Dictionaries for sparse representation and recovery of reflectances

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ABSTRACT

The surface reflectance function of many common materials varies slowly over the visible wavelength range. For this reason, linear models with a small number of bases (5-8) are frequently used for representation and estimation of these functions. In other signal representation and recovery applications, it has been recently demonstrated that dictionary based sparse representations can outperform linear model approaches. In this paper, we describe methods for building dictionaries for sparse estimation of reflectance functions. We describe a method for building dictionaries that account for the measurement system; in estimation applications these dictionaries outperform the ones designed for sparse representation without accounting for the measurement system. Sparse recovery methods typically outperform traditional linear methods by 20-40% (in terms of RMSE).

Keywords: Reflectance estimation, sparse recovery, dictionary learning

1. INTRODUCTION

Light incident on a surface can be absorbed, transmitted, or reflected. The complete interaction of light at the surface is difficult to predict from first principles and is a function of many variables. An important first-order approximation for imaging is to assume that objects reflect energy equally in all directions, and the reflectance is only a function of wavelength. In typical imaging applications, only the visible range of roughly [400,700] nm is considered.

In digital imaging applications, light scattered from surfaces is gathered by the lens and converted to an irradiance at the sensor surface, In color imaging analyses, the irradiance image, which is commonly referred to as a color signal, is often discretized by sampling the visible wavelength interval every 10 nm. The resulting length 31 vector has been found to well represent common illuminants and surface reflectances.[1] In fact, for illuminants other than fluorescent lights, it has been shown that the representative Munsell set of spectra[2] is adequately sampled in the visible range at every 20 nm.[3] The accuracy of such coarse sampling in color calculations reveals the slow modulation as a function of wavelength of natural irradiance signals.

If the spectral power distribution of the illuminant is known, reflectance functions can be estimated from data collected using a digital camera augmented by a small number of optical filters.[4] Because only a few sample measurements are available, the wavelength composition of the incident light is critically undersampled; hence, it is impossible to guarantee accurate estimation of the reflectance function. Despite this limitation, low dimensional capture devices perform well because of the statistical structure of the input signals. Reflectance functions tend to be smooth functions of wavelength, are bound between 0 and 1, and they fall within a small subset of all such possible functions.

Nearly all algorithms that estimate reflectance from a small number of color sensors are based on the recognition that there is a much higher likelihood of observing some wavelength functions than others. The most complete way to incorporate such knowledge is to use Bayesian methods.[5] A full description of the likelihood distributions required for optimal performance, however, may be beyond current understanding. A simpler and more practical approach is to summarize our knowledge of the likely wavelength functions by creating a low dimensional linear model of the wavelength functions and to choose our estimate from this linear subspace.[6,7] Purely linear methods are computationally efficient, but they fail to take advantage of a great deal of the regularity that is present in the original data. Another approach is to use an intermediate strategy between Bayesian and linear models, suggested by DiCarlo and Wandell.[8] They proposed a two-step estimation in which we combine a linear estimate with values in a look-up table. The table is designed by encoding the typical estimation

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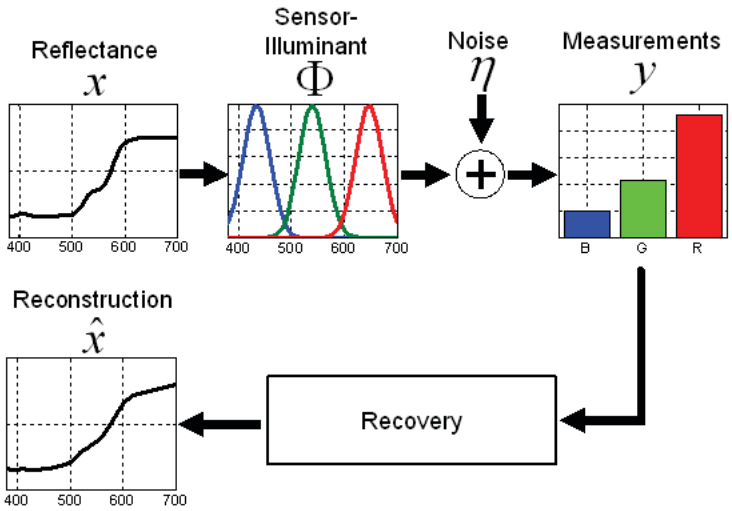

Figure 1. Overview of spectral recovery from color measurements. A surface reflectance is measured by three camera sensors. The illuminant is incorporated into the sensor spectral responsivities. Noise is added to produce the $k = 3$ measured values. The recovery process converts the k responses into an estimated reflectance function.

errors of the linear model for different parts of the sensor space. A summary of various estimation methods is reviewed elsewhere.[9]

Here, we evaluate a new approach based on sparse representations to estimate reflectances of objects from a small number of sensor measurements acquired under known illuminants. Sparse representations have been successful in various digital imaging applications, such as in compression[10] and denoising.[11,12] Here, we describe one method of sparse reflectance recovery. The proposed method extends our previous work on spectral representations and recovery.[13] We show that sparse methods outperform conventional linear methods used for estimating reflectances.

2. SPARSE RECOVERY OF REFLECTANCE FROM COLOR MEASUREMENTS

We analyze the problem of recovering a discretely sampled reflectance function, $x \in \mathbb{R}^n$, from a small number of sensor measurements, $y \in \mathbb{R}^k$. The relationship between the reflectance function and measurements is: $y = \Phi x + \eta$, where the rows of $\Phi \in \mathbb{R}^{k,n}$ combine the sensor filters and the illuminant. Measurement noise is represented by $\eta \in \mathbb{R}^k$. Figure 1 gives an an overview of the reflectance recovery problem.

The recovery method uses the assumption that the signal is well approximated by a sparse coefficient vector in a known fixed basis, or dictionary, given by the matrix $D \in \mathbb{R}^{n,n}$. We say a discrete signal, $\theta \in \mathbb{R}^n$, is sparse if $\|\theta\|_0 \leq m$ where m is small relative to n and $\|\cdot\|_0$ is the ℓ^0 pseudo-norm that counts the number of non-zero elements of the vector. We consider only dictionaries that are complete, but not overcomplete, bases of the space of sampled reflectance functions.

The reflectance estimate for sparse recovery is $\widehat{x} = D\widehat{\theta}$, where

$$\widehat{\theta} = \arg\min_{\theta} \|y - \Phi D\theta\|_2^2 + \tau\|\theta\|_1. \tag{1}$$

The minimization comprises two terms that are balanced by a regularization parameter, τ. The first term measures the difference between the observed and predicted measurements that are derived from the recovered reflectance, $D\widehat{\theta}$. The first term is not necessarily zero because the measurements contain noise. Minimizing the second term encourages sparsity of $\widehat{\theta}$.[14,15] In applications, the value of τ that produces the least error depends on measurement noise level and statistics of the data.

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3. BACKGROUND: DICTIONARIES FOR SPARSE REPRESENTATIONS

Since we estimate the recovered spectra using a sparse linear combination of vectors from a dictionary, the dictionary should be chosen to well represent the data. We define the sparse representation error of a dictionary as the average ℓ^2 error between a spectra and its best representation in the dictionary under a specific sparsity constraint on the coefficients: $\min_\theta E\left(\|x - D\theta\|_2\right)$ such that $\|\theta\|_0 \leq m$. Note that θ depends on x, and which coefficients are non-zero depends on the particular spectral vector that is being represented.

This problem of sparse representation is closely related to the design of a basis for compression of spectral signals. Note that there are no sensor measurements involved in this sparse representation problem in contrast with the sparse recovery method in Section 2. When performing sparse recovery, the average error of the resultant estimate is bounded below by the sparse representation error.

For some data sets such as images, predefined dictionaries such as the bases for the discrete cosine and wavelet transforms provide reasonable sparse representations. Although these standard dictionaries have the advantage of being computationally efficient, they perform poorly for reflectance data. In this case, dictionaries with superior performance can be learned from a representative training set. We now present and evaluate several algorithms for generating dictionaries to yield sparse representations of training data.

3.1 PCA

The most commonly used dictionary for representation of spectra is derived from Principal Components Analysis (PCA).[2,16] The PCA basis is orthonormal and has 'optimal energy compaction' in the sense that the first PCA vector is in the direction of maximum variance of the training data. The second PCA vector is orthogonal to the first and in the direction of maximum residual variance. When the PCA basis is used for sparse representations, the first few coefficients are generally non-zero for all encoded reflectances.

3.2 Dictionary Learning Algorithms

Algorithms designed specifically to learn a dictionary try to minimize the sparse representation error for a set of test data under a given sparsity constraint. These algorithms try to solve

$$\min_{D,\Theta} \|X - D\Theta\|_F^2 \text{ subject to } \|\theta_i\|_0 \leq m, \|d_i\|_2 = 1, \forall i, \tag{2}$$

where $X \in \mathbb{R}^{n,p}$ is the training data, $\Theta \in \mathbb{R}^{n,p}$ is a matrix of the sparse coefficients with ith column θ_i, and d_i is the ith column of D. Here we use the Frobenius norm given by $\|A\|_F = \sqrt{\sum_{i,j} |a_{ij}|^2}$. The unit length constraint on the dictionary vectors does not change the value of the minimization due to a possible scaling of Θ and D without any resultant change in the representations. This constraint is included so that the minimizers are unique.

Dictionary learning algorithms generally try to solve Problem (2) by repeatedly estimating solutions to the following two problems in succession.

$$\widehat{\Theta} = \arg\min_{\Theta} \|X - \widehat{D}\Theta\|_F^2 \text{ subject to } |\theta_i|_0 \leq m, \forall i \text{ for fixed } \widehat{D} \tag{3}$$

$$\widehat{D} = \arg\min_{D} \|X - D\widehat{\Theta}\|_F^2 \text{ for fixed } \widehat{\Theta}. \tag{4}$$

This formulation parallels the well-known K-means algorithm (also known as the generalized Lloyd algorithm) for vector quantization. Some of these dictionary learning algorithms can be viewed as generalizations of the K-means algorithm.[17,18]

Problem (3) seeks the optimal sparse representation of the training data in a known dictionary and is sometimes called the sparse approximation or sparse coding stage. This problem is NP-hard.[19] For most applications, finding the exact solution is not feasible so approximation algorithms are used to obtain an estimate. The Matching Pursuit (MP),[20] Orthogonal Matching Pursuit (OMP),[21] FOCal Underdetermined System Solver (FOCUSS),[22,23] and Basis Pursuit[15] algorithms are possible choices to find the sparse representation. Although

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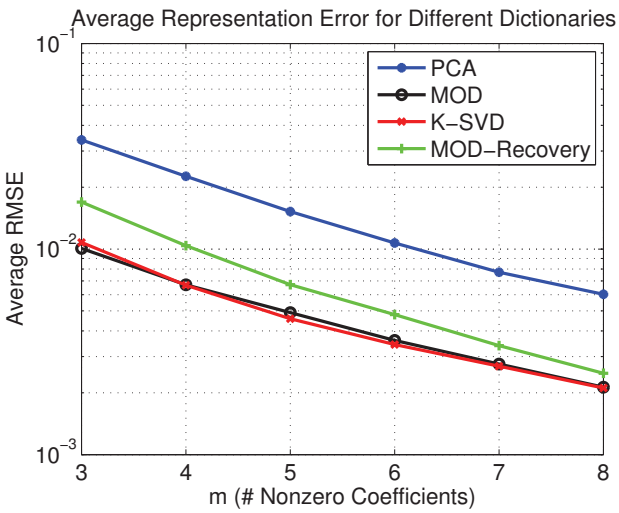

Figure 2. Average representation error over the test set of 100 reflectance spectra for optimal sparse representations using dictionaries from PCA, MOD, K-SVD, and MOD-Recovery algorithms.

dictionary learning algorithms may suggest a particular pursuit algorithm, any one can be used in nearly all dictionary learning algorithms.

Problem (4) is the dictionary learning stage and seeks the optimal dictionary given a sparse representation. Dictionary learning algorithms primarily differ only in how they solve this problem, hence these algorithms can be viewed as dictionary update methods. Note the dictionary found in Problem (4) is normalized so all of the columns have unit norm before being used in Problem (3).

The Maximum Likelihood (ML),[24] Method of Optimal Directions (MOD),[17,25,26] and FOCUSS-CNDL[27,28] algorithms approach dictionary learning in exactly this manner. The K-SVD[18,29] and Regularized Dictionary Learning (RDL)[30] algorithms employ this approach with a slightly different formulation when updating the dictionary. For the dictionary update, the K-SVD algorithm iterates through each vector in the dictionary, and while fixing the other dictionary vectors and coefficients, solves for the optimal dictionary vector and corresponding coefficients with the same support as the previous coefficient vector. The RDL algorithm incorporates the unit norm constraint into Problem (4) instead of enforcing it after solving for the dictionary.

Differentiating the right side of (4) with respect to D and setting it equal to 0 yields $(X - D\widehat{\Theta})\widehat{\Theta}^T = 0$. Assuming $\widehat{\Theta}\widehat{\Theta}^T$ is invertible, the solution is given by

$$D = X\widehat{\Theta}^+ = X\widehat{\Theta}^T(\widehat{\Theta}\widehat{\Theta}^T)^{-1} = \widetilde{R}_{X\widehat{\Theta}}\widetilde{R}^{-1}_{\widehat{\Theta}\widehat{\Theta}}, \tag{5}$$

where $\widehat{\Theta}^+$ is the pseudoinverse of $\widehat{\Theta}$, $\widetilde{R}_{X\widehat{\Theta}}$ is the estimated cross-correlation between X and $\widehat{\Theta}$, and $\widetilde{R}_{\widehat{\Theta}\widehat{\Theta}}$ is the estimated autocorrelation of $\widehat{\Theta}$. The MOD algorithm uses this for the dictionary update stage while the ML and FOCUSS-CNDL algorithms use gradient descent.

3.3 Representation Results

We trained dictionaries using each of the above methods. In each case, the training set was a collection of 450 measured reflectance spectra of common objects. These spectra were measured with a spectraradiometer and contain samples of common color test charts, skin, and other natural objects that were sampled every 10 nm between 380 nm and 700 nm to give length 33 vectors.[4] The MOD and K-SVD* algorithms were run for 500 iterations using OMP with four non-zero coefficients for the sparse representation stage and the dictionary initialized with data vectors.

*Software available at `http://www.cs.technion.ac.il/~elad/software/`.

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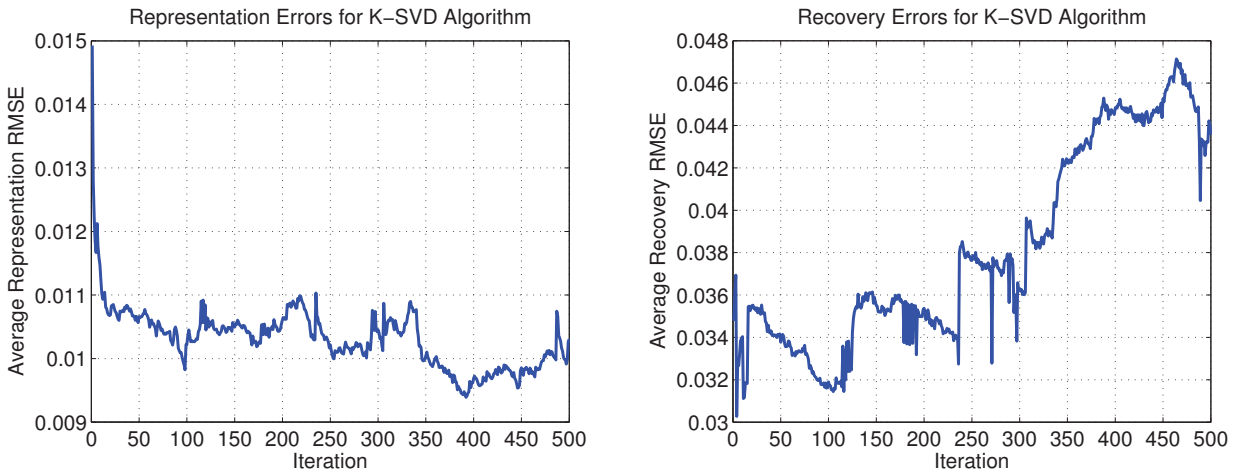

(a) (b)

Figure 3. Performance of dictionaries at each iteration of the K-SVD algorithm when used for (a) sparse representation of the training set and (b) sparse recovery of the test set. The sparse representations were found using OMP with at most four non-zero coefficients. The estimates from sparse recovery were derived from measurements using four equally spaced Gaussian filters and additive white Gaussian noise at SNR of 35 dB.

We evaluated the dictionaries by finding sparse representations for each vector in a test set of 100 spectra of similar objects and measured in the same manner as the training set. For each test vector and dictionary, the optimal representation using at most m non-zero coefficients was found by finding the optimal coefficient values for all possible selections of used dictionary vectors. Figure 2 shows the average representation error over the test set for dictionaries derived with the algorithms in this section and with the MOD-Recovery algorithm presented in the next section. We see that the MOD and K-SVD dictionaries have similar sparse representation performances while the PCA dictionary has significantly worse performance. For instance, using the MOD or K-SVD dictionaries with at most three non-zero coefficients has approximately the same representation quality as using the PCA dictionary with at most six non-zero coefficients.

4. DICTIONARY LEARNING FOR SPARSE RECOVERY

4.1 Description of Proposed Algorithms

How can we choose a dictionary for sparse recovery? One idea is to choose the dictionary that has the best sparse representation (Equation (2)). This dictionary imposes a lower bound on the sparse recovery error. However, this is not a good strategy. An optimal dictionary for representation may perform poorly when used for recovery. We illustrate the dissociation between optimizing for representation and recovery in Figure 3. The left panel shows that as the K-SVD algorithm progresses, new dictionaries are learned that tend to have a decreasing representation error. In contrast, the panel on the right shows that for these same dictionaries the sparse recovery error increases.

Hence, we select a dictionary designed specifically for recovery. The proposed dictionary for recovery will differ from the sparse representation dictionary because it depends on the measurement instrument. We seek a dictionary that minimizes the error between the test data and the prediction in Equation (1). Specifically we try to solve

$$\min_{D} \|X - D\widehat{\Theta}\|_F^2 \text{ where } \widehat{\theta}_i = \arg\min_{\theta_i} \|y_i - \Phi D\theta_i\|_2^2 + \tau\|\theta_i\|_1, \tag{6}$$

where $\widehat{\theta}_i$ is the ith column of $\widehat{\Theta}$ and $y_i = \Phi x_i$ are simulated noise-free measurements. We remove the measurement noise so the dictionary learning algorithm does not fit the noise. Paralleling the approach used in Sec. 3, we

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solve (6) by repeatedly solving the following problems

$$\widehat{\theta}_i = \arg\min_{\theta_i} \|y_i - \Phi\widehat{D}\theta_i\|_2^2 + \tau\|\theta_i\|_1 \text{ for fixed } \widehat{D} \tag{7}$$

$$\widehat{D} = \arg\min_{D} \|X - D\widehat{\Theta}\|_F^2 \text{ for fixed } \widehat{\Theta}. \tag{8}$$

As before, the vectors in the dictionary found in Problem (8) are normalized before being used in Problem (7).

Note that the sparse recovery problem, (7), relies on the training data only through the simulated instrument measurements; the sparse representation problem in Sec. 3 requires knowledge of the full spectral curves of the training data. The sparse recovery problem is equivalent to the intended use of the dictionary, recovery of a signal from measurements using Problem (1). If one prefers to use a different procedure for recovery, then that procedure should be used instead of Problem (7).

The dictionary update stage for sparse recovery in Problem (8) is identical to the dictionary update stage for sparse representation in Problem (4). We propose using the dictionary update methods described in Sec. 3. The modified algorithms for recovery that use (7) instead of (3) shall be denoted by adding `-Recovery` to the end of the algorithm name.

We now address an issue that rarely appears in the sparse representation algorithms but may occur frequently for certain applications of the recovery algorithms. In some cases, a vector in the dictionary is not used for the recovery of any element of the training set. When performing the dictionary update, this is problematic because the values of the unused dictionary vector are irrelevant when solving Problem (8), so we have no way of updating them. This issue occurs more frequently when the number of measurements is small compared to the number of atoms in the dictionary.

If a dictionary element is unused, the corresponding row of $\widehat{\Theta}$ is identically 0. To solve this problem, we propose removing the rows in $\widehat{\Theta}$ that are identically zero, which allows one to update the dictionary as before. The resulting dictionary contains too few vectors; we complete the dictionary by adding the leading vectors from the SVD of the residuals, $X - \widehat{D}\widehat{\Theta}$ where $\widehat{D}$ is the dictionary from the previous iteration. The added vectors represent the maximal variation of the residuals. The addition of these vectors yields better performance and convergence than introducing the data vectors that have the largest recovery error as suggested for the K-SVD.[18]

None of the dictionary learning algorithms discussed here guarantee a monotonic decrease in the objective function. The stopping rule must allow performance to degrade in hope of achieving a superior dictionary at

Algorithm 1 MOD-Recovery Algorithm

Input: Training data of representative reflectances, X; number of vectors in dictionary, r; set of possible values of τ; maximum number of iterations, N.

Output: Dictionary $\widehat{D}$

1: Initialize $\widehat{D}$ with r random vectors from X.
2: **for** iteration = 1 to N **do**
3: **Sparse recovery:**
   i. Solve Problem (7) for each value of τ.
   ii. Choose $\widehat{\Theta}$ as the estimate that yields the smallest average MSE, $\|X - \widehat{D}\widehat{\Theta}\|_F^2$.
4: **Dictionary update:**
   i. Let q be the number of rows of $\widehat{\Theta}$ that are identically zero. If $q \neq 0$, find the SVD decomposition $U\Sigma V = \left(X - \widehat{D}\widehat{\Theta}\right)$, and save the columns of U corresponding to the largest q singular values.
   ii. Remove the rows of $\widehat{\Theta}$ that are identically 0.
   iii. Form new dictionary, $\widehat{D}$, from the columns of $X\widehat{\Theta}^+$ and the q saved vectors.
   iv. Normalize the columns of $\widehat{D}$.
5: **end for**
6: **return** $\widehat{D}$ from the iteration that resulted in the smallest average MSE.

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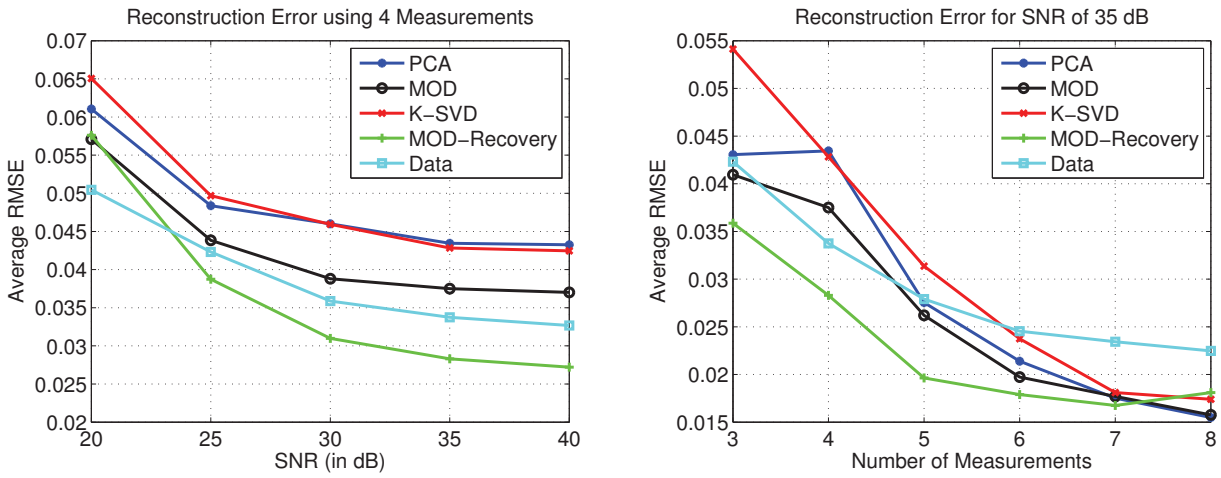

(a) (b)

Figure 4. Average RMSE for sparse recovery using different dictionaries for (a) various SNR levels using fixed measurement method containing four Gaussian filters and (b) various number of measurements from Gaussian filters for fixed SNR of 35 dB.

later iterations. Consequently, we choose the dictionary from the iteration with the smallest recovery error of the training data. This can yield significant improvement over choosing the dictionary found at the last iteration. For simplicity, we use a fixed number of iterations (500) as the stopping criterion.

In the analyses below, we extended the MOD algorithm (Algorithm 1) for the recovery application.[17,26] We chose the MOD algorithm for its simplicity and approximately equivalent sparse representation performance as the K-SVD algorithm.

4.2 Dictionary selection performance

We analyzed the algorithms using a simulated measurement instrument comprising various numbers of sensor-illuminant responsivities with Gaussian ($\sigma = 25$ nm) shapes; the sensor-illuminant function centers were evenly spaced over the range from 380 nm to 700 nm. The measurements were corrupted with additive normally distributed white noise at various levels.

The sparse recovery step in the MOD-Recovery algorithm requires searching over a set of values of τ to find a minimum error solution of Problem (7). We chose $\tau \in \{2\alpha\|\Phi^T y\|_\infty\}$ where $\alpha = 10^{-.25r}$ and r is an integer between 0 and 20, inclusive. We also use these values for τ when recovering each vector from the test set using Problem (1), and then choose the value of τ that gives the minimum average RMSE. Note this approach will give the optimal value of τ from the set of possible values, although this technique cannot be used in practice and heuristics must be employed. We solved Problems (1) and (7) using the Gradient Projection for Sparse Reconstruction (GPSR) algorithm.[31†] We used the GPSR-BB mode without debiasing for 25 iterations at each τ value. We employed continuation to solve for the series of values of τ starting with the largest and decreasing as recommended by the authors of the algorithm.[31] Continuation increases the speed and accuracy of the algorithm and is necessary to avoid algorithm failure for small values of τ.[32]

The sparse recovery performance under various conditions is summarized in Figure 4. We evaluated several dictionaries, different numbers of measurements, and a range of noise levels. For this application, the MOD-Recovery dictionaries have superior performance compared to those derived using the PCA, MOD, and K-SVD algorithms. The dictionary labeled `Data` was formed by randomly selecting 33 vectors from the training set, which yielded very impressive recovery performance considering its simplicity.

[†]Software available at `http://www.lx.it.pt/~mtf/GPSR/`.

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5. COMPARISONS OF SPARSE AND TRADITIONAL METHODS

We now compare sparse recovery using the best dictionary with two traditional methods for estimating spectra from color measurements, the Wiener filter and PCA subspace reconstruction. Noisy measurements for each of the 100 spectra in the test set were simulated, and reflectance signals were estimated using each of the recovery methods.

The Wiener filter is the linear shift-invariant filter that minimizes the mean squared error of the estimate under certain assumptions about the signal and noise.[33] The estimate using the Wiener filter, W, is

$$\widehat{x} = Wy = \widetilde{R}_{XX}\Phi^T(\Phi\widetilde{R}_{XX}\Phi^T + \widetilde{R}_{\eta\eta})^{-1}y, \tag{9}$$

where the estimated autocorrelation matrix $\widetilde{R}_{XX}$ is found from the training data and $\widetilde{R}_{\eta\eta} = \sigma_\eta^2 I$ where σ_η^2 is the noise variance and I is the identity matrix.

In PCA subspace reconstruction, the estimate's deviation from the data mean is restricted to a linear subspace spanned by the first few PCA vectors. The idea is that all reasonable reflectance functions lie very close to this set so restricting the reconstructions to this subspace imposes our a priori knowledge of the likely reflectance functions. The solution has the form

$$\widehat{x} = P\widehat{\theta} + \overline{x}, \tag{10}$$

where $\overline{x}$ is the mean reflectance function of the training data and P is a matrix whose columns are the first few principal components. The solution minimizes the estimation error between the measurements and the predicted measurements of the reflectance estimate, $\|\Phi\widehat{x} - y\|_2^2$. If the number of PCA terms exceeds the number of measurements in y, multiple solutions exist. In this case, we choose the coefficient vector, θ, with the smallest

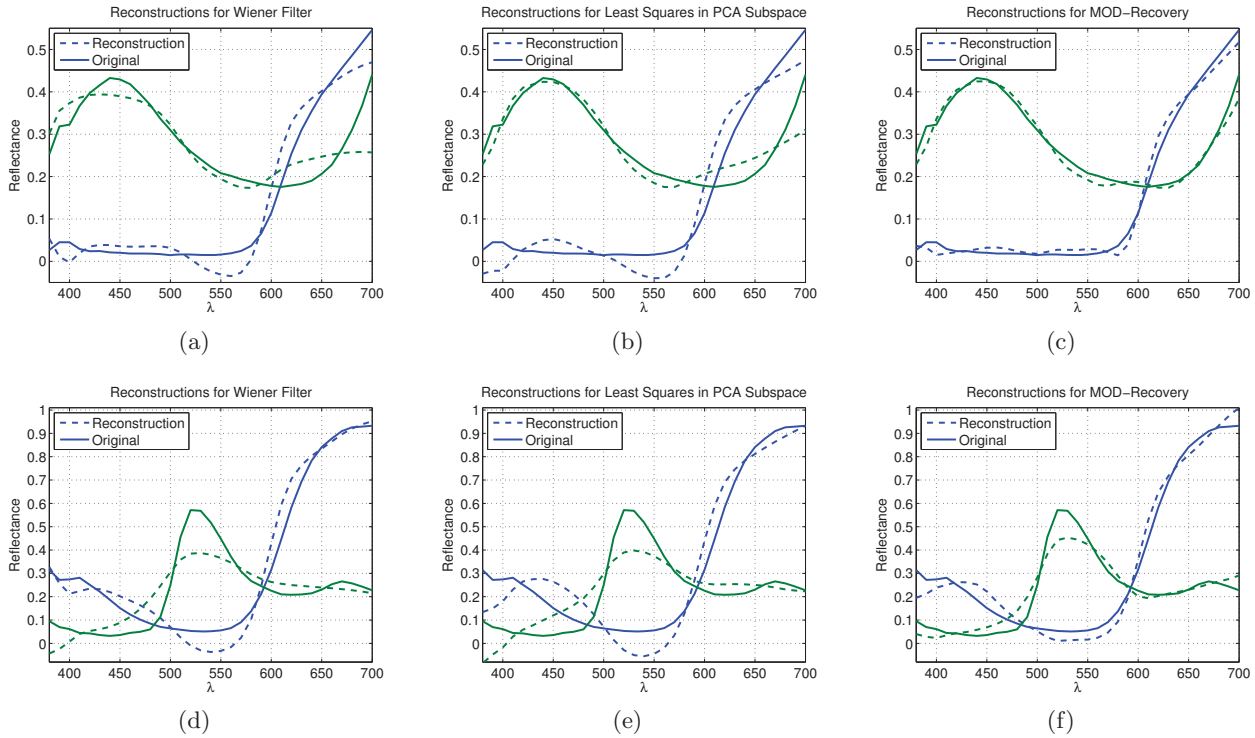

Figure 5. Each plot contains two spectra and reconstructions from four measurements with Gaussian sesnsor-illuminant filters at SNR of 35 dB. Spectra were chosen from the test set based on their reconstruction error for MOD-Recovery. Spectra were chosen in two groups. Panels (a-c) have typical reconstructions (50% of the test set had higher error). Panels (d-f) have poor reconstructions (only 10% of the test set had higher error).

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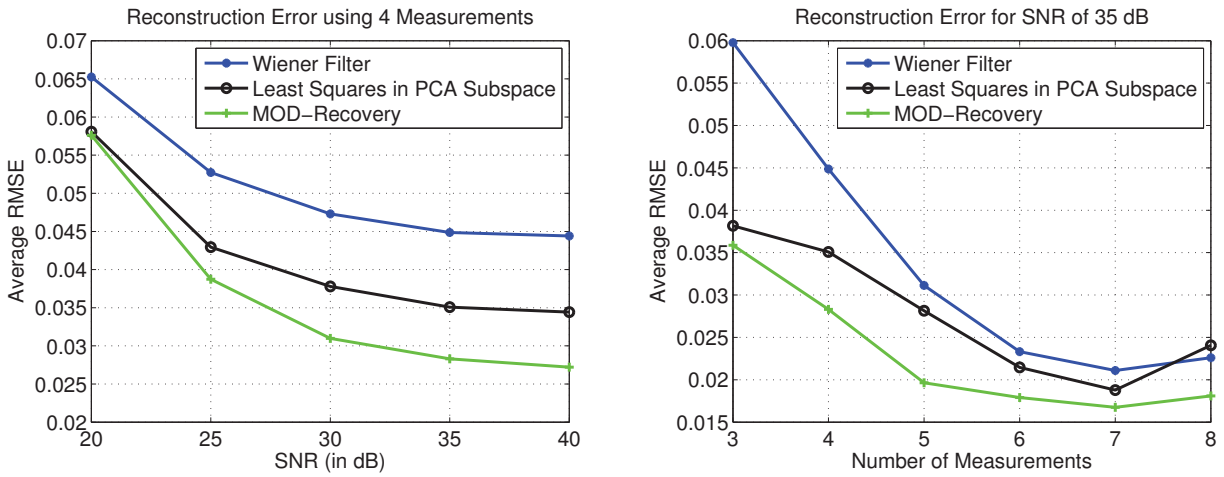

(a) (b)

Figure 6. Reconstruction error for different recovery methods vs (a) SNR for 4 Gaussian filters and (b) number of Gaussian filters for SNR of 35 dB.

ℓ^2 norm. The solution is found using the pseudo-inverse[9]

$$\widehat{\theta} = (\Phi P)^{+}(y - \Phi\overline{x}). \tag{11}$$

The optimal number of PCA vectors to include in the subspace depends on both the number of measurements and the noise level. For example, if more measurements with a higher SNR are available, one can make a better estimate by using more PCA components. We chose 8 PCA components for all of the presented results because this generated the best overall performance.

Figure 5 shows spectra and their reconstructions using the Wiener filter (left column), PCA subspace (middle), and sparse recovery using the MOD-Recovery dictionary (right). The panels compare typical and poor sparse recovery examples with the estimates from traditional methods.

Figure 6 compares the three recovery methods averaged over the entire test set. The separate curves and panels illustrate results using various numbers of measurements and noise levels. The proposed method with the MOD-Recovery dictionary outperforms the Wiener filter and PCA subspace reconstruction. The RMSE improvement is on the order of 20% to 40%.

6. CONCLUSIONS

We developed a method for estimating reflectance functions from a small number of color measurements using sparse methods. We adjusted existing algorithms designed for representation to learn dictionaries for recovery. Recovery-based dictionaries offer superior performance compared to representation-based dictionaries. The sparse recovery method combined with our dictionaries offers superior reconstruction compared to traditional methods (Wiener filter and PCA reconstruction). However, the sparse recovery method is significantly more computationally intensive than these approaches.

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