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Quantized nonnegative matrix factorization

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Quantized Nonnegative Matrix Factorization

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Abstract—Even though Nonnegative Matrix Factorization (NMF) in its original form performs rank reduction and signal compaction implicitly, it does not explicitly consider storage or transmission constraints. We propose a Frobenius-norm Quantized Nonnegative Matrix Factorization algorithm that is 1) almost as precise as traditional NMF for decomposition ranks of interest (with in 1-4dB), 2) admits to practical encoding techniques by learning a factorization which is simpler than NMF’s (by a factor of 20-70) and 3) exhibits a complexity which is comparable with state-of-the-art NMF methods. These properties are achieved by considering the quantization residual via an outer quantization optimization step, in an extended NMF iteration, namely QNMF. This approach comes in two forms: QNMF with 1) quasi-fixed and 2) adaptive quantization levels. Quantized NMF considers element-wise quantization constraints in the learning algorithm to eliminate defects due to post factorization quantization. We demonstrate significant reduction in the cardinality of the factor signal values set for comparable Signal-to-Noise-Ratios in a matrix decomposition task.

Index Terms—low rank; nmf; quantization;

I. INTRODUCTION

Nonnegative Matrix Factorization (NMF) is a fundamental tool in Signal Processing and Machine Learning, which is used for portfolio optimization [1] and Blind Source Separation [2], [3], [4]. The appeal of NMF is that it learns an adaptive basis (set of vectors) and sparse coefficients: NMF represents an input stimulus ensemble as a linear combination of elements from a representative set of learned NMF basis functions.

Given the matrix \( V \), NMF decomposes \( V \) into the product of two matrices, \( W \in \mathbb{R}^{M \times R} \) and \( H \in \mathbb{R}^{R \times N} \). All matrices have exclusively nonnegative elements, \( M > R, N > R \). NMF-Frobenius’ objective is the squared-\( \ell_2 \) norm:

\[
f(V\|WH) = \frac{1}{2} \sum_{m,n} |V_{m,n} - (WH)_{m,n}|^2. \tag{1}
\]

A suitable step-size parameter, proposed by Lee and Seung in [5], results in two alternating, multiplicative, gradient descent updating algorithms:

\[
W \leftarrow W \odot VH^T \odot WHH^T, \tag{2}
\]

\[
H \leftarrow H \odot W^T V \odot W^T WH \tag{3}
\]

where \( \odot \) represents element-wise multiplication, and \( \odot \) is element-wise division. The NMF solution is generally not unique [6], [7], or exact. For every invertible \( A \) we have a potential factorization [8], [9],

\[
V \approx (WA)(A^{-1}H). \tag{4}
\]

In recent work, [7] the authors solved the uniqueness problem, and addressed the inexactness of NMF, by introducing the idea that rank-1 NMF approximations are closures. Using this restriction, the solution space was constrained to the extent that the approximation could be replaced by equality in (Eqn. 4). The Nonnegative Matrix Approximation (NMA) in (Eqn. 4), described by Lee and Seung in [5] is used in many applications. Typically any member of the set of NMA’s that meets an arbitrary accuracy constraint suffices: this apparent freedom motivates the present contribution, namely QNMF, which produces factors which have a small set of possible entry values, and are thus amenable to efficient storage (via a supplementary compression process).

Definition 1: A valid NMF solution is a pair of matrices \( \{W, H\} \) which are element-wise nonnegative \( W_{m,r} \geq 0, H_{r,n} \geq 0 \), that satisfy the accuracy condition \( ||V - WH||^2 \leq \eta \), where \( \eta \in \mathbb{R} \) is an arbitrary small positive number. The set of valid NMFs is denoted

\[
S = \{\{W, H\} | ||V - WH||^2 \leq \eta\}. \tag{5}
\]

We consider the problem of transmission and storage of the approximation in (Eqn. 4). We use additional criteria to select members of \( S \) with appropriate properties —here the crucial property is that the factors are element-wise integer and that this set of integers has low cardinality.

We consider the factorization-quantization-reconstruction scenario described in Fig.1. Our hypothesis is that traditional NMF may yield an inefficient representation for transmission. The inputs matrix \( V \in \mathbb{R}^{M \times N} \) is factorized-quantized into the product of two integer matrices \( W' \in \mathbb{Z}^{M \times R} \) and \( H' \in \mathbb{Z}^{R \times N} \) and two quantization step-size (scalars or) vectors, \( \Delta W \) and \( \Delta H \).

\[
Q \rightarrow W' \mapsto W, H' \mapsto H, \text{Recons.} \rightarrow V
\]

Fig. 1. QNMF reconstruction: The input matrix \( V \) is real valued and factorized into two real-valued factors \( W', H \) in the NMF block. The NMF factors are then quantized using either fixed step-size quantization or adaptive stepsize quantization producing integer valued factors \( W \in \mathbb{Z}^{M \times R}, H \in \mathbb{Z}^{R \times N} \). Adaptive quantization optimization is denoted by the double ended arrows from the step-size to the NMF optimization routine. The resulting factorization has the same dimensions as \( V \) but it is integer valued, \( V' \in \mathbb{Z}^{M \times N} \).
The operation, \( \text{diag} \), constructs a square matrix with the vector \( x \)'s elements on the diagonal. The factors produced by an inner NMF \( \hat{W} \in \mathbb{R}^{M \times R}, \hat{H} \in \mathbb{R}^{R \times N} \) (for example à la Lee and Seung in [5]) are scalar, or element-wise quantized –quantized by a quantizer which acts separately on each component of \( \hat{W} \) and \( \hat{H} \) as part of the learning routine.

Definition 2: A Quantized NMF solution is a member of the set \( S_\eta \)

\[
S_\eta = \{ (\hat{W}, \hat{H}) | ||V - \hat{W}\text{diag}\Delta_w\text{diag}\Delta_h\hat{H}||^2 \leq \eta \}.
\]

The crucial observation in this paper, is that if quantization error minimization is alternated with factorization updates, we can learn members of the set \( S_\eta \) which are as accurate as element-wise-continuous-valued NMF.

We have introduced the QNMF mixing model. In § II we motivate NMF in light of related quantized expansions. We examine the effects of quantization on NMF in § III. We contribute a family of QNMF algorithms in § IV. We perform a numerical evaluation of QNMF in § V and discuss future research directions in § VI.

II. RELATED WORK

The requirement for QNMF arises when many measurements can be taken at a sensing location but only a low-rank approximation is required at a receiver/decision making entity or storage entity. For example, the authors of [10] consider the Matrix Completion problem: they recover and classify Wireless Sensor Network data while minimizing the number of samples that is acquired, processed, and transmitted. In essence a low rank matrix is recovered from a small number of randomly sampled entries. However, quantization is not considered in the learning algorithm. More generally, scaling the algorithms [1], [2], [3], [4] to large scale data may be problematic; what is required is a good quality low-rank compressible approximation. How can we best estimate \( V \) from \( \hat{W} \) and \( \hat{H} \) in these situations? How does the quality of the \( \hat{V} \) depend on the properties of \( \hat{W}, \hat{H}, \Delta_w, \text{and} \Delta_h \)? These fundamental questions are addressed here for the first time by introducing QNMF. The effects of QNMF with respect to the appropriate perceptual quality measure in these domains is deferred to future work. Other potential applications for QNMF include matrix decomposition/missing data estimation in wireless sensor networks [11].

Entropy-based distortion measures and bit allocations for compression are often based on the mean-squared error [12], [13], [14]. This motivates our selection of the Frobenius-norm for QNMF. Our goal is to learn the parameters \( \{ \hat{W}, \hat{H}, \Delta_w, \Delta_h \} \) so that the reconstruction error \( f = ||V - \hat{V}||^2 \) is minimized. The properties of an NMF in the presence of coefficient quantization have not been explored. We contribute algorithms to learn NMF of this form by considering quantization as part of the alternating minimizing low-rank factorization. The effects of coefficient quantization on representations in \( \mathbb{R}^N \) using overcomplete sets of vectors are investigated in [14]. We empirically investigate the distortion as a function of the rank parameter \( R \) and the cardinality of the set of values the factorization takes (which we call “simplicity”). This is the first paper that examines the effects of quantization on a nonnegative matrix factorization. If NMF is to scale to big data analysis, efficient storage of the factors is one problem that must be addressed. Uniform quantization is selected in this paper because the authors of [15] demonstrate that it has an output entropy which is asymptotically smaller than that of any other quantizer, independent of the density function or the error criterion. An excellent quantization survey is found in [16]. Finally, given that NMF learns basis functions with different scales, we introduce a step-size parameter for each column (row) of \( \hat{W} (\hat{H}) \) to improve its simplicity.

We introduce some notation. \( U(0, 1) \) is used to represent a uniform distribution from the domain \((0, 1)\). \( U_{NM} \) represents a matrix of size \( M \times N \) –each element is independently drawn from \( U(0, 1) \). The subscript is frequently omitted. A vector of \( R \) ones is denoted by \( \mathbf{1}_R \).

III. QUANTIZED NMF FRAMEWORK

We propose a Quantized Nonnegative Matrix Factorization algorithm that is 1) almost as precise as traditional NMF, 2) admits to practical encoding techniques 3) and exhibits a complexity which is comparable with state-of-the-art NMF methods in § IV. These properties are achieved by considering the quantization residual, via an outer quantization optimization step, in an extended NMF iteration. The use of the quantized activations, for example, in the optimization of the W-update reduces the propagation of the quantization error to subsequent NMF iterations. We consider the effects of quantization on NMF here.

<table>
<thead>
<tr>
<th>QNMF Algorithm and its Acronym</th>
<th>QNMF</th>
<th>Acronym</th>
<th>Quantizer</th>
<th>Adaptive</th>
</tr>
</thead>
<tbody>
<tr>
<td>Round random</td>
<td>roundrand</td>
<td>round or round</td>
<td>x</td>
<td></td>
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<tr>
<td>Floor random</td>
<td>floorrand</td>
<td>[ ] or [ ]</td>
<td>x</td>
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<tr>
<td>Round random Adaptive</td>
<td>roundadapt</td>
<td>[ ] or [ ]</td>
<td>✓</td>
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<tr>
<td>Floor random Adaptive</td>
<td>flooradapt</td>
<td>round or round</td>
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</table>

QNMF Framework: Table ?? describes the quantized NMF framework underpinning the results in this paper. It is composed of an inner NMF optimization routine (consisting of an unshaded row for the h-update and the w-update) in lines 5 and 8, which is wrapped by an outer quantization updating routine (the shaded rows in Table ??) in lines 6, 7, 9, 10 and 12. The algorithm presented in Table ?? is simple: 1) the quantization steps are randomly initialized (less than one), and 2) the quantization steps are fixed for the entire NMF iteration. These short-comings conspire to produce a factorization algorithm which may not converge monotonically –we provide two enhancements which improve convergence in § IV. First we motivate these algorithms by examining quantization error.
Classical Statistical Analysis: To understand why monotonicity is an issue, we consider the effects of the outer routine on the inner routine. A first step is to consider the affect of reconstructing a vector \( v = V_{:,n} \) when the corresponding activation vector estimate \( h = H_{:,n} \) has been degraded in some unspecified way. Lines 5-7 in Table ?? provide an example of the introduction of quantization error. Our analysis provides an understanding of the effects of the outer quantization routine where degradation due to quantization is modelled as additive white noise. After each inner NMF h-update (line 5) we have

\[
v = Wh + E,
\]

where the functions \( W \) are assumed fixed and \( E \) captures element-wise Gaussian noise in the estimate. Suppose we want \( \beta \) to approximate element-wise Gaussian noise in the estimate. Suppose we want where the functions \( W \) are modelled as additive white noise. After each inner NMF h-update (line 5) we have

\[
\beta \approx v - Wh - W_\beta + E = -W_\beta.
\]

However, the appeal of NMF is that the objective function

\[
f(h) = \arg \min_h ||v - Wh||^2
\]

is monotonically decreased by application of the \( W \) or \( H \) update. Perturbation \( \beta \) caused by quantization may cause the objective to be increased. In short, if \( h^{t+1} \) minimizes \( f(\cdot) \), then \( f(h^{t+1}) \leq f(h^t) \), but then if application of quantization reverses this ordering,

\[
f(Q(h^{t+1})) \leq f(h^t) \quad \text{or} \quad f(Q(h^{t+1})) > f(h^t),
\]

NMF loses its appealing monotonic convergence property. We consider a number of strategies for addressing the problem of quantizing \( H \) and \( W \) such that \( f(h) \) and \( f(w) \) are minimized. The quantization functions in this paper are uniform mid-tread [16].

IV. MONOTONICALLY DECREASING QNMF

We introduce 1) random-quasi fixed ‘floorrand’ and ‘roundrand’ QNMFs and 2) adaptive QNMFs, namely ‘flooradapt’ and ‘roundadapt’ QNMF (cf. Table. I), for the framework in Table. ?? This constitutes replacing lines 1,2,6,9 and 12 in Table. ?? with a new outer optimization routine.

Random Quasi-Fixed Quantizer: A probabilistic method for finding the quantization functions that minimize the objective, \( f \), after each NMF update has been applied (in Table. ??) is presented in Table II. This approach is more efficient than exhaustive enumeration of the quantization functions provided that the goal is merely to find an acceptable solution in a fixed amount of time, rather than the best possible solution. This is compatible with the goal of monotonic convergence of NMF. Consider, there are \( 2^{RN} \) and \( 2^MR \) possible quantization functions for \( H \) and \( W \).

Table II summarizes the approach for random quasi-fixed ‘floorrand’ quantization of the \( H \) matrix—a similar technique is applied to the \( W \) matrix, but omitted for brevity. We first investigate if a floored quantizer, applied to each element of \( H \), minimizes \( f \) after the NMF \( H \)-update has been applied. If minimization is achieved quantization is applied and QNMF proceeds. If the objective is not minimized by the floored quantization functions we perform Bernoulli trials to generate a new array of random scalar quantizers where the floor and ceil functions are chosen randomly for each element of the quantization function. The probability of choosing a ‘floor’ is...
p; decreasing this probability increases the probability of introducing a ceil element in the quantization function. Our goal is to slowly migrate away from the original floored quantization function until a suitable quantizer is found. Multiple Bernoulli trials (≈ 100) are used to generate quantization functions with the probability of a floor for each equal to p. If after many random candidate quantization functions have been applied, the objective is not minimized for a fixed quantization step size, ∆h, the step-size is divided by two and the process is repeated with the smaller step-size. ‘floorrand’ QNMF is described as follows: Lines 6, 7, 9 and 10 in Table II are augmented to include the generation of the new ‘floorrand’ quantizer in Table II. random quantization is invoked independently for the matrices HH and WW. Once the new step-sizes are generated, they are maintained for the remainder of the optimization unless they are further decreased.

Empirical evidence suggests that fixing p = 0.5 and s = 0 for the duration of this simulation provides acceptable convergence (cf. the discussion in § V). ‘roundrand’ quasi-fixed QNMF operates in a similar manner: the floor function in Line 6 in Table II is replaced by the round function. If line 6 uses a round down quantizer in the previous Bernoulli trial, line 7 uses a round-up quantizer with probability p.

Adaptive Quantizer: The quantization step-sizes in the randomized algorithms ‘floorrand’ and ‘roundrand’ QNMF are quasi-fixed –they are only changed if the Bernoulli randomization routine fails to find a valid solution after exhausting all p. We derive new update rules for the step-size parameters for adaptive QNMF using the Frobenius-norm.

\[ \|V - \hat{W} \text{diag} \Delta_w \text{diag} \Delta_h \hat{H}\|^2 \] (14)

is non-increasing under the updates rules for the step-size

\[ \Delta_{H,r} \leftarrow \Delta_{H,r} - \frac{(W^T V \odot \hat{H})_1}{(W^T \text{diag} \Delta_h \hat{H})_1} \] (15)

\[ \Delta_{W,r} \leftarrow \Delta_{W,r} - \frac{(W V W^T \odot \hat{W})}{(W \text{diag} \Delta_h \hat{H}^T \odot \hat{W})} \] (16)

Table III lists the ordering of the adaptive QNMF algorithm. Although these updates are guaranteed to monotonically decrease the objective, the quantization step after the initial NMF H and W updates may introduce an error which is larger than the minimization improvement achieved by applying the updates above, and also by NMF. The aggregate effect of quantization and step-size optimization may cause the objective to increase after the application of these operations. We have observed that in practice adaptive QNMF typically converges (for s = 0 and fixed). Put simply, if a sufficient number of quantization levels have been assigned to the algorithm QNMF reduces to the original Lee and Seung NMF. In future work we will analyze the relationship between the quantization error and expected error reduction due to the application of an NMF.

The control of algorithm flow of ‘flooradapt’ and ‘roundadapt’ QNMF is summarized in Table III. In lines 2a or b and lines 6a or b either floor or round randomized quantizers are applied to the factors –the quantizer gives its name to the adaptive algorithm: ‘flooradapt’ and ‘roundadapt’ QNMF.

V. Empirical Evaluation

Our empirical evaluation explores the efficacy of using QNMF as an algorithm for lossy compression-factorization. We use Donoho and Stodden’s NMF Swimmers database to evaluate QNMF’s convergence. The Swimmers are an element-wise integer-valued data-set V m,n ∈ {1, 39}; NMF does not produce an element-wise integer factorization of this data-set. Taking our inspiration from Occam’s Razor, we seek a simpler factorization –element-wise finite-resolution data-sets call for an NMF algorithm that generates a factorization with a finite number of different values in the entries. Our choice of the Swimmers is motivated by the fact that the correct factorization, and thus rank parameter R = 16, is known. Knowledge of R is important in our analysis of QNMF as choosing an R that is too large (small) generates a low(high) factorization distortion. Our goal is to isolate the effect of quantized updates from the rank selection problem, the Swimmers are suitable.

QNMF Convergence and Complexity: We plot the objective function of the variants of QNMF for the first 100 iterations of QNMF in Fig. V when they are applied to the Swimmers data-set with R = 16. Lee-Seung’s Frobenius NMF is plotted as a benchmark method. Each factorization is initialized with the same initial matrices. Firstly, the accuracy of all of factorizations, measured using the squared \( \ell_2 \)-norm,
is approximately the same. We conclude that the distortion penalty associated with learning a finite-precision factorization over the traditional NMF is small. Secondly, although we have not given a proof of convergence for QNMF, the success of these methods in numerous trials (cf. Table IV) suggests that whilst monotonic convergence is not guaranteed the techniques converge to a good-simple solution. To highlight the convergence property and also the complexity of QNMF, we plot time-series for the factors, \( W \) and \( H \) respectively, which record the counts of the numbers of Bernoulli trials required to decrease the objective function at each iteration. We make the following observations: 1) initially a relatively large number of Bernoulli trials is required for all algorithms; 2) the number of Bernoulli trials reduces to a small number as the quality of the QNMF improves; 3) on first inspection this number of Bernoulli trials may seem onerous, however modern computers have multiple cores and these Bernoulli trials are easily run in parallel; 4) when the Bernoulli count reaches the maximum number of Bernoulli trials (1000 trials for the rounded QNMF and 100 trials for floored QNMF), the quantization function has failed to minimize the objective. The rounded QNMF algorithms only increase the objective \(1 - 3\) times. These objective increases occur at the start of the iteration. In some respects this behaviour is analogous to finding a good set of initial matrices, or starting NMF from multiple initial conditions.

The primary factor that causes the objective function to increase is the error introduced by the quantization step. A useful performance measure to evaluate the convergence of QNMF is the Quantization Efficiency, which is defined as: 
\[
\omega_Q = \frac{SNR_{Q_{NMF}}}{SNR_{NMF}}
\]
for a given rank. Fig. 3 illustrates the quantization efficiency of the quantization functions computed at each iteration. The quantization efficiency is the ratio of the SNR of the NMF generated updates post and pre quantization. The floored algorithms outperform the rounded algorithms. The convergence in Fig. 3 mirrors that in Fig. V; the variance in the quantization error appears to converge as the distortion measure converges.

QNMF is as precise as NMF for the same rank, but simpler: We demonstrate that QNMF gives a similar quality of decomposition, in terms of the mean SNR, as a NMF of the same rank in Fig. 4 for the Swimmers and for the standard “Cameraman” test image in Table IV. In addition, we illustrate that QNMF learns a simpler decompositions in Fig. 5 for the swimmers and in Table IV for the Cameraman. The input matrix is generated for the Cameraman by blocking (8x8 pixel blocks) the image and placing the vectorized block in the columns of \( V \). We perform 50 Monte Carlo runs and plot the average SNR and cardinality \( C(\{W\}) + C(\{H\}) \) for a range of ranks \(10 \leq R \leq 20\) for the Swimmers and for \(10 \leq 40\) for the Cameraman. We compute the cardinality because estimating the differential entropy of NMF or QNMF decompositions, the ideal performance metric, is fraught with difficulty [17]. This discussion underlines the problem with quantizing traditional NMF. Producing a histogram of the
columns (rows) of $W$ ($H$), and then finding the discrete entropy, may produce misleading results because 1) QNMF produces integer factors and NMF produces nonnegative factors, using the same histogram bin selection for these two completely different types of data can generate drastically different discrete entropies; 2) the rows and columns of QNMF and NMF may be permuted and scaled; 3) adaptive QNMFs optimize the quantization step-size across the rows and columns, using a uniform step-size to quantize a NMF to compute its discrete entropy means that we are not comparing like-for-like. In addition, computing the performance of NMF and QNMF with respect to some post-processing compression routine, introduces the possibility that the compression routine favours QNMF. We plot the mean cardinality of the QNMF. The cardinality of the set of entries of NMF is $MR + RN$. The ‘floorrand’ and ‘flooradapt’ QNMF are the best QNMF algorithms with respect to SNR. For all NMFs the accuracy increases as $\text{SNR} \rightarrow \infty$. Table IV shows that QNMF is with in 4 dB of NMF. The ‘floorrand’ and ‘flooradapt’ QNMF are the best QNMF algorithms with approximately the same accuracy. Table IV demonstrates QNMF has a factor of 20-70 fewer levels than NMF for the $W$ matrix and a factor of 500-1000 fewer levels for $H$. Experiments on the Peppers and Barbara images in the supplementary material further support these results.

VI. DISCUSSION

The rationale for the Bernoulli quantization is clear; if the current quantization functions increase the objective, a matrix of quantization functions which have a high probability ($p < 1$) of being a ‘floor’ or ‘round’ but minimize the objective is a satisfactory substitute. Moreover, the number of candidate random quantizers generated for each $p$ is bounded –This bound is much smaller than the total number of possible floor-ceiling matrix permutations, typically $\ll 2^{RN}, 2^{HM}$. In terms of the step-size division process for the round quantizer, when the $\Delta_h$ is small (relative to the variation in the signal being measured [15]), the MSE produced by the rounding operation is approximately $\sigma^2_h = \frac{1}{12} \Delta_h^2$. This relationship underpins the initialization of the quantization step-sizes. Recall that in this paper the step-sizes are initialized to be less than one, the largest signal value is 39. Successive halving of the interval $\Delta_h$ causes the variance to reduce according to: $\sigma^2_{h/2} = \frac{1}{12} \Delta_h^2$. In effect as $\Delta_h \rightarrow 0$ the quantization error is reduced and QNMF begins to approximate the original NMF –a related analysis holds for the floor and not-round functions. It is reasonable to assume that in the limit QNMF reduces to original NMF. In short, monotonic convergence is feasible (for a large enough $s$). Successive halving (of $\Delta_h$) in this manner exhibits favourable complexity. In practice, we have observed that the number of Bernoulli trials required to achieve minimization using the random quantizers is small. Moreover step-size division is rarely required, in fact $s$ is fixed for all our experiments.

VII. CONCLUSIONS

Our first conclusion is that QNMF is more amenable to storage than NMF due to its reduced factor-cardinality. It trades-off only 1-4dB to achieve a reduction of 20-70 (500-1000) times the cardinality of the $W$ ($H$) matrix element set to achieve this reduction. We make the recommendation that based on the cardinality gains achieved by QNMF, efficient and accurate compression-factorization can achievable using QNMF. A second conclusion is that our empirical convergence evaluation of QNMR substantiates the claim that quantization does not significantly affect convergence. In future work we will give a more formal analysis of QNMF convergence and consider the impact of quantization on domain specific perceptual measures.

REFERENCES


