \leq j \leq n} \) introduced in (5), and the smooth function \( f(\cdot) \) computes their average.

It is well known from the law of large numbers (LLN) that the empirical mean \( S_n \) of a large number of independent random variables stays very close to the true mean, which is...
equal to the average sampling ratio \( \xi \) in our case. In particular, by the standard Chebyshev inequality [33], we know that

\[
\Pr\{S_n - E[S_n] > \varepsilon\} \leq \frac{\text{Var}[x_j]}{n\varepsilon^2}, \quad (12)
\]

for every positive \( \varepsilon \).

One drawback of the bound in (12) is that it is overly loose, providing only a linear rate of decay for the error probabilities as \( n \to \infty \). In contrast, the concentration inequalities provide much tighter bounds with exponential decays. In this work, we will use one particular inequality due to S. Bernstein [34]:

**Lemma 1 (Bernstein Inequality [34]):** Let \( X_1, \ldots, X_n \) be a sequence of independent random variables. Suppose that \( l_j \leq X_j \leq u_j \) for all \( j \), where \( u_j \) and \( l_j \) are constants. Let \( S_n = (1/n) \sum_{j=1}^n X_j \), and \( M = \max_{1 \leq j \leq n} (u_j - l_j)/2 \). Then for every positive \( \varepsilon \),

\[
\Pr\{S_n - E[S_n] > \varepsilon\} \leq \exp \left(-\frac{n\varepsilon^2}{2 \left( \frac{1}{n} \sum_{j=1}^n \text{Var}[X_j] + Mx/3 \right)} \right). \quad (13)
\]

To see how Bernstein’s inequality can give us a better probability bound for the empirical sampling ratio \( S_n \), we note that \( X_j = l_j \) in our case. Thus, \( M = 1 \) and \( E[S_n] = \xi \). Moreover, if the sampling pattern is uniform, i.e., \( p = [\xi, \ldots, \xi]^T \), we have

\[
\frac{1}{n} \sum_{j=1}^n \text{Var}[X_j] = \frac{1}{n} \sum_{j=1}^n p_j (1 - p_j) = \xi (1 - \xi).
\]

Substituting these numbers into (13) yields an *exponential* upper bound on the error probability, which is plotted and compared in Fig. 4 against the LLN bound in (12) and against the true probabilities estimated by Monte Carlo simulations. It is clear that the exponential bound provided by Bernstein’s inequality is much tighter than that provided by LLN.

\[\text{Fig. 4. Comparison of the concentration of measure bound (13), the LLN bound (12), and the true error probability \( \Pr[S_n - E[S_n] > \varepsilon] \) as estimated by Monte Carlo simulations. Fixing \( n = 10^6 \), we plot the bounds and probabilities for different values of \( \varepsilon \).}\]

### B. General Error Probability Bound for MCNLM

We now derive a general bound for the error probabilities of MCNLM. Specifically, for any \( \varepsilon > 0 \) and any sampling pattern \( p \) satisfying the conditions that \( 0 < p_j < 1 \) and \( \frac{1}{n} \sum_{j=1}^n p_j = \xi \), we want to study

\[
\Pr\{[Z(p) - z] > \varepsilon\}, \quad (14)
\]

where \( z \) is the full NLM result defined in (1) and \( Z(p) \) is the MCNLM estimate defined in (11).

**Theorem 1:** Assume that \( w_j > 0 \) for all \( j \). Then for every positive \( \varepsilon \),

\[
\Pr\{[Z(p) - z] > \varepsilon\} \leq \exp\left(-n\varepsilon^2\right) + \exp\left(\frac{n\varepsilon^2}{2 \left( \frac{1}{n} \sum_{j=1}^n \text{Var}[X_j] + (\mu_B \varepsilon) M_\alpha/6 \right)} \right), \quad (15)
\]

where \( \mu_B \) is the average similarity weights defined in (10), \( \alpha_j = w_j (x_j - z - \xi) \), \( \beta_j = w_j (x_j - z + \varepsilon) \), and

\[
M_\alpha = \max_{1 \leq j \leq n} \frac{|\alpha_j|}{p_j}, \quad \text{and} \quad M_\beta = \max_{1 \leq j \leq n} \frac{|\beta_j|}{p_j}.
\]

**Proof:** See Appendix A. \[\Box\]

**Remark 1:** In a preliminary version of our work [35], we presented, based on the idea of martingales [36], an error probability bound for the special case when the sampling pattern is uniform. The result of Theorem 1 is more general and applies to any sampling patterns. We also note that the bound in (15) quantifies the deviation of a ratio \( Z(p) = A(p)/B(p) \), where the numerator and denominator are both weighted sums of independent random variables. It is therefore more general than the typical concentration bounds seen in the literature (see [37], [38]), where only a single weighted sum of random variables (i.e., either the numerator or the denominator) is considered.

**Example 2:** To illustrate the result of Theorem 1, we consider a 1D signal as shown in Fig. 5(a). The signal \( |x_j|_{j=1}^n \) is a piecewise continuous function corrupted by i.i.d. Gaussian noise. The noise standard deviation is \( \sigma = 5/255 \) and the signal length is \( n = 10^4 \). We use MCNLM to denoise the 5001-th pixel, and the sampling pattern is uniform with \( p_j = \xi = 0.05 \) for all \( j \). For \( \varepsilon = 0.01 \), we can compute that \( \frac{1}{n} \sum_{j=1}^n \alpha_j^2 = 1.335 \times 10^{-4} \), \( \frac{1}{n} \sum_{j=1}^n \beta_j^2 = 1.452 \times 10^{-4} \), \( \mu_B = 0.3015 \), \( M_\alpha = 0.458 \), and \( M_\beta = 0.617 \). It then follows from (15) that

\[
\Pr\{[Z(p) - z] > 0.01\} \leq 6.516 \times 10^{-6}.
\]

This bound shows that the random MCNLM estimate \( Z(p) \), obtained by taking only 5% of the samples, stays within one percent of the true NLM result \( z \) with overwhelming probability. A complete range of results for different values of \( \varepsilon \) are shown in Fig. 5(b), where we compare the true error probability as estimated by Monte Carlo simulations with the analytical upper bound predicted by Theorem 1. We see from the “zoomed-in” portion of Fig. 5(b) that the analytical bound approaches the true probabilities for \( \varepsilon \geq 0.005 \).
proporcional to $\xi$ still keeping the error probability small, a larger $n$ in the right-hand side of (16) is negligible. For example, when $k$ as a function of $\varepsilon$. In this plot, the "crosses" denote the true probabilities as estimated by $10^5$ independent trials and the "circles" denote the analytical upper bound predicted by Theorem 1. For easy comparisons, we also provide a zoomed-in version of the plot in the insert.

C. Special Case: Uniform Sampling Patterns

Since the error probability bound in (15) holds for all sampling patterns $p$, we will use (15) to design optimal nonuniform sampling patterns in Section IV. But before we discuss that, we first consider the special case where $p$ is a uniform sampling pattern to provide a convenient and easily interpretable bound on the error probabilities.

Proposition 1 (Uniform Sampling): Assume that the sampling pattern is uniform, i.e., $p = \xi \mathbf{1}$. Then for every $\varepsilon > 0$ and every $0 < \xi \leq 1$,

$$
\Pr \left[ |Z(p) - z| > \varepsilon \right] \leq \exp \left\{ -n \xi \right\} + 2 \exp \left\{ -n \mu_B f(\varepsilon) \xi \right\},
$$

(16)

where $f(\varepsilon) \overset{\text{def}}{=} \varepsilon^2 / \left(2(1 + \varepsilon)(1 + 7\varepsilon/6)\right)$.

Proof: See Appendix B.

To interpret (16), we note that, for large $n$, the first term on the right-hand side of (16) is negligible. For example, when $n = 10^4$ and $\xi = 0.01$, we have $e^{-n \xi} = 3.7 \times 10^{-44}$. Thus, the error probability bound is dominated by the second term, whose negative exponent is determined by four factors:

1. The size of the reference set $\mathcal{X}$. If all other parameters are kept fixed or strictly bounded below by some positive constants, the error probability goes to zero as an exponential function of $n$. This shows that the random estimates obtained by MCNL can be very accurate, when the size of the image (for internal denoising) or the size of the dictionary (for external denoising) is large.

2. Sampling ratio $\xi$. To reduce the sampling ratio $\xi$ while still keeping the error probability small, a larger $n$, inversely proportional to $\xi$, is needed.

3. Precision $\varepsilon$. Note that the function $f(\varepsilon)$ in (16) is of order $O(\varepsilon^2)$ for small $\varepsilon$. Thus, with all other terms fixed, a $k$-fold reduction in $\varepsilon$ requires a $k^2$-fold increase in $n$ or $\xi$.

4. Patch redundancy $\mu_B$. Recall that $\mu_B = \frac{1}{n} \sum_{j=1}^{n} w_j$, with the weights $\{w_j\}$ measuring the similarities between a noisy patch $y_j$ and all patches $\{x_j\}_{j=1}^n$ in the reference set $\mathcal{X}$. Thus, $\mu_B$ serves as an indirect measure of the number of patches in $\mathcal{X}$ that are similar to $y_j$. If $y_j$ can find many similar (redundant) patches in $\mathcal{X}$, its corresponding $\mu_B$ will be large and so a relatively small $n$ will be sufficient to make the probability small; and vice versa.

Using the simplified expression in (16), we derive in Appendix C the following upper bound on the mean squared error (MSE) of the MCNL estimation:

Proposition 2 (MSE): Let the sampling pattern be uniform, with $p = \xi \mathbf{1}$. Then for any $0 < \xi \leq 1$,

$$
\text{MSE}_p \overset{\text{def}}{=} \mathbb{E}_p \left[ (Z(p) - z)^2 \right] \leq e^{-n \xi} + \frac{1}{n \xi} \left( \frac{52}{3 \mu_B} \right).
$$

(17)

Remark 2: The above result indicates that, with a fixed average sampling ratio $\xi$ and if the patch redundancy $\mu_B$ is bounded from below by a positive constant, then the MSE of the MCNL estimation converges to zero as $n$, the size of the reference set, goes to infinity.

Remark 3: We note that the $\text{MSE}_p$ stated in Proposition 2 is a measure of the deviation between the randomized solution $Z(p)$ and the deterministic (full NLM) solution $z$. In other words, the expectation is taken over the different realizations of the sampling patterns, with the noise (and thus $z$) fixed. This is different from the standard $\text{MSE}$ used in image processing (which we denote by $\text{MSE}_N$), where the expectation is taken over different noise realizations.

To make this point more precise, we define $\varepsilon^*$ as the ground truth noise free image, $Z(p, \eta)$ as the MCNL solution using a random sampling pattern $p$ for a particular noise realization $\eta$. Note that the full NLM result can be written as $Z(1, \eta)$ (i.e., when the sampling pattern $p$ is the all-one
vector.) We consider the following two quantities:

\[ \text{MSE}_\eta = \mathbb{E}_\eta[(Z(1, \eta) - z^*)^2] \tag{18} \]

and

\[ \text{MSE}_{\eta,p} = \mathbb{E}_{\eta,p}[(Z(p, \eta) - z^*)^2] \tag{19} \]

The former is the MSE achieved by the full NLM, whereas the latter is the MSE achieved by the proposed MCNLM. While we do not have theoretical bounds linking \( \text{MSE}_\eta \) to \( \text{MSE}_{\eta,p} \) (as doing so would require the knowledge of the ground truth image \( z^* \)), we refer the reader to Table I in Sec. V, where numerical simulations show that, even for relatively small sampling ratios \( \zeta \), the MSE achieved by MCNLM stays fairly close to the MSE achieved by the full NLM.

IV. OPTIMAL SAMPLING PATTERNS

While the uniform sampling scheme (i.e., \( p = \zeta 1 \)) allows for easy analysis and provides useful insights, the performance of the proposed MCNLM algorithm can be significantly improved by using properly chosen nonuniform sampling patterns. We present the design of such patterns in this section.

A. Design Formulation

The starting point of seeking an optimal sampling pattern is the general probability bound provided by Theorem 1. A challenge in applying this probability bound in practice is that the right-hand side of (15) involves the complete set of weights \( \{w_j\} \) and the full NLM result \( z \). One can of course compute these values, but doing so will defeat the purpose of random sampling, which is to speed up NLM by not computing all the weights \( \{w_j\} \). To address this problem, we assume that

\[ 0 < w_j \leq b_j \leq 1, \tag{20} \]

where the upper bounds \( \{b_j\} \) are either known a priori or can be efficiently computed. We will provide concrete examples of such upper bounds in Section IV-B. For now, we assume that the bounds \( \{b_j\} \) have already been obtained.

Using (20) and noting that \( 0 \leq x_j, z \leq 1 \) (and thus \( |x_j - z| \leq 1 \)), we can see that the parameters \( \{a_j, b_j\} \) in (15) are bounded by

\[ |a_j| \leq b_j(1 + \varepsilon) \quad \text{and} \quad |b_j| \leq b_j(1 + \varepsilon), \]

respectively. It then follows from (15) that

\[
\Pr[|Z(p) - z| > \varepsilon] \leq \exp \left\{ -n\xi \right\} + 2 \exp \left\{ \frac{-n(\mu Bc)^2}{2(b_j(1 + \varepsilon))^2} \right\},
\]

where \( \mu \) is the uniform sampling scheme (i.e., single image) denoising where there is often a spatial term in the similarity weight, i.e.,

\[ w_j = w_j^s w_j^f. \tag{25} \]

One example of the spatial weight can be found in (4). Since \( w_j^f \leq 1 \), we always have \( w_j \leq w_j^f \). Thus, a possible choice is to set

\[ b_j = w_j^f. \tag{26} \]
The advantage of the above upper bound is that $b_j$ is a function of the spatial distance $d_{ij}$ between a pair of pixels, which is independent of the image data $X$ and $Y$. Therefore, it can be pre-computed before running the MCNLM algorithm. Moreover, since $\{b_j\}$ is spatially invariant, they can be reused at all pixel locations.

2) Bounds From Intensity Information: For external image denoising, the patches in $X$ and $Y$ do not have any spatial relationship, as they can come from different images. In this case, the similarity weight $w_j$ is only due to the difference in pixel intensities (i.e., $w_j = w_j'$), and thus we cannot use the spatial bounds given in (26). To derive a new bound for this case, we first recall the Cauchy-Schwarz inequality: For any two vectors $u, v \in \mathbb{R}^d$ and for any positive-definite weight matrix $\Lambda \in \mathbb{R}^{d \times d}$, it holds that

$$|u^T \Lambda v| \leq \|u\|_\Lambda \|v\|_\Lambda.$$  

Setting $u = y - x_j$, we then have

$$w_j = e^{-\|y-x_j\|_\Lambda^2/(2\lambda_r^2)} \leq e^{-(x_j^T y - y^T \Lambda y)/(2\lambda_r^2 \|y\|_\Lambda^2)} \leq e^{-(x_j^T y - y^T y)^2} = b_j', \tag{27}$$

where

$$y \defeq \Lambda v / (\sqrt{2\lambda_r} \|v\|_\Lambda).$$

The vector $v$ can be any nonzero vector. In practice, we choose $v = 1$ with $\Lambda = \text{diag}[1/d, \ldots, 1/d]$ and we find this choice effective in our numerical experiments. In this case,

$$b_j' = \exp \left\{-((x_j^T 1 - y^T 1)^2/(2\lambda_r^2 \|y\|_\Lambda^2)) \right\}.$$  

Remark 6: To obtain the upper bound $b_j'$ in (27), we need to compute the terms $y^T s$ and $x_j^T s$, which are the projections of the vectors $y$ and $x_j$ onto the one-dimensional space spanned by $s$. These projections can be efficiently computed by convolving the noisy image and the images in the reference set with a spatially-limited kernel corresponding to $s$. To further reduce the computational complexity, we also adopt a two-stage importance sampling procedure in our implementation, which allows us to avoid the computation of the exact values of $\{b_j\}$ at most pixels. Details of our implementation are given in a supplementary technical report [39].

Remark 7: Given the oracle sampling pattern, it is possible to improve the performance of NLM by deterministically choosing the weights according to the oracle sampling pattern. We refer the reader to [11], where similar approaches based on spatial adaptations were proposed.

Example 3: To demonstrate the performance of the various sampling patterns presented above, we consider denoising one pixel of the Cameraman image as shown in Fig. 6(a). The similarity weights are in the form of (25), consisting of both a spatial and a radiance-related part. Applying the result of Theorem 2, we derive four optimal sampling patterns, each associated with a different choice of the upper bound, namely, $b_j = w_j$, $b_j = b_j'$, $b_j = b_j''$, and $b_j = b_j'''$. Note that the first choice corresponds to an oracle setting, where we assume that the weights $\{w_j\}$ are known. The latter three are practically achievable sampling patterns, where $b_j'$ and $b_j''$ are defined in (26) and (27), respectively.

Fig. 6(b)–(e) show the resulting sampling patterns. As can be seen in the figures, various aspects of the oracle sampling pattern are reflected in the approximated patterns. For instance, the spatial approximation has more emphasis at the center than the peripherals whereas the intensity approximation has more emphasis on pixels that are similar to the target pixel.

To compare these sampling patterns quantitatively, we plot in Fig. 7 the reconstruction relative error associated with different patterns as functions of the average sampling ratio $\xi$. Here, we set $h_r = 15/255$ and $h_s = 50$. For benchmark, we also show the performance of the uniform sampling pattern. It is clear from the figure that all the optimal sampling patterns outperform the uniform pattern. In particular, the pattern obtained by incorporating both the spatial and intensity information approaches the performance of the oracle scheme.

V. EXPERIMENTAL RESULTS

In this section we present additional numerical experiments to evaluate the performance of the MCNLM algorithm and compare it with several other accelerated NLM algorithms.
A benchmark of ten standard test images are used for this experiment. For each image, we add zero-mean Gaussian noise with standard deviations equal to $\sigma = \frac{10}{255} \cdot 20 \cdot \frac{255}{255} \cdot 30 \cdot \frac{255}{255} \cdot 40 \cdot \frac{255}{255} \cdot 50$, to simulate noisy images at different PSNR levels. Two choices of the spatial search window size are used: $21 \times 21$ and $35 \times 35$, following the original configurations used in [1].

The parameters of MCNLM are as follows: The patch size is $5 \times 5$ (i.e., $d = 25$) and $A = I/d$. For each choice of the spatial search window size (i.e., $\rho = 21$ or $\rho = 35$), we define $h_s = (\rho/2)/3$ so that three standard deviations of the spatial Gaussian will be inside the spatial search window. The intensity parameter is set to $h_r = 1.3\sigma/255$.

In this experiment, we use the spatial information bound (26) to compute the optimal sampling pattern in (40). Incorporating additional intensity information as in (27) would further improve the performance, but we choose not to do so because the PSNR gains are found to be moderate in this case due to the relatively small size of the spatial search window. Five average sampling ratios, $\xi = 0.05, 0.1, 0.2, 0.5, 1$, are evaluated. We note that when $\xi = 1$, MCNLM is identical to the full NLM.

For comparisons, we test the Gaussian KD tree (GKD) algorithm [28] with a C++ implementation (ImageStack [40]) and the adaptive manifold (AM) algorithm [29] with a MATLAB implementation provided by the authors. To create a meaningful common ground for comparison, we adapt MCNLM as follows: First, since both GKD and AM use SVD projection [20] to reduce the dimensionality of patches, we also use in MCNLM the same SVD projection method by computing the 10 leading singular values. The implementation of this SVD step is performed using an off-the-shelf MATLAB code [41]. We also tune the major parameters of GKD and AM for their best performance, e.g., for GKD we set $h_r = 1.3\sigma/255$ and for AM we set $h_r = 2\sigma/255$. Other parameters are kept at their default values as reported in [28] and [29]. For completeness, we also show the results of BM3D [3].

Table I and Table II summarize the results of the experiment. Additional results, with visual comparison of denoised images, can be found in the supplementary technical report [39]. Since MCNLM is a randomized algorithm, we report the average PSNR values of MCNLM over 24 independent runs using random sampling pattern and 20 independent noise realizations. The standard deviations of the PSNR values over the 24 random sampling patterns are shown in Table II. The results show that for the 10 images, even at a very low sampling ratio, e.g., $\xi = 0.1$, the averaged performance of MCNLM (over 10 testing images) is only about 0.35 dB to 0.7 dB away (depending on $\sigma$) from the full NLM solution. When the sampling ratio is further increased to $\xi = 0.2$, the PSNR values become very close (about a 0.09 dB to 0.2 dB drop depending on $\sigma$) to those of the full solution.

In Table III we report the runtime of MCNLM, GKD and AM. Since the three algorithms are implemented in different environments, namely, MCNLM in MATLAB/C++ (.mex), GKD in C++ with optimized library and data-structures, and AM in MATLAB (.m), we caution that for internal (i.e., single-image) denoising, the contribution of MCNLM is mainly of a theoretical nature: It provides the theoretical foundation and a proof-of-concept demonstration to show the effectiveness of a simple random sampling scheme to accelerate the NLM algorithm. More work is needed to explore the application of similar ideas to more advanced image denoising algorithms.

As we will show in the following, the practical usefulness of the proposed MCNLM algorithm is more significant in the setting of external dictionary-based denoising, for which the classical NLM is still a leading algorithm enjoying theoretical optimality as the dictionary size grows to infinity [13].

B. External Dictionary-Based Image Denoising

To test MCNLM for external dictionary-based image denoising, we consider the dataset of Levin and Nadler [13], which contains about 15,000 training images (about $n \approx 10^{10}$ image patches) from the LabelMe dataset [42]. For testing, we use a separate set of 2000 noisy patches, which are mutually exclusive from the training images. The results are shown in Fig. 8.

Due to the massive size of the reference set, full evaluation of (1) requires about one week on a 100-CPU cluster, as reported in [13]. To demonstrate how MCNLM can be used to speed up the computation, we repeat the same experiment on a 12-CPU cluster. The testing conditions of the experiment are identical to those in [13]. Each of the 2000 test patches is corrupted by i.i.d. Gaussian noise of standard deviation

Fig. 7. Denoising results of using different sampling schemes shown in Fig. 6. Setting of experiment: noise $\sigma = 15/255$, $h_s = 50$, $h_r = 15/255$, patch size $5 \times 5$. 

Fig. 8. Performance of external dictionary-based denoising using different sampling schemes.
TABLE I
SINGLE IMAGE DENOISING BY MCNLM, USING THE OPTIMAL GAUSSIAN SAMPLING PATTERN. THE CASE WHEN $\xi = 1$ IS EQUIVALENT TO THE STANDARD NLM [2]. GKD REFERS TO [28], AM REFERS TO [29], BM3D REFERS TO [3]. SHOWN IN THE TABLE ARE PSNR VALUES (IN dB).
THE RESULTS OF MCNLM IS AVERAGED OVER 24 INDEPENDENT TRIALS OF USING DIFFERENT SAMPLING PATTERNS, AND OVER 20 INDEPENDENT NOISE REALIZATIONS.

<table>
<thead>
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<th>$\xi$</th>
<th>0.05</th>
<th>0.1</th>
<th>0.2</th>
<th>0.5</th>
<th>1</th>
<th>GKD</th>
<th>AM</th>
<th>BM3D</th>
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<tbody>
<tr>
<td>$\sigma$</td>
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<td>31.56</td>
<td>31.60</td>
<td>31.60</td>
<td>31.13</td>
<td>28.88</td>
<td>33.14</td>
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<td>26.85</td>
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<td>22.70</td>
<td>24.21</td>
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</tr>
</tbody>
</table>

$\sigma$ = 18/255. Patch size is fixed at 5 x 5. The weight matrix is $\Lambda = I$. We consider a range of sampling ratios, from $\xi = 10^{-6}$ to $\xi = 10^{-2}$. For each sampling ratio, 20 independent trials are performed and their average is recorded. Here, we show the results of the uniform sampling pattern and the optimal sampling pattern obtained using the upper bound in (27). The
results in Fig. 8 indicate that MCNLM achieves a PSNR within 0.2dB of the full computation at a sampling ratio of 10^{-3}, a speed-up of about 1000-fold.

VI. CONCLUSION

We proposed Monte Carlo non-local means (MCNLM), a randomized algorithm for large-scale patch-based image filtering. MCNLM randomly chooses a fraction of the similarity weights to generate an approximated result. At any fixed sampling ratio, the probability of having large approximation errors decays exponentially with the problem size, implying that the approximated solution of MCNLM is tightly concentrated around its limiting value. Additionally, our analysis allows the derivation of optimized sampling patterns that exploit partial knowledge of weights of the types that are readily available in both internal and external denoising applications. Experimentally, MCNLM is competitive with other state-of-the-art accelerated NLM algorithms for single-image denoising in standard tests. When denoising with a large external database of images, MCNLM returns an approximation close to the full solution with speed-up of three orders of magnitude, suggesting its utility for large-scale image processing.

APPENDIX

A. Proof of Theorem 1

For notational simplicity, we shall drop the argument p in A(p), B(p) and Z(p), since the sampling pattern p remains fixed in our proof. We also define A/B = 1 for the case when B = 0. We observe that

Pr[|Z - z| > ε] = Pr[|A/B - z| > ε]
= Pr[|A/B - z| > ε ∩ B = 0]
+ Pr[|A/B - z| > ε ∩ B > 0]
≤ Pr[B = 0]
+ Pr[|A - zB| > εB ∩ B > 0]
≤ Pr[B = 0] + Pr[|A - zB| > εB].

(28)

By assumption, w_j > 0 for all j. It then follows from the definition in (8) that B = 0 if and only if I_j = 0 for all j. Thus,

Pr[B = 0] = \prod_{j=1}^{n} (1 - p_j) = \exp \left\{ \sum_{j=1}^{n} \log(1 - p_j) \right\}
= \exp \left\{ -\sum_{j=1}^{n} p_j \right\} \leq \exp \{-n\zeta\}.

(29)

Here, (b1) holds because log(1 - p) ≤ -p for 0 ≤ p ≤ 1; and (b2) is due to the definition that \zeta = \frac{1}{n} \sum_{j=1}^{n} p_j.

Next, we provide an upper bound for Pr[|A - zB| > εB] in (28) by considering the two tail probabilities Pr[A - zB > εB] and Pr[A - zB < -εB] separately. Our goal here is to rewrite the two inequalities so that Bernstein’s inequality in Lemma 1 can be applied. To this end, we define

\alpha_j = w_j(x_j - z - \epsilon) and \ y_j = \alpha_j \left( \frac{I_j}{p_j} - 1 \right).

We note that \epsilon = \mu_A/\mu_B, where \mu_A and \mu_B are defined in (9) and (10), respectively. It is easy to verify that

Pr[A - zB > εB] = Pr \left\{ \frac{1}{n} \sum_{j=1}^{n} Y_j > \frac{1}{n} \sum_{j=1}^{n} \alpha_j \right\}
= Pr \left\{ \frac{1}{n} \sum_{j=1}^{n} Y_j > \epsilon \mu_B \right\}.

(30)

The random variables Y_j are of zero-mean, with variance

\text{Var}[Y_j] = \frac{\alpha_j^2}{p_j} \text{Var}[I_j] = \frac{\alpha_j^2}{p_j} \frac{1 - p_j}{p_j}.

Using Bernstein’s inequality in Lemma 1, we can then bound the probability in (30) as

Pr[A - zB > εB]
\leq \exp \left\{ -\frac{n(\mu_B \epsilon)^2}{2 \left( \frac{1}{n} \sum_{j=1}^{n} \alpha_j^2 \left( \frac{1-p_j}{p_j} \right) + M'_\alpha(\mu_B \epsilon)/3 \right) } \right\},

(31)

where the constant M'_\alpha can be determined as follows. Since

\begin{cases}
\alpha_j (1 - p_j)/p_j, & \text{if } I_j = 1, \\
\alpha_j, & \text{if } I_j = 0,
\end{cases}

it holds that

M'_\alpha = \max_{1 \leq j \leq n} \left( \frac{1}{2} \left| \alpha_j \left( \frac{1 - p_j}{p_j} - \alpha_j \right) \right| \right) = \max_{1 \leq j \leq n} \left( \frac{|\alpha_j|}{2p_j} \right).
The other tail probability, i.e., $\Pr[A - zB < -\epsilon B]$, can be bounded similarly. In this case, we let
\[
\beta_j \overset{\text{def}}{=} w_j(x_j - z + \epsilon) \quad \text{and} \quad \bar{\beta}_j \overset{\text{def}}{=} -\beta_j \left( \frac{1}{p_j} - 1 \right).
\]
Then, following the same derivations as above, we can show that
\[
\Pr[A - zB < -\epsilon B] \leq \exp \left\{ -n(\mu_B \epsilon)^2 \right\}
\]
where $M'_\beta = \max_{1 \leq j \leq n} (|\beta_j| / 2p_j)$. Substituting (29), (31) and (32) into (28), and defining $M_a = 2M'_a$, $M_B = 2M'_B$, we are done.

**B. Proof of Proposition 1**

The goal of the proof is to simplify (15) by utilizing the fact that $0 \leq x_j \leq 1$, $0 \leq z \leq 1$, $0 \leq w_j \leq 1$ and $p = \xi$. To this end, we first observe the following:
\[
|a_j| = w_j |x_j - z - \epsilon| \leq w_j |x_j - z + \epsilon| \leq w_j (1 + \epsilon).
\]
Consequently, $M_a$ is bounded as
\[
M_a = \max_{1 \leq j \leq n} \left( \frac{|a_j|}{p_j} \right) \overset{(a)}{\leq} \frac{1 + \epsilon}{\xi},
\]
where in (a) we used the fact that $w_j \leq 1$. Similarly,
\[
|\beta_j| \leq w_j (1 + \epsilon) \quad \text{and} \quad M_B \leq \frac{1 + \epsilon}{\xi}.
\]
Therefore, the two negative exponents in (15) are lower bounded by the following common quantity:
\[
\frac{n(\mu_B \epsilon)^2}{2 \left( \sum_{j=1}^n w_j^2 (1 + \epsilon)^2 \right)} \overset{(b)}{\geq} \frac{n\xi^2(\mu_B \epsilon)^2}{2 \left( \sum_{j=1}^n w_j (1 + \epsilon)^2 + \mu_B \epsilon (1 + \epsilon) / 6 \right)}
\]
\[
= \frac{n\xi^2(\mu_B \epsilon)^2}{2 \left( \sum_{j=1}^n w_j (1 + \epsilon)^2 + \mu_B \epsilon (1 + \epsilon) / 6 \right)}
\]
\[
= \frac{n\xi^2 \mu_B \epsilon^2}{2(1 + \epsilon)(1 + 7\epsilon/6)},
\]
where in (b) we used the fact that $0 \leq w_j \leq 1 \Rightarrow 0 \leq w_j^2 \leq w_j$. Defining $f(\epsilon) \overset{\text{def}}{=} \epsilon^2 / (2(1 + \epsilon)(1 + 7\epsilon/6))$ yields the desired result.

**C. Proof of Proposition 2**

The MSE can be computed as
\[
\mathbb{E}\left[ (Z(p) - z)^2 \right] \overset{(a)}{=} \int_0^\infty \Pr\left[ (Z(p) - z)^2 > \epsilon \right] d\epsilon
\]
\[
\overset{(b)}{=} \int_0^1 \Pr\left[ (Z(p) - z)^2 > \epsilon \right] d\epsilon
\]
where (a) is due to the “layer representation” of the expectations (See [43, Ch. 5.6]), and (b) is due to the fact that $|Z(p) - z| \leq 1$. Then, by (16), we have that
\[
\int_0^1 \Pr\left[ (Z(p) - z)^2 > \epsilon \right] d\epsilon
\]
\[
\leq \epsilon^{-n\xi^2} + 2 \int_0^1 \exp \left\{ -n\mu_B f(\sqrt{\epsilon}) \right\} d\epsilon.
\]
By the definition of $f(\epsilon)$, it is easy to verify $f(\sqrt{\epsilon}) \geq 3\epsilon/26$. Thus,
\[
\int_0^1 \Pr\left[ (Z(p) - z)^2 > \epsilon \right] d\epsilon
\]
\[
\leq \epsilon^{-n\xi^2} + 2 \int_0^1 \exp \left\{ -n\mu_B (3\epsilon/26) \right\} d\epsilon
\]
\[
\leq \epsilon^{-n\xi^2} + \frac{1}{n^\xi} \left( \frac{52}{3\mu_B} \right).
\]

**D. Proof of Theorem 2**

By introducing an auxiliary variable $t > 0$, we rewrite (P) as the following equivalent problem

\[
\begin{align*}
\text{minimize} & \quad \frac{1}{n} \sum_{j=1}^n b_j^2 / p_j + Mt \\
\text{subject to} & \quad \frac{b_j}{p_j} \leq t, \quad \sum_{j=1}^n p_j = n\xi, \quad 0 < p_j \leq 1.
\end{align*}
\]

Combining the first and the third constraint, (33) becomes

\[
\begin{align*}
\text{minimize} & \quad \frac{1}{n} \sum_{j=1}^n b_j^2 / p_j + Mt \\
\text{subject to} & \quad \sum_{j=1}^n p_j = n\xi, \quad \frac{b_j}{p_j} \leq p_j \leq 1.
\end{align*}
\]

We note that the optimal solution of (P) can be found by first minimizing (34) over $p$ while keeping $t$ fixed.

For fixed $t$, the lower bound $b_j / t$ in (34) is a constant with respect to $p$. Therefore, by applying Lemma 2 in Appendix E, we obtain that, for any fixed $t$, the solution of (34) is
\[
p_j(t) = \max \left( \min \left( b_j \tau(t), 1 \right) \right), \quad \tau(t) \quad \text{is the unique solution of the following equation with respect to the variable $x$:}
\]
\[
\sum_{j=1}^n \max \left( \min \left( b_j x, 1 \right) \right) = n\xi
\]
In order to make (34) feasible, we note that it is necessary to have
\[
t \geq \max_{1 \leq j \leq n} b_j \quad \text{and} \quad \frac{1}{n^\xi} \sum_{j=1}^n b_j.
\]
The first constraint is due to the fact that $b_j / t \leq p_j \leq 1$ for all $j$, and the second constraint is an immediate consequence by substituting the lower bound constraint $b_j / t \leq p_j$ into the equality constraint $\sum_{j=1}^n p_j = n\xi$. For $t$ satisfying (36), Lemma 3 in Appendix E shows that $\tau_t = \tau^*$ is a constant with respect to $t$. Therefore, (35) can be simplified as
\[
p_j(t) = \max \left( c_j, b_j / t \right),
\]
where $c_j \overset{\text{def}}{=} \min(b_j \tau^*, 1)$ is a constant in $t$. 

Substituting (37) into (34), the minimization of (34) with respect to \( t \) becomes

\[
\min_t \phi(t) = \frac{1}{n} \sum_{j=1}^{n} \frac{b_j^2}{\max(c_j, b_j/t)} + Mt.
\]

subject to \( t \geq \frac{1}{n \xi^2} \sum b_j \), and \( t \geq \max_{1 \leq j \leq n} b_j \). \hfill (38)

Here, the inequality constraints follow from (36).

Finally, the two inequality constraints in (38) can be combined to yield

\[
t = \max \left( \frac{1}{n \xi^2} \sum_{j=1}^{n} b_j, \max_{1 \leq j \leq n} b_j \right) = t^*.
\] \hfill (39)

Since the function \( f(x) = \max(c, x) \) is non-decreasing for any \( c \in \mathbb{R} \), it follows that \( \max(c_j, b_j/t) \leq \max(c_j, b_j/t^*) \), and hence \( \phi(t) \geq \phi(t^*) \). Therefore, the minimum of \( \phi \) is attained at

\[
t = \max \left( \frac{1}{n \xi^2} \sum_{j=1}^{n} b_j, \max_{1 \leq j \leq n} b_j \right).
\]

E. Auxiliary Results for Theorem 2

**Lemma 2:** Consider the optimization problem

\[
(P') \quad \begin{array}{l}
\text{minimize} \quad \sum_{j=1}^{n} \frac{b_j^2}{p_j} \\
\text{subject to} \quad \sum_{j=1}^{n} p_j = \xi \quad \text{and} \quad \delta_j \leq p_j \leq 1.
\end{array}
\]

The solution to \((P')\) is

\[
p_j = \max(\min(b_j \tau, 1), \delta_j), \quad \text{for } 1 \leq j \leq n.
\] \hfill (40)

where the parameter \( \tau \) is chosen so that \( \sum_{j=1}^{n} p_j = n \xi \).

**Proof:** The Lagrangian of \((P')\) is

\[
\mathcal{L}(p, \lambda, \eta, v) = \sum_{j=1}^{n} \frac{b_j^2}{p_j} + v \left( \sum_{j=1}^{n} p_j - n \xi \right)
\]

\[
+ \sum_{j=1}^{n} \lambda_j (p_j - 1) + \sum_{j=1}^{n} \eta_j (\delta_j - p_j),
\] \hfill (41)

where \( p = [p_1, \ldots, p_n]^T \) are the primal variables, \( \lambda = [\lambda_1, \ldots, \lambda_n]^T \), \( \eta = [\eta_1, \ldots, \eta_n]^T \) and \( v \) are the Lagrange multipliers associated with the constraints \( p_j \leq 1 \), \( p_j \geq \delta_j \) and \( \sum_{j=1}^{n} p_j = n \xi \), respectively.

The first order optimality conditions imply the following:

- **Stationarity:** \( \nabla_p \mathcal{L} = 0 \). That is, \(-\frac{b_j^2}{p_j^2} + \lambda_j - \eta_j + v = 0 \).
- **Primal feasibility:** \( \sum_{j=1}^{n} p_j = n \xi \), \( p_j \leq 1 \), and \( p_j \geq \delta_j \).
- **Dual feasibility:** \( \lambda_j \geq 0 \), \( \eta_j \geq 0 \), and \( v \geq 0 \).
- **Complementary slackness:** \( \lambda_j (p_j - 1) = 0 \), \( \eta_j (\delta_j - p_j) = 0 \).

The first part of the complementary slackness implies that for each \( j \), one of the following cases always holds: \( \lambda_j = 0 \) or \( p_j = 1 \).

Case 1: \( \lambda_j = 0 \). In this case, we need to further consider the condition that \( \eta_j (\delta_j - p_j) = 0 \). First, if \( \eta_j = 0 \), then \( p_j \geq \delta_j \). Substituting \( \lambda_j = \eta_j = 0 \) into the stationarity condition yields \( p_j = b_j / \sqrt{v} \). Since \( \delta_j \leq p_j \leq 1 \), we must have \( b_j \leq \sqrt{v} \leq b_j / \delta_j \). Second, if \( p_j = \delta_j \), then \( \eta_j > 0 \). Substituting \( p_j = \delta_j \) and \( \lambda_j = 0 \) into the stationarity condition yields \( \eta_j = \sqrt{v} - b_j^2 / \delta_j^2 \). Since \( \eta_j > 0 \), we have \( \sqrt{v} > b_j / \delta_j \).

Case 2: \( p_j = 1 \). In this case, \( \eta_j (\delta_j - p_j) = 0 \) implies that \( \eta_j = 0 \) because \( p_j = 1 > \delta_j \). Substituting \( p_j = 1 \), \( \eta_j = 0 \) into the stationarity condition suggests that \( \lambda_j = b_j^2 / v \). Since \( \lambda_j > 0 \), we have \( \sqrt{v} < b_j \).

Combining these two cases, we obtain

\[
p_j = \begin{cases} \delta_j, & \text{if } b_j < \delta_j \sqrt{v}, \\ b_j / \sqrt{v}, & \text{if } \delta_j \sqrt{v} \leq b_j \leq \sqrt{v}, \\ 1, & \text{if } b_j > \sqrt{v}. \end{cases}
\]

By defining \( \tau = 1 / \sqrt{v} \), we prove (40).

It remains to determine \( v \). This can be done by using the primal feasibility condition that \( \frac{1}{n} \sum_{j=1}^{n} p_j = \xi \). In particular, consider the function \( g(t) \) defined in (24), where \( \tau = 1 / \sqrt{v} \). The desired value of \( v \) can thus be obtained by finding the root of the equation \( g(\tau) \). Since \( g(\tau) \) is a monotonically increasing piecewise-linear function, the parameter \( v \) is uniquely determined, so is \( p \).

**Lemma 3:** Let \( g_t(x) = \sum_{j=1}^{n} \max(\min(b_j x, 1), b_j / t) \), and for any fixed \( t \), let \( t_\tau \) be the solution of the equation \( g_t(x) = n \xi \). For any \( t \geq t^* \), where \( t^* \) is defined in (39), \( t_\tau = t^* \) for some constant \( t^* \).

**Proof:** First, we claim that

\[
g_t(x) = \begin{cases} \sum_{j=1}^{n} b_j / t, & x \leq 1/t, \\ \sum_{j=1}^{n} \min(b_j x, 1), & x > 1/t. \end{cases}
\] \hfill (42)

To show the first case, we observe that \( b_j / t \leq 1 \) implies \( b_j x \leq b_j / t \leq 1 \).

\[
g_t(x) = \sum_{j=1}^{n} \max(\min(b_j x, 1), b_j / t) = \left( \sum_{j=1}^{n} b_j \right) / t.
\]

For the second case, since \( x > 1/t \), it follows that \( b_j / t < b_j x \).

\[
g_t(x) = \sum_{j=1}^{n} \min(b_j x, 1).
\]

Now, by assumption that \( t \geq 1 / n \xi \sum_{j=1}^{n} b_j \), it follows from (42) that

\[
g_t \left( \frac{1}{t} \right) \leq n \xi.
\] \hfill (43)

Since \( g_t(x) \) is a constant for \( x \leq 1/t \) or \( x \geq 1 / \min_1 b_j \), the only possible range for \( g_t(x) = n \xi \) to have a solution is when \( 1/t < x < 1 / \min_1 b_j \). In this case, \( g_t(x) = \sum_{j=1}^{n} \min(b_j x, 1) \) is a strictly increasing function in \( x \) and so the solution is unique. Let \( t^* \) be the solution of \( g_t(x) = n \xi \). Since \( \sum_{j=1}^{n} \min(b_j x, 1) \) does not involve \( t \), it follows that \( t^* \) is a constant in \( t \).
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REFERENCES

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