Recovery and Generalization in Over-Realized Dictionary Learning

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Abstract

In over two decades of research, the field of dictionary learning has gathered a large collection of successful applications, and theoretical guarantees for model recovery are known only whenever optimization is carried out in the same model class as that of the underlying dictionary. This work characterizes the surprising phenomenon that dictionary recovery can be facilitated by searching over the space of larger over-realized models. This observation is general and independent of the specific dictionary learning algorithm used. We thoroughly demonstrate this observation in practice and provide a theoretical analysis of this phenomenon by tying recovery measures to generalization bounds. We further show that an efficient and provably correct distillation mechanism can be employed to recover the correct atoms from the over-realized model. As a result, our meta-algorithm provides dictionary estimates with consistently better recovery of the ground-truth model.

1 Introduction

Latent variable models have been very successful for a variety of unsupervised learning problems, from regularizing inverse problems of different kinds to enabling clustering, classification or other down-stream supervised learning problems [Bengio et al., 2013]. We focus on sparse representation models, which posit that data $x \in \mathcal{X} \subseteq \mathbb{R}^d$ admits a sparse decomposition in terms of a redundant dictionary $D \in \mathcal{D} \subseteq \mathbb{R}^{d \times p}$, where $p > d$ and $\mathcal{D}$ is an appropriate constraint set. In other words, $x = D\gamma$, where the number of nonzero entries $\|\gamma\|_0 \leq k \ll d$. These models are most useful when the model $D$ is learned from a collection of samples $\{x_i\}_{i=1}^n$, thus allowing for greater sparsity or representation power. This task goes by the name of dictionary learning, and many algorithms have been proposed over the last two decades to (most often approximately) solve this problem [Aharon et al., 2006a, Mairal et al., 2010, Engan et al., 1999, Olshausen and Field, 1997, Arora et al., 2015].

A central problem in dictionary learning is that of model recovery. More precisely, assuming that the training samples follow such a generative model, $x_i = D\gamma_i$, and one has access to a learning algorithm that provides an estimate $\hat{D}$, how close will the obtained model be from the true generating dictionary? There exist by now a rich literature on these questions. Some of these results are concerned with providing recovery guarantees for popular and practical dictionary learning methods, such as the K-SVD [Aharon et al., 2006b, Schnass, 2014] or simpler online learning algorithms [Olshausen and Field, 1997, Arora et al., 2015]. Others instead propose new algorithms with recovery guarantees, most often in an alternating minimization manner [Agarwal et al., 2016, 2014, Arora et al., 2014a, b, Arora and Risteski, 2017], while other results study local identifiability [Geng and Wright, 2014, Gribonval et al., 2015a] or fundamental limits and min-max optimal bounds [Shakeri et al., 2018, Jung et al., 2016]. Naturally, these guarantees depend on the minimum number of
training samples, \( n \), as well as on the parameters of the model: \( d, p \) and \( k \), the particular distribution of the non-zero values, and possibly the amount of noise contamination in the observations.

Though dictionary learning algorithms vary, by and large they share the following common scheme: given the constraint set \( \mathcal{D}_p \) of the ground-truth model, typically \( \mathcal{D}_p = \{ \mathbf{D} \in \mathbb{R}^{d \times p} : \| \mathbf{D} \|_2 = 1 \ \forall \ i \in \{1, \ldots, p\} \} \), and given a collection of \( n \) samples from this model, one searches for an estimate \( \hat{\mathbf{D}} \in \mathcal{D}_p \) by means of some optimization approach. The first question we pose in this work is the following: \textit{Why should one limit to the set } \( \mathcal{D}_p \textit{ instead of searching over a larger class of models?} \) Somewhat surprisingly, we will show that dictionary recovery can be consistently improved if one allows the learning algorithm to search for models \( \hat{\mathbf{D}} \in \mathcal{D}_{p'} \subset \mathbb{R}^{d \times p'} \), where \( p' > p \). In other words, we will search for a larger set of atoms than those that are strictly necessary to sparsely represent the training data – an over-realized model.

While it is certainly natural that a larger model of \( p' > p \) atoms can approximate the training samples better than one with \( p \) atoms, it is not immediately obvious that this might lead to a better overall dictionary recovery. After all, how can one evaluate model recovery if the estimate and ground-truth models belong to different spaces? To this end, we propose a new distance metric and show that it can be upper bounded by a function of the empirical risk (i.e. training error) and the generalization gap, both of which are computable. This result links recovery guarantees to generalization bounds, allowing us to characterize the behaviour observed in our experiments, and leading to a uniform upper bound to the recovery error. We then study a second driving question: \textit{given a trained model } \( \hat{\mathbf{D}} \in \mathcal{D}_{p'} \textit{, can one distill from it an estimate } \hat{\mathbf{D}} \in \mathcal{D}_p \textit{ and, in doing so, improve the recovery of the true dictionary?} \) We will answer this question in the affirmative, providing a provably correct algorithm under incoherence assumptions. As a result, we will provide a meta-algorithm for dictionary learning via over-realized models that improves model recovery over conventional (non over-realized) approaches.

The study of over-realized models in unsupervised learning has received some – but limited – attention in the past. The work in [Dasgupta and Schulman, 2007] showed more than a decade ago that the recovery of \( k \) clusters by k-means [Lloyd, 1982] can be improved by a two-step process, whereby in the first round one uses more random guesses as initialization (more precisely, \( \mathcal{O}(k \log k) \)). To the best of our knowledge, the recent and inspiring work in [Buhai et al., 2019] is the first to provide a provably correct algorithm under incoherence assumptions. As a result, we will provide a meta-algorithm for dictionary learning via over-realized models that improves model recovery over conventional (non over-realized) approaches.

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**Overview** We first introduce our notation and provide the necessary background in Section 2. We then address the recovery problem in the over-realized case in Section 3, providing examples and presenting our main theoretical result. Section 4 tackles the question of the distillation of larger models, and provides a provably correct algorithm as well as extensive empirical evidence. We finally delineate final remarks and conclude in Section 5.

## 2 Preliminaries

We consider data \( \mathbf{x} \in \mathbb{R}^d \), and a redundant dictionary \( \mathbf{D}_0 \in \mathcal{D}_p, p > d. \) We consider the following generative model for \( \mathbf{x} \) throughout this work, providing a sampling distribution \( \mathcal{P} \): a sparse representation \( \gamma \in \mathbb{R}^p \) is sampled from a set of \( k \)-sparse vectors by (i) sampling its support \( S \) uniformly from the set of all possible \( \binom{p}{k} \) supports of cardinality \( k \), and (ii) sampling its non-zero values i.i.d from a distribution \( \mathcal{P}, \gamma_i \sim \mathcal{P} \ \forall i \in S \) with mean zero and unit variance (for simplicity). Samples are then obtained as \( \mathbf{x} = \mathbf{D}_0 \gamma \). Given \( \mathbf{x} \) and \( \mathbf{D}_0 \), the problem of retrieving the representation \( \gamma \) is termed...
sparse coding, and it involves solving a problem of the form
\[
\min_{\gamma} \frac{1}{2} \|x - D_0 \gamma\|_2^2 + g(\gamma),
\]
where \(g(\gamma)\) is a sparsity-promoting function that regularizes the ill-posed recovery problem. Typical choices for \(g\) are the non-convex and non-smooth \(\ell_0\) pseudo-norm, or its convex relaxation, the \(\ell_1\) norm. Alternatively, \(g\) may denote an indicator function over a constraint set, such as
\[
g_k(\gamma) = \begin{cases} 
0 & \text{if } \|\gamma\|_0 \leq k, \\
+\infty & \text{otherwise}. 
\end{cases}
\]

In either case, numerous pursuit algorithms exist that allow for the provable recovery of \(\gamma\) under assumptions like restricted isometry property [Candes and Tao, 2005] or incoherence [Tropp, 2004, Donoho and Elad, 2003], or approximations in the case of noisy measurements. When \(g(\gamma) = \|\gamma\|_1\), the problem is termed Basis Pursuit DeNoising or Lasso [Tibshirani, 1996] (and Basis Pursuit when an \(\ell_1\) ball is used as a constrained set). Alternatively, one may employ greedy algorithms such as the popular Orthogonal Matching Pursuit (OMP) [Pati et al., 1993], which approximates the solution to the \(\ell_0\)-constrained problem.

When the dictionary is not known, the dictionary learning problem attempts to recover an estimate as close as possible to the ground-truth model given a set of \(n\) training samples \(x_i\) from it. The quality of a dictionary in approximating a sample \(x\) is measured by the function value of the cost above, namely
\[
f_{x_i}(D) := \inf_{\gamma \in \mathbb{R}^p} \frac{1}{2} \|x - D \gamma\|_2^2 + g(\gamma).
\]

In this way, the dictionary learning problem can be written as
\[
\min_{D \in D_p} \frac{1}{n} \sum_{i=1}^{n} f_{x_i}(D).
\]

The resulting optimization problem is non-convex and hard to analyze in general [Tillmann, 2014], but this has not prevented the development of many (and very successful) algorithms. One such methods is the Online Dictionary Learning (ODL) from [Mairal et al., 2010], which minimizes (4) in an online manner. In a nutshell, given a current estimate for the dictionary, this algorithm iterates between drawing a sample (or a mini-batch thereof) at random, then employing a pursuit algorithm to minimize (1), and finally updating the dictionary so as to minimize a surrogate of the cost in (4). The approach is general in that it can accommodate different pursuit algorithms for different penalty functions \(g(\gamma)\), and it scales well to large datasets. The very popular K-SVD Aharon et al. [2006a], on the other hand, is a batch-learning approach that alternates between sparse coding (typically with OMP) and dictionary update, which is characteristically carried out column-by-column by performing rank-1 approximations to atom-wise residual.

Recovery
A central question is this setting is that of model recovery, which asks how far the recovered estimate \(\hat{D} \in D_p\) is from the ground-truth dictionary, \(D_0 \in D_p\). To formalize this question one needs an appropriate measure of distance between matrices. The problem in (4) is permutation (and sign) invariant: the columns of the dictionary can be arbitrarily permuted (or multiplied by \(-1\)) without modifying the cost \(f_x(D)\). Thus, different measures of recovery have been used in previous works accounting for such invariance, such as [Arora et al., 2015]
\[
\min_{\hat{P} \in \Pi} \|D_0 - \hat{D} \hat{P}\|_F^2,
\]

where \(\Pi\) is the set of signed permutation matrices, i.e orthogonal matrices that contain only \(\{0, \pm 1\}\). Several works have studied recovery questions over the last decade. Some of these show local linear convergence to the global optimum (i.e. the true model) via alternating minimization employing \(\ell_1\) penalty functions [Agarwal et al., 2014, 2016] or to an \(\epsilon\)-close optimum via \(\ell_0\) constraints [Arora...
et al., 2015]. In the simpler case of orthonormal dictionaries the optimization landscape is better understood [Zhai et al., 2019], as in the case of learning only one atom [Sun et al., 2015, Qu et al., 2019]. In these settings, these non-convex problems have a benign geometry structure that allows for provable algorithms. On the other hand, [Jung et al., 2016] develops minimax risk bounds for dictionary recovery, and [Shakeri et al., 2018] studies these as a function of their tensor structure. All of these results, however, analyze the conventional setting whereby the constraint sets of the ground-truth dictionary and the one enforced during optimization are the same.

**Generalization Error** From a statistical learning standpoint, the dictionary learning problem consists in finding a model $D \in \mathcal{D}_p$ that minimizes the above function in expectation over the population, i.e.,

$$\hat{D} \in \arg\min_{D \in \mathcal{D}_p} \mathbb{E}_{x \sim P} [f_x(D)].$$

(6)

Since one does not typically have access to the underlying distribution, the empirical risk minimization algorithm (ERM) minimizes the empirical estimate of the above risk, which is precisely the problem in Eq. (4). In this context, a central question is given by the generalization error, which quantifies the extent to which the empirical error, $R_S(D) = \frac{1}{n} \sum_{i=1}^{n} f_i(D)$, differs from its expectation in Eq. (6). Uniform bounds have recently been developed for these models in [Maurer and Pontil, 2010, Vainsencher et al., 2011, Seibert, 2019]. More specifically, with overwhelming probability over the sample $S$, the work in [Gribonval et al., 2015b] shows that

$$\sup_{D \in \mathcal{D}_p} \left| R_S(D) - \mathbb{E}_{x \sim P} [f_x(D)] \right| \leq \eta_n.$$

(7)

The generalization error above, $\eta_n$, depends on the model capacity, the number of samples, as well as the data distribution and properties of the penalty function $q$. Slightly more specifically, $\eta_n$ is $O(\sqrt{(dp) \log n/n})$, where $(dp)$ is the number of parameters in the dictionary with $p$ atoms. This type of bounds are very useful, since they provide an upper bound to the expected error given the empirical risk, and they reflect a natural trade-off between the model size (number of atoms, $p$) and the number of training samples, $n$. The bound above holds not just for norms and norm-like regularization functions (like the $\ell_1$ norm) but also for indicator sets as $g_k$ in (2). We will keep our derivations maximally general by simply referring to $\eta_n$, and we refer the reader to [Gribonval et al., 2015b] for further details on the involved constants.

3 Searching for over-realized dictionaries

In this work we focus on the over-realized setting, in which the minimization in Eq. (4) is done over a class of dictionaries $\mathcal{D}_{p'}$, with $p' > p$, i.e. larger than the original model. One might wonder as to the need for this change. After all, there exists indeed a global minimum ($D_0$) with $p$ atoms that achieves both zero training and testing errors. Nonetheless, one should keep in mind that the optimization landscape of these optimization problems is still not fully understood, and practical local-search algorithms may converge to a local minimum due to the high non-convexity of the problem (4).

We first require a distance measure between dictionaries of potentially different sizes. We will use the following definition for the distance between a dictionary $D_0 \in \mathcal{D}_p$ and an estimate $\hat{D} \in \mathcal{D}_{p'}$:

$$d(D_0, \hat{D}) = \frac{1}{p} \sum_{i=1}^{p} \min_{j \in [p']} \min_{\epsilon \in \{-1, 1\}} \|D_0^i - \epsilon \hat{D}_j\|_2^2.$$

(8)

Note that this distance is zero if and only if there exists a match for each of the atoms in $D_0$ in the estimated $\hat{D}$, irrespective the size $p'$, and it provides a generalization of the above (5).

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1 We will use $D_0^i$ to denote the $i^{th}$ column, or atom, from $D_0$.

2 Note that our definition in Eq. (8) generalizes that in Eq. (5) by allowing the set of permutation matrices to become column-selection (non-square) ones.
We now explore the first question posed above, namely: can one obtain an estimate with better generalization error and lower recovery error by searching in a hypothesis class bigger than that of the original dictionary? As a motivating example, we construct the following experimental setting. Data is sampled as described in the previous section from a ground truth dictionary (with normalized Gaussian atoms) of size $50 \times 70$, from representations with cardinality $k = 3$. We construct 300 such samples for training, leaving 1000 to estimate the population statistics. As a learning algorithm, we employ ODL\cite{Mairal2010} for 2000 iterations, which are more than sufficient for convergence. We employ OMP for the sparse coding step.

In Figure 1a we depict the risk, or error, on both training and test sets, as a function of the number of atoms in the estimated dictionary $\hat{D}$, from 70 (the size of the ground-truth model) to 500. We repeat the experiment 20 times, and present the mean together with the 25% and 75% percentiles. Interestingly, both train and testing errors, shown in Figure 1a, improve with increasing dictionary size $p' > p$ within some range. More surprisingly, the distance from the estimate to the ground truth $D_0$ also improves as one searches for bigger dictionaries. Note that because of our definition of distance in Eq. (8), a small distance implies a close recovery of the true atoms, irrespective of the “extra” ones. At the same time, this behaviour is tightly related to that of model capacity and over-fitting: while increased dictionary size allows for better recovery, the limited training size eventually results insufficient to train the larger model and the generalization error increases (while perfectly fitting the training data). This is verified in Figure 1c and Figure 1d, seeing that the generalization error – and dictionary recovery – is precisely controlled by the size of the training set. In this figure, only the means of the 20 realizations are depicted for the sake of clarity.

3.1 Recovery guarantees via generalization bounds

While the behaviour observed in Figure 1a and Figure 1c is well understood in the statistical learning literature, this is still surprising in light of the fact that there exist a ground truth model with just $p$ atoms that achieves zero risk. Moreover, how this relates to improved recovery of the ground-truth dictionary in over-realized settings – as shown in Figure 1b and Figure 1d – is, to the best of our knowledge, unknown. Learning bounds and recovery guarantees for dictionary learning have so far remain mostly separated. We will now precisely connect the model recovery error with its expected risk, providing a theoretical characterization for this phenomenon.

Let $f_{\gamma,s}(D) = \inf_{\|\gamma\|_0 \leq s} \frac{1}{2} \|x - D\gamma\|_2^2$ denote the risk measured with $s$ non-zero coefficient. We will denote the mutual coherence of a dictionary by $\mu(D) = \max_{i \neq j} |\langle D_i, D_j \rangle|$ (recall that columns

\footnote{Available at spams-devel.gforge.inria.fr/}.
are normalized). Furthermore, for a given atom in the estimate dictionary, \( \hat{D}_j \), consider its closest atom in the ground truth dictionary, \( D_{i(j)} \). Then, let \( \nu = \max_j \max_{k \neq i(j)} \left| \langle D_j, D_k^\prime \rangle \right| \). In words, \( \nu \) quantifies the coherence between \( \hat{D} \) and \( D_0 \) after excluding the closest neighbor of each atom. While this expression might seem somewhat convoluted, this simply reduces to the traditional mutual coherence of the dictionary, \( \mu(D_0) \), in the case that \( \hat{D} = D_0 \).

With these definitions, we have the following central Lemma.

**Lemma 3.1.** For a ground-truth dictionary \( D_0 \in \mathbb{R}^{d \times p} \) generating samples \( x_i = D_0 \gamma_i \), where \( \gamma_i \) are \( k \)-sparse with non-zeros sampled i.i.d from a zero mean and unit variance distribution, and for any estimate \( \hat{D} \in \mathcal{D}_{p'} \), we have that

\[
\frac{2}{k} \mathbb{E}_{x \sim \mathcal{D}} \left[ f_x^k(\hat{D}) \right] \leq d(\hat{D}, D_0) \leq \frac{4}{k} \mathbb{E}_{x \sim \mathcal{D}} \left[ f_x^k(\hat{D}) \right] - \frac{2}{k} \zeta_k(k-1).
\]

where \( \zeta_k := \max \{ 0, 1 - (k-2)\mu(D_0) - 2\nu^2 \} \).

Note that this result links the recovery distance, \( d(\hat{D}, D_0) \), with the expected risk, as measured by \( f_x^k(\hat{D}) \) and \( f_x^k(D) \). We will comment on further implications of this shortly, but first we present our main result as a consequence the Lemma 3.1, which is of practical relevance. Employing the generalization bound from Eq. (7), we can bound the dictionary distance by measurable and computable quantities, as presented in the main result.

**Theorem 3.2.** For a ground-truth dictionary \( D_0 \in \mathbb{R}^{d \times p} \) generating samples \( x_i \) with sparsity of \( k \), and for any estimate \( \hat{D} \in \mathcal{D} \), with overwhelming probability, we have that

\[
\frac{k}{4} d(\hat{D}, D_0) \leq \frac{1}{n} \sum_{i} f_{x_i}^k(\hat{D}) - \frac{1}{2} \zeta_k(k-1) + \eta_n,
\]

where \( \eta_n = \mathcal{O}(\sqrt{dp \log n/n}) \).

First, this result shows that the distance to the true model can be upper bounded by the empirical risk up to a generalization error and a model-dependent quantity. This reflects an important implicit trade-off: the dictionary recovery error can be decreased by increasing the model capacity (dictionary size) as long as the generalization error is kept small by increasing the sample size appropriately. This is indeed the behaviour observed in Figure 1d above. Second, the term \( \zeta_k(k-1) \) appearing in both results above, accounts for the fact that the upper bound is constructed via \( f_x^k \), as opposed to \( f_x^{[k]} \). Indeed, note that this term vanishes when \( k = 1 \). When \( k > 1 \), the empirical estimate of \( f_x^{[k]} \) will necessarily be greater than zero. It is in these cases where the term \( \zeta_k(k-1) \) provides a non-trivial tighter bound, as long as \( k \leq 2 + 1/\mu(D_0) - 2\nu^2/\mu(D_0) \), which are mild conditions. We now provide a sketch of the proof of Lemma 3.1, and defer the complete proof to Appendix A.

**Proof sketch:** The upper and lower bound for \( d(\hat{D}, D) \) are obtained independently, though with similar proof techniques. For the upper bound, the risk \( \mathbb{E}[f_x^k(\hat{D})] \) can be expressed analytically in closed form for each sample \( x \). We then decompose the resulting expression for the expectation in three terms. Relying on the fact that the non-zero entries are drawn i.i.d with mean zero and unit variance, one of these vanishes; another term can be lower bounded by \( \zeta_k(k-1) \), while the remaining term can be lower bounded by a quantity proportional to the dictionary distance \( d(\hat{D}, D_0) \). Arranging accordingly provides the bound above. The lower bound relies on constructing an analytical (and potentially suboptimal) solution for the sparse coding problem involved in \( f_x^{[k]}(\hat{D}) \) relying on the atoms that are closest to \( D_0 \), upper bounding this risk. A series of algebraic manipulations and the final evaluation of the expectation over the distribution of supports provide the final upper bound on \( \mathbb{E}[f_x^k(\hat{D})] \) as a function of the distance \( d(D_0, \hat{D}) \).

These results provide an answer in support of learning larger dictionaries, not only to minimize the expected risk but also to obtain estimates with small distance to the ground-truth model. However, a question remains: how can one *distill* the estimated over-realized \( \hat{D} \) to recover the best \( p \) atoms that are the closest to the real model? This is the question we address in the next section.
4 Distilling the over-realized model

In this section, we will first show that the recovered dictionary in the over-realized model exhibit two distinct behaviors: any recovered atom is either (very) close to a true atoms in $D_0$, or is significantly far apart from all atoms in $D_0$. We will also show that this clustering behaviour correlates with the atom usage in the estimated model. From this observation, we will then develop a provably correct pruning strategy based on the atom’s usage frequency. This distillation approach will recover an estimate of the original size with a lower recovery error than the traditional (non over-realized) learning approach.

As before, given 500 training samples created as the linear combination of $k = 3$ atoms from a ground-truth dictionary $D_0$ with 70 atoms in 50 dimensions, we train an over-realized dictionary $\hat{D}$ with 100 atoms using ODL (with OMP for sparse coding). We then measure, per estimated atom $\hat{D}_i$, the similarity to its closest neighbor in the ground-truth $D_0$ (computed as $-\log \|D_0^{(j)} - \hat{D}_i\|_2^2$). We plot these similarities as a function of the atom’s usage: the relative number of times it is used by the training samples upon completion of training. The results are depicted in Figure 2a, and two observations are worth noting: the recovered atoms either have a high similarity with those in the ground-truth dictionary or are markedly distinct, with a clear separation between groups. This is similar to the observation made in [Buhai et al., 2019] in the context of noisy-or networks and approximate sparse coding. Second, there exists a strong correlation between the former measure – which cannot be computed in practise, i.e. without access to the original model – and the number of times an estimated atom is used by the training samples – which can.

Following this observation, we then propose the following simple meta-algorithm: after learning an over-realized dictionary, we keep the $p$ most frequently used atoms by the training samples. Other works have suggested similar approaches that prune the over-realized model to a subset of components and then continue the optimization with these as better initializations [Dasgupta and Schulman, 2007]. This is not needed in our setting, however, likely due to the significant more accurate coding step. Figure 2b illustrates the same experiment as that in Figure 1a and Figure 1b, though now with the statistics provided by our distillation strategy. While clearly the distillation procedure introduces some errors, it still provides a considerable advantage over the traditional approach (i.e. training with the original size $p$) by significantly diminishing the recovery error. This is further explained by the details in Figure 2a, comparing the atoms chosen by this distillation procedure and the oracle choices – those atoms that are the closest to the ground-truth dictionary. As can be seen, most atoms picked by this strategy coincide with the oracle ones.

4.1 Theoretical guarantees for distillation

We now strengthen our argument for our distillation strategy. In the following result, we show that if the atom usage of the over-realized estimate $\hat{D}$ is measured via OMP (with $k = 1$), and $D$ contains
such that $x$

Theorem 4.1. we must only select atoms in atoms, as our condition only requires correct atoms within it. On the other hand, is milder than the one for OMP, leading to relaxed and improved guarantees. This is natural, since have the following result, which is proved in Appendix B.

Let $D_0 \in \mathbb{R}^{d \times p}$ and consider, without loss of generality, that $D = [D_0, A] \in \mathbb{R}^{d \times p'}$ with $D_0 \in \mathbb{R}^{d \times m}$, with $m \leq p'$, such that $d(D_0^i, D_0) \leq \epsilon$ for all $i \in \{1, \ldots, m\}$, and $d(A_j, D_0) > \epsilon$ for all $j \in \{1, \ldots, p' - m\}$. In other words, $D_0$ contains all those $m$ atoms that are $\epsilon$-close to those in $D_0$, while $A$ contains those that are further away. Additionally, we require that each atom in $D_0$ has at least one $\epsilon$-neighbor in $D_0$; i.e., $d(D_0^i, D_0) \leq \epsilon$ for all $i \in \{1, \ldots, p\}$. We allow $m \geq p$ since the over-realized estimate $\hat{D}$ may naturally contain several atoms that close to a real one. Also suppose that both $D_0$ and $\hat{D}$ are column-wise normalized for simplicity. Let us denote by $\mu(D_0, A) = \max_{i,j} |\langle D_0^i, A_j \rangle|$ the mutual coherence between $D_0$ and $A$. With these definitions, we have the following result, which is proved in Appendix B.

Theorem 4.1. Let $x$ be a $k$-sparse signal under $D_0$, i.e., there exists $\gamma \in \mathbb{R}^p$ with $\|\gamma\|_0 \leq k$ such that $x = D_0 \gamma$, and let $\hat{D}$ be defined as above. Then, $\arg\max_k |x^T \hat{D}_i| \in [m]$ as long as $k \leq \frac{1}{\mu(D_0)} \frac{1}{\mu(D_0, A)}$.

Note that, on one hand, if the distance $\epsilon = 0$ and we replace $\mu(D_0, A)$ with $\mu(D_0)$, our condition can be compared to the traditional incoherence condition for OMP that requires $k < \frac{1}{\mu(D_0)}(1 + \frac{1}{\mu(D_0, A)})$. As shown by the results in Figure 2a, we indeed observe that the similarity in the un-related atoms to those in $D_0$ is quite low, i.e., $\mu(D_0, A)$ is very small. Then, and our condition above (with $\epsilon = 0$) is milder than the one for OMP, leading to relaxed and improved guarantees. This is natural, since we must only select atoms in $\hat{D}$ that belong to $D_0$ as opposed to demanding the recovery of the correct atoms within it. On the other hand, $A$ itself is allowed to be coherent, even with repeated atoms, as our condition only requires $\mu(D_0, A)$ to be small. Lastly, the result above is more general in that we allow for $\epsilon > 0$, which better reflects the empirical behavior reflected in Figure 2a.

Figure 3: Risk and Dictionary error (log$_{10}$ thereof, lower is better) of the estimate provided by traditional dictionary learning (i.e. $D \in D_p$) and that resulting from the proposed over-realized approach (i.e. $D \in D_{p'}$) followed by distillation to the original size, over a number of parameters (sparsity, dimension and redundancy).
4.2 Applicability to different model parameters and algorithms

Thus far we have employed the same experimental setting (dimension, dictionary size and sparsity) for all the above examples for simplicity. However, the reported findings are general and hold for a variety of parameters and algorithms. We now demonstrate this in Figure 3 where we report the risk and dictionary error for the estimates produced by learning a dictionary (with ODL+OMP) in the traditional setting (i.e., $\hat{D} \in D_p$) and that produced by searching over a larger set (i.e., $\hat{D} \in D_{p'}$, with $p' > p$) followed by our distillation strategy. In this way, all reported measures are computed on estimates of the same size as the original model. Note that an important improvement in risk, but most importantly in dictionary recovery, is observed across a wide range of parameters. Moreover, the phenomenon is general not just across different model parameters but also to different learning algorithms and regularization functions $g$. In Appendix C we show that similar behaviour (albeit less pronounced) can be obtained by employing: (i) the ODL method from [Mairal et al., 2010] with an $\ell_1$ regularizer, i.e. employing Lasso for sparse coding, and (ii) the batch algorithm K-SVD [Aharon et al., 2006a].

5 Conclusions

In this work we showed that learning over-realized dictionaries can be beneficial not just to provide lower training and population risk, but to also improve the recovery of the underlying model. Our characterization of this phenomenon relies on the connection between the recovery error and the expected risk, enabling thus an upper bound to the former in terms of the empirical risk and a generalization gap. Moreover, we showed that an estimate of the original size can be distilled from the over-realized model, consistently improving the recovered dictionary across different model parameters and algorithms.

At the same time, several questions remain un-answered. It is still unclear what determines the optimal degree of over-realization (oracle choices were employed in the above experiments). A complete understanding of the reasons behind the benefits of over-realization is still missing, and is likely to involve an optimization perspective. In the $p' > p$ setting, the learning problem (4) might become more amenable to practical optimization algorithms, which thus may find a better solution. Similar phenomena have also been studied in k-means [Lloyd, 1982], training neural networks with ReLu units [Safran and Shamir, 2018], and noisy OR-network [Buhai et al., 2019]. Further research in this direction will enable to characterize the reported results better, and might extend the application of these ideas to other unsupervised machine learning models.

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Appendix

A Recovery Guarantees

Lemma 3.1. For a ground-truth dictionary \( D_0 \in \mathbb{R}^{d \times p} \) generating samples \( x_i = D_0 \gamma_i \), where \( \gamma_i \) are \( k \)-sparse with non-zeros sampled i.i.d. from a zero mean and unit variance distribution, and for any estimate \( \hat{D} \in D \), with overwhelming probability, we have that

\[
(2/k) \mathbb{E}[f_x^{(1)}(D)] \leq d(\hat{D}, D_0) \leq \frac{4}{k} \mathbb{E}[f_x^{(1)}(D)] - \frac{2}{k} \zeta(k - 1).
\]  

(11)

where \( \zeta_k := \max \{0, 1 - (k - 2)\mu(D) - 2\nu^2\} \).

Proof. Recall that \( x \) is sampled from distribution \( \mathbb{P}_k \) by first sampling its support at \( S \) from a uniform distribution of all possible supports with \( k \) elements, followed by sampling the non-zeros of its representation given the support, \( \gamma_S \sim \mathbb{P}_k \). These non-zero entries are sampled i.i.d. from a distribution with mean zero and variance of 1. The sample is finally constructed as \( x = D_0 \gamma_S \).

Upper bound Let us first show the upper bound. Let \( S = \text{supp}(\gamma) \). Then,

\[
f_x^{(1)}(\hat{D}) = \inf_{\alpha: \|\alpha\|_1 = 1} \frac{1}{2} \|x - \hat{D}\alpha\|_2^2
\]

(12)

\[
= \min \min_j \frac{1}{2} \|D_S \gamma_S - \hat{D}_j \alpha_j\|_2^2
\]

(13)

\[
= \frac{1}{2}\|D_S \gamma_S - \hat{D}_j^T D_S \gamma_S\|_2^2,
\]

(14)

where the last inequality follows by solving for the optimal \( \alpha_j^* = \hat{D}_j^T x \), and \( j^* \) denotes the optimal choice of the atom index, given by (recall atoms are normalized)

\[
j^* = \arg \min_j \|x - \hat{D}_j \alpha_j^*\|_2^2 = \arg \max_j |\langle D_S \gamma_S, \hat{D}_j \rangle|.
\]

(15)

See [Elad, 2010, Section 3.1] for a more detailed derivation. Let us denote by \( D_i \) the closest atom to \( \hat{D}_j \) in \( S \); i.e. \( i = \arg \min_{k \in S} \min_{\epsilon \in \{+1,-1\}} \|D_k - \epsilon \hat{D}_j\|_2 \). Then, expand the expression above as follows

\[
2f_x^{(1)}(\hat{D}) = \|D_i \gamma_i + D_{S\setminus i} \gamma_{S\setminus i} - \hat{D}_j \hat{D}_j^T (D_i \gamma_i + D_{S\setminus i} \gamma_{S\setminus i})\|_2^2
\]

(16)

\[
= \|\langle D_i - \hat{D}_j, \hat{D}_j^T D_i\rangle \gamma_i + \langle I - \hat{D}_j, \hat{D}_j^T D_{S\setminus i} \rangle \gamma_{S\setminus i}\|_2^2
\]

(17)

\[
= \|\langle D_i - \hat{D}_j, \hat{D}_j^T D_i\rangle \gamma_i\|_2^2 + \|\langle I - \hat{D}_j, \hat{D}_j^T D_{S\setminus i} \rangle \gamma_{S\setminus i}\|_2^2 + \ldots
\]

(18)

\[
= 2\langle D_i - \hat{D}_j, \hat{D}_j^T D_i\rangle \gamma_i + \langle I - \hat{D}_j, \hat{D}_j^T D_{S\setminus i}\rangle \gamma_{S\setminus i}\}
\]

(19)

\[
= A_i + B_i + C_i.
\]

(20)

Let us now analyze \( \mathbb{E}_{x \sim p}[2f_x^{(1)}(\hat{D})] = \mathbb{E}_{x \sim p}[A_i] + \mathbb{E}_{x \sim p}[B_i] + \mathbb{E}_{x \sim p}[C_i] \).

Consider first

\[
\mathbb{E}_{x \sim p}[A_i] = \mathbb{E}_{x \sim p}[\|\langle D_i - \hat{D}_j, \hat{D}_j^T D_i\rangle \gamma_i\|_2^2]
\]

(21)

\[
= \mathbb{E}_S \mathbb{E}_{\gamma_S}[\|D_i - \hat{D}_j \cdot (\hat{D}_j^T D_i)\|_2^2]\mathbb{1}_{\gamma_S}
\]

(22)

\[
= \mathbb{E}_S \|D_i - \hat{D}_j \cdot (\hat{D}_j^T D_i)\|_2^2
\]

(23)

\[
= \frac{k}{p} \sum_{i=1}^p \|D_i - \rho_i \hat{D}_j \|_2^2,
\]

(24)
where we used the fact that $E[\gamma_i^2] = 1$ and we defined $\rho_i := \hat{D}_j^T D_i$.

Looking at the third term,

$$
\frac{1}{2} \mathbb{E}_{x \sim p} \left[ C_i \right] = \mathbb{E}_{x \sim p} \left[ \langle (D_i - \hat{D}_j, \hat{D}_j^T D_i) \gamma_i, (I - \hat{D}_j, \hat{D}_j^T) D_{S \setminus \gamma_{S \setminus i}} \rangle \right] = \mathbb{E}_{x \sim P} \left[ \left( (D_i - \rho_i \hat{D}_j, \gamma_i), (I - \hat{D}_j, \hat{D}_j^T) D_{S \setminus \gamma_{S \setminus i}} \right) \right] = \mathbb{E}_{x \sim P} \left[ \sum_{q \in S \setminus i} \mathbb{E}_{\gamma_i} \left[ \langle (D_i - \rho_i \hat{D}_j, \gamma_i), (I - \hat{D}_j, \hat{D}_j^T) D_q \gamma_q \rangle \right] \right] = 0
$$

because $E[\gamma_i \gamma_q] = E[\gamma_i] E[\gamma_q] = 0$, since the variables are independent and of zero mean. Thus, so far we have that

$$
E_{x \sim p} \left[ f_i^{[1]}(\hat{D}) \right] = \frac{k}{2p} \sum_{i=1}^p \|D_i - \rho_i \hat{D}_j\|^2 + \frac{1}{2} \mathbb{E}_{x \sim p} \left[ B_i \right].
$$

First, note that $E_{x \sim p} \left[ B_i \right] > 0$. Consider a tighter lower bound as follows

$$
E_{x \sim p} \left[ B_i \right] = \mathbb{E}_{x \sim p} \left[ \| (I - \hat{D}_j, \hat{D}_j^T) D_{S \setminus \gamma_{S \setminus i}} \|_2 \right] \geq \mathbb{E}_{x \sim p} \left[ \| D_{S \setminus \gamma_{S \setminus i}} \|_2 + \| \hat{D}_j, \hat{D}_j^T D_{S \setminus \gamma_{S \setminus i}} \|_2 - 2 \mathbb{E}_{x \sim p} \left[ D_{S \setminus \gamma_{S \setminus i}} \right] \right] \geq \mathbb{E}_{x \sim p} \left[ \| D_{S \setminus \gamma_{S \setminus i}} \|_2 - 2 \mathbb{E}_{x \sim p} \left[ \sum_{k \in S \setminus i} \hat{D}_j^T D_k \right] \right] \geq \mathbb{E}_{x \sim p} \left[ \| D_{S \setminus \gamma_{S \setminus i}} \|_2 - 2 \mathbb{E}_{x \sim p} \left[ \sum_{k \in S \setminus i} \gamma_k \right] \right] \geq \mathbb{E}_{x \sim p} \left[ \| D_{S \setminus \gamma_{S \setminus i}} \|_2 - 2 \max_{k \in S \setminus i} \| \hat{D}_j^T D_k \|_2 \right] \geq \mathbb{E}_{x \sim p} \left[ \| D_{S \setminus \gamma_{S \setminus i}} \|_2 - 2 \nu^2 (k - 1) \right]
$$

where we used the fact that $\mathbb{E}_{x \sim p} \left[ \left( \sum_{k \in S \setminus i} \gamma_k \right)^2 \right] = k - 1$ since the variables are independent and have variance of 1. Additionally, we defined $\nu = \max_{x \in p} \max_{k \in S \setminus i} \| \hat{D}_j^T D_k \|$, with $i^* = \arg \max_{x \in p} \| \hat{D}_j^T D_k \|$. In other words, $i^*$ denotes the nearest neighbor in $\mathcal{D}$ for every $\hat{D}_j$. Continuing from above,

$$
E_{x \sim p} \left[ B_i \right] \geq \mathbb{E}_{x \sim p} \left[ \| D_{S \setminus \gamma_{S \setminus i}} \|_2 - 2 \nu^2 (k - 1) \right] \geq \mathbb{E}_{x \sim p} \left[ (1 - \delta_{k-1}) \| \gamma_{S \setminus i} \|_2^2 - 2 \nu^2 (k - 1) \right] \geq (1 - (k - 2) \mu(D))(k - 1) - 2 \nu^2 (k - 1) = \max \{ 1 - (k - 2) \mu(D) - 2 \nu^2 \} \geq 0
$$

where $\delta_{k-1}$ is the $(k - 1)$-RIP constant of $\mathcal{D}$, and we then used the bound with the mutual coherence $\delta_k \leq (k - 1) \mu(D)$. In the last line, we added the condition that $E_{x \sim p} \left[ B_i \right] \geq 0$. 

13
Thus, defining \( \zeta_k := \max \{0, [1 - (k - 2)\mu(D) - 2\nu^2]\} \), we can write

\[
\mathbb{E}_{x \sim \mathcal{P}}[f^{[1]}(\hat{D})] \geq \frac{k}{2p} \sum_{i=1}^{p} \|D_i - \rho_i \hat{D}_{j^*}\|_2^2 + \frac{1}{2} [(1 - (k - 2)\mu(D) - 2\nu^2)](k - 1) \tag{43}
\]

\[
\geq \frac{k}{2p} \sum_{i=1}^{p} \|D_i - \rho_i \hat{D}_{j^*}\|_2^2 + \frac{1}{2} \zeta_k(k - 1). \tag{44}
\]

Finally, recalling the definition of \( \rho_i \) (and that the atoms have unit norm) note that

\[
\|D_i - (\hat{D}_{j^*})^T \hat{D}_{j^*}\|_2^2 \geq \frac{1}{2} \min(\|D_i - \hat{D}_{j^*}\|_2^2, \|D_i + \hat{D}_{j^*}\|_2^2) = \frac{1}{2} d(D_i, \hat{D}_{j^*})
\]

Recall that \( \hat{D}_i \) is the closest atom to \( \hat{D}_{j^*} \) out of those in the support \( S \), and their distance might be equal or larger to the closest atom in \( \hat{D} \) to \( D_i \); i.e.

\[
d(D_i, \hat{D}_{j^*}) \geq \min_j d(D_i, \hat{D}_j).
\]

Thus,

\[
- \frac{1}{p} \sum_{i=1}^{p} \min_j d(D_i, \hat{D}_j) = d(D, \hat{D}) = \frac{4}{k} \mathbb{E}_{x \sim \mathcal{P}}[f^{[1]}(\hat{D})] - \frac{2}{k} \zeta_k(k - 1). \tag{45}
\]

**Lower bound** Let us know focus on the lower bound for \( d(\hat{D}, D) \). For any \( S \), let \( \hat{D}_S \) contain the atoms from \( D \) that are closest to the ones in \( D_S \), i.e.,

\[
d(D_S(i), \hat{D}_S(i)) = d(D_S(i), \hat{D}_i), \forall i \leq k.
\]

Then,

\[
f^{[k]}_x(\hat{D}) = \inf_{\alpha : \|\alpha\|_2 = k} \frac{1}{2} \|x - \hat{D}\alpha\|_2^2
\]

\[
\leq \min_{\hat{D}_S} \frac{1}{2} \|D_S \gamma_S - \hat{D}_S \hat{\alpha}_S\|_2^2
\]

\[
= \frac{1}{2} \|D_S \gamma_S - \hat{D}_S(D_S^T \hat{D}_S)^{-1} \hat{D}_S^T \gamma_S\|_2^2
\]

which implies

\[
\mathbb{E}_{\gamma_S}[f^{[k]}_x(\hat{D})] = \frac{1}{2} \mathbb{E}_{\gamma_S}[\|D_S \gamma_S - \hat{D}_S(D_S^T \hat{D}_S)^{-1} \hat{D}_S^T \gamma_S\|_2^2]
\]

\[
= \frac{1}{2} \sum_{i=1}^{k} \|D_S(i) - \hat{D}_S(D_S^T \hat{D}_S)^{-1} \hat{D}_S^T D_S(i)\|_2^2
\]

\[
\leq \frac{1}{2} \sum_{i=1}^{k} \|D_S(i) - \hat{D}_S(i) \hat{D}_S(i)\|_2^2
\]

\[
\leq \frac{1}{2} \sum_{i=1}^{k} d(D_S(i), \hat{D}_S(i)) = \frac{1}{2} \sum_{i=1}^{k} d(D_S(i), D),
\]

where the first line utilizes the fact that each entry of \( \gamma_S \) is i.i.d. with variance 1, and the third line follows because \( \|D_S(i) - \hat{D}_S(D_S^T \hat{D}_S)^{-1} \hat{D}_S^T D_S(i)\|_2^2 \) is the projection residual of \( D_S(i) \) onto the subspace spanned by \( \hat{D}_S \), which smaller than the one onto a particular column of \( D_S \). The last line follows because

\[
\|a - aa^T b\|_2^2 = \|a\|^2 - (a^T b)^2 \leq \min \{\|a\|^2 - 2(a^T b) + \|b\|^2, \|a\|^2 + 2(a^T b) + \|b\|^2\} = d(a, b)
\]
for any unit norm vectors $a, b \in \mathbb{R}^d$. Thus, finally,

$$
\mathbb{E}[f_{x}^{[k]}(\hat{D})] = \mathbb{E}_S \left[ \mathbb{E}_{\gamma} \left[ f_{x}^{[k]}(\hat{D}) \right] \right] S
$$

$$
\leq \frac{1}{2} \mathbb{E}_S \left[ \sum_{i=1}^{k} d(D_{S(i)}, \hat{D}) \right]
$$

$$
= \frac{1}{2} \frac{(k-1)}{(k)} \sum_{i=1}^{p} d(D_i, \hat{D}) = \frac{1}{2} \frac{(p-1)^p}{(k-1)^{p-k}} \sum_{i=1}^{p} d(D_i, \hat{D}) = \frac{1}{2} \frac{k^p}{p} \sum_{i=1}^{p} d(D_i, \hat{D})
$$

$$
\leq \frac{k}{2} d(D, \hat{D}).
$$

\Box

B  Pruning Guarantees

Let $D_0 \in \mathbb{R}^{d \times p}$ and consider, without loss of generality, that $\hat{D} = [\hat{D}_0, A] \in \mathbb{R}^{d \times p'}$ with $\hat{D}_0 \in \mathbb{R}^{d \times m}$, with $m \leq p'$, such that $d(\hat{D}_0, D_0) \leq \epsilon$ for all $i \in \{1, \ldots, m\}$, and $d(A_i, D_0) > \epsilon$ for all $j \in \{1, \ldots, p' - m\}$. In other words, $D_0$ contains all those $m$ atoms that are $\epsilon$-close to those in $\hat{D}_0$, while $A$ contains those that are further away. Additionally, we require that each atom in $D_0$ has at least one $\epsilon$-neighbor in $\hat{D}_0$; i.e. $d(D_0^0, \hat{D}_0) \leq \epsilon$ for all $i \in \{1, \ldots, p\}$. We allow $m \geq p$ since the over-realized estimate $\hat{D}$ may naturally contain several atoms that close to a real one. Also suppose that both $D_0$ and $\hat{D}$ are column-wise normalized for simplicity. Let us denote by $\mu(D_0, A) = \max_{i,j} |\langle D_0^i, A_j \rangle|$ the mutual coherence between $D_0$ and $A$. With these definitions, we have the following result:

\textbf{Theorem 4.1.} 0 Let $x$ be a $k$-sparse signal under $D_0$, i.e., there exists $\gamma \in \mathbb{R}^p$ with $||\gamma||_0 \leq k$ such that $x = D_0 \gamma$. Then, $\arg \max_k |x^T d_i| \in [m]$ as long as

$$
k \leq \frac{1 - \frac{\epsilon}{2} + \sqrt{\epsilon} + \mu(D_0) }{\mu(D_0) + \sqrt{\epsilon} + \mu(D_0, A)}.
$$

\textbf{Proof of Theorem 4.1.} Without of loss generality, we assume that the entries of $\gamma$ are placed in the decreasing order of the values $|\gamma_i|$. Recall that we require each atom in $D_0$ has at least one $\epsilon$-neighbor in $\hat{D}_0$; i.e. $d(D_0^i, \hat{D}_0) \leq \epsilon$ for all $i \in \{1, \ldots, p\}$. For simplicity, we assume $d(D_0^i, \hat{D}_0) = ||D_0^i - \hat{D}_0|| \leq \epsilon$ for all $i \in \{1, \ldots, p\}$, i.e., the $i$-th column of $D_0$ (or $\hat{D}$) is $\epsilon$-close to the $i$-th atom of $D_0$.

To show the atom that has the largest correlation with $x$ must be within the first $m$ columns of $\hat{D}$, we need to find $i \in [m]$ such that

$$
|x^T D_0^i| > |x^T A_i|, \quad \forall \ell.
$$

Towards that goal, we choose $i = 1$ (as $|\gamma_1|$ is the largest sparse coefficient) to get

$$
|x^T D_0^0| = \sum_{i=1}^{k} |\gamma_i (D_0^i)^T \hat{D}_0^0| \geq (1 - \frac{\epsilon}{2}) |\gamma_1| - (\mu(D_0) + \sqrt{\epsilon}) \sum_{i=2}^{k} |\gamma_i|
$$

$$
\geq \left(1 - \frac{\epsilon}{2} - (k - 1)(\mu(D_0) + \sqrt{\epsilon}) \right) |\gamma_1|,
$$

where the first inequality follows because

$$
(D_0^0)^T \hat{D}_0^0 = 1 - \frac{1}{2} ||D_0^0 - \hat{D}_0^0||_2^2 \geq 1 - \frac{\epsilon}{2}
$$

and

$$
(D_0^0)^T \hat{D}_0^0 = (D_0^0)^T D_0^0 + (D_0^0)^T (\hat{D}_0^0 - D_0^0) \leq \mu(D_0) + ||D_0^0 - \hat{D}_0^0||_2 \leq \mu(D_0) + \sqrt{\epsilon}
$$

15
for all $2 \leq i \leq p$. On the other hand, we have

$$|x^\top A_\ell| = \left| \sum_{i=1}^{k} \gamma_i (D^i_0)^\top A_\ell \right| \leq \mu(D_0, A) \sum_{i=1}^{k} |\gamma_i| \leq k \mu(D_0, A) |\gamma_1| , \forall \ell,$$

which together with (48) and (46) gives (47), implying that the chosen element by the first step of OMP must correspond to the one that is close to the correct dictionary, $D_0$.

C Numerical Results

Figure 4: Risk and Dictionary error ($\log_{10}$ thereof, lower is better) of the estimate provided by traditional dictionary learning (i.e. $\hat{D} \in \mathcal{D}_p$) and that resulting from the proposed over-realized approach (i.e. $\hat{D} \in \mathcal{D}_p'$) followed by distillation to the original size, over a number of parameters (sparsity, dimension and redundancy). Algorithm: ODL+Lasso.
Figure 5: Risk and Dictionary error ($\log_{10}$ thereof, lower is better) of the estimate provided by traditional dictionary learning (i.e. $\hat{D} \in D_p$) and that resulting from the proposed over-realized approach (i.e. $\hat{D} \in D_p'$) followed by distillation to the original size, over a number of parameters (sparsity, dimension and redundancy). Algorithm: K-SVD.