Mutual information based detection of TNT content by Nuclear Quadrupole Resonance.

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***Abstract*— A mutual information based approach for the analysis of signals obtained by nuclear quadrupole resonance (NQR) measurements to detect TNT content is proposed. We apply the method to real NQR data obtained under laboratory conditions and compare ROC curves for the presented method with those of the popular demodulation technique and the matched-filter detector. Our results show mutual information to be an extremely sensitive technique, especially for very low signal-to-noise ratio, as in the case of NQR based TNT detection.**

I. Introduction

In this letter we report on a highly sensitive entropy based method for the detection of explosive content in data obtained by nuclear quadrupole resonance (NQR) measurements. NQR signals result from the relaxation of nuclear quadrupole momenta to their original thermal equilibrium position after an initial, high power RF pulse has been applied which causes a splitting of the Zeeman energy levels due to the interaction of the nuclear quadrupole with the electric field gradient. This equilibrium is a function of the electromagnetic field in the vicinity of the quadrupole active nuclei resulting in a spectrum that is very specific with respect to chemical compounds. Because of its high potential value in remote explosive detection there is renewed interest in NQR methods for landmine and UXO detection, as well as for securing high risk areas such as airports by non-intrusive means. Although applicable in principle to any type of NQR based detection, the target application of focus in this paper will be humanitarian landmine detection. The main drawback of NQR based landmine detection is the inherently low power of the returned echoes. We present a mutual information based method and compare ROC curves with both matched filter detection and the popular demodulation technique. Our results show mutual information to be a very powerful technique, especially for a very low signal to noise ratio, as in the case of NQR based TNT detection.

II. Landmines and nuclear quadrupole resonance

The bulk of landmines is still detected using metal detectors because all landmines contain at least a small amount of metal content in the detonator and the metal detector gives a clear signal that is trusted by field workers. However the very high sensitivity of the metal detector needed to reliably detect landmines, also increases large false alarm rate. As a result on average 100 to 1000 objects are wrongly classified as potential mines for each real mine encountered causing substantial overhead in time, energy and cost. As an example, consider the data from the Cambodian Mine Action Centre (CMAC) taken between March 1992 to October 1998, as cited in [1]. Over this six year period approximately 90,000 antipersonnel mines were cleared but an additional 200 million scrap items were excavated in the process. The probability of false alarm was therefore 99.7%. A possible solution involves the use of nuclear quadrupole resonance techniques. A necessary condition for the use of NQR is the presence of a substance with a nuclear quadrupole moment, such as the naturally stable nitrogen isotope ^{14}N, (with a natural abundance of 99.64 %) with nuclear spin-1 and corresponding nuclear quadrupole moment. The vast majority of explosives in mass-produced landmines contain ^{14}N and can at least in principle be detected by NQR. An exception is the PFM-1 landmine which contains a liquid explosive. The rapid molecular tumbling, characteristic of the liquid state, averages the quadrupole interaction to zero, effectively eliminating the applicability of any current NQR technique. Typical landmine NQR transition frequencies lie in the range between 0 and 6 MHz, actual values depending mostly on the electric field gradient tensor which is primarily determined by the charge distribution of the electrons that bind the nitrogen to the rest of the explosive. The resulting NQR signal is therefore highly dependent on the chemical structure of the sample, and delivers a potentially very reliable classification with an accompanying very low false alarm rate. The main challenge for NQR techniques is the extremely low energy content of the signal resulting in a very low signal to noise ratio (SNR). To improve the SNR many repetitions of the experiment are necessary. The most popular method is to set up an appropriate sequence of RF pulses, and register the returned echo after each such pulse. The rate at which repetition is physically informative is bound from below in a fundamental way by the physical parameters of the nuclear relaxation process which is a result of two different mechanisms called the spin-spin relaxation and the spin-lattice relaxation [2]. The relaxation time that characterizes the spin-lattice relaxation, denoted $T_{1\rho}$, determines the time necessary for the system to regain its original thermal equilibrium state, and gives a bound on how quickly one entire pulse sequence can be initiated after another. The spin-spin relaxation time, often denoted T_2, is indicative of the decoherence as a result of spin-spin interactions and determines the time between refocusing pulses *within* one spin echo sequence. Spin-spin relaxation times are generally (much) shorter than spin-lattice relaxation times. For most explosives, the characteristic relaxation times are short enough so that NQR detection becomes feasible. Unfortunately this is not true for $\alpha-$trinitrotoluene (TNT), the active compound of approximately 60% of the landmines, because TNT has relaxation times that lead to prohibitively long detection times within the operational limits of landmine detection. It is therefore projected that an NQR based landmine detector will probably serve mainly as a confirmation sensor, i.e. a detector that is employed to decrease the false alarm rate only after a metal detector or a ground penetrating radar system has detected a potential landmine [3]. It is interesting to note that the hardware for an NQR detector is very similar to a metal detector. Hence a dual metal/NQR detector is feasible in which the metal detector mode serves as a primary sensor and after an alarm the detector is switched to its NQR operation mode to serve as a confirmation detector. Whether used as a confirmation or as a primary detector NQR detection efficiency for TNT will benefit greatly from a reduction in the time necessary for reliable detection. Because one cannot shorten the relaxation parameters of TNT much effort has gone into cleverly designing the emitted RF pulse [4], [5], [6], [7] and improving the hardware of antenna and receiver [8], [9]. Besides these efforts it is worthwhile to pursue better signal analytic detection techniques [10], [11], [12], [13], [14].

III. The decision problem for NQR and detection schemes

It would lead us to far to give a detailed account of the theory of NQR and refer the interested reader to [2], [15], [16] for excellent introductions. However, for our present purpose, we need only the bare basics. What causes the NQR signal, is the relaxation of nuclear quadrupole momenta which changes the magnetization projected along the direction of the solenoid. In the case of ^{14}N, we are dealing with a spin-1 system so that the relevant quantum mechanical subspace is spanned by just three orthogonal vectors. In a quantum mechanical descriptions of NQR, the state of the system is a classical statistical mixture of pure quantum states, described by a density operator $\hat{\rho}$ belonging to the class of linear, positive operators that sum to one when they act upon a complete set of eigenvectors. The dynamics of the density operator $\hat{\rho}$ is governed by the unitary evolution that solves the Schrödinger equation

$$\frac{d\hat{\rho}(t)}{dt} = -\frac{i}{\hbar}[\hat{H}, \hat{\rho}(0)] \tag{1}$$

Here $\hbar$ is the Planck constant divided by 2π, $\hat{H}$ is the interaction Hamiltonian of the NQR subsystem and $\hat{\rho}(0)$ the initial density operator. Data analysis for NQR experiments starts from the quadrature components $V(t)$, which are a result of the change in the magnetization M. The expectation of the magnetization $\langle \hat{M}_z \rangle$ in the direction of the axis of symmetry of the solenoid (here the z-axis), is obtained by tracing over the product of the state $\hat{\rho}_{sys}$ (the mixture of quadrupole active spin-1 states) with the magnetization operator $\hat{\mu}_z$ along that spatial axis:

$$\langle \hat{M}_z \rangle = Tr(\hat{\mu}_z \hat{\rho}_{sys}) \tag{2}$$

With N the number of turns in a solenoid of area A, Q the quality factor of the coil, and μ_0 the magnetic permeability in free space, we have

$$V(t) = QN\frac{d(\mu_0 \langle \hat{M}_z \rangle A)}{dt} \tag{3}$$

As the two quadrature components are always 90 degrees out of phase, they form a pair of quantities that can be expressed as a single complex quantity.

The actual problem of detecting the presence of TNT can be quite complex, but in its most basic form we have to decide between the case when there is TNT present in the soil and when there is no NQR active substance at all. Complicating factors, such as temperature dependence of the spectrum[1], or the presence RF interference, other explosives, other crystalline forms, or harmless but still NQR active components, are necessary extensions to make field application of this method possible. Needless to say, this will decrease the statistical performance of the detection method. For each detection method, we will briefly indicate how it may be extended to incorporate such effects. The analysis we present is however aimed at comparing the statistical performance of different detection methods in this most basic setting. If no NQR signal is present, the measured quadrature components are modelled as pure noise components V_{noise}. The alternative hypothesis assumes there is TNT present in the soil, and we will have a NQR active density operator. The measured quadrature components are then be modelled as the superposition of the noise free components V_{TNT} with the noise components V_{noise}..

$$\begin{aligned} H_0 &: \quad V(t) = V_{noise}(t) \\ H_1 &: \quad V(t) = V_{TNT}(t) + V_{noise}(t) \end{aligned} \tag{4}$$

The decision problem is then to decide from a measured $V(t)$ whether H_0 or H_1 applies. All three methods we will present shortly require prior knowledge of the signal. Although this is in varying degrees true for many detection methods, it is especially true for NQR based detection due to the inherently high specificity of the method. Even chemical degradation of the explosive over time will alter the NQR spectrum. Hence in field applications this prior knowledge can only be obtained through calibration of the detector on the spot. Such a calibration is time consuming, especially since the location of the resonances depends on the temperature of the sample, so we need to model the explosives' response as a function of the temperature. An example where extensive laboratory measurements are used to produce a good model of the NQR response for TNT as a function of temperature and fraction of multiple polymorphic forms can be found in [18]. This requirement may invalidate these methods for applications which require rapid demining of unknown explosives, such as is the case for military demining. However, we are concerned here with humanitarian demining which has very different requirements [3]. In many instances it is known what type of mines are to be expected and it is possible to spend a few days for calibrating the detector. In our data analysis we have calibrated our detector with the same data that is being used to test the performance of the detector. To avoid the risk of cross-contaminating the results, the reference signal was obtained by forming the sum of all signals except the one that is under examination. Verification of the results when no such

[1] This complication presents no fundamental problem to any of the methods we will present and, however important to the actual demining problem (see, for example, [11] and [17]), is not taken into account here .

precautionary measure is taken show this to be of little or no consequence in terms of overall performance of any of the detection methods.

A. The Demodulation technique

A popular method to establish the presence of a given substance in a NQR tested sample, is the so-called demodulation technique. This method consists of calculating an estimate $\sigma(\nu_n)$ of the power spectral density $S(\nu)$ of the signal $s(t_n)$, $n = 1, \ldots, 256$, by first fast Fourier transforming the signal and taking its modulus squared. Let us call $\nu_{\max}$ the frequency $\nu_{\max} = \arg(\max(S(\nu)))$ where one expects the spectral line with the highest intensity in presence of TNT at a given temperature. The value of the *estimated* power spectral density $\sigma(\nu_{\max})$ evaluated at the frequency $\nu_{\max}$, is then the test statistic for a threshold detector. If $\sigma(\nu_{\max})$ exceeds a given threshold H_1 is accepted; if not, H_0 is adopted. The estimated $\sigma(\nu_n)$ will in general deviate from $S(\nu)$ at the precise values ν_n, but may be approximately regarded as an average over the interval $[\frac{\nu_n-\nu_{n-1}}{2}, \frac{\nu_{n+1}-\nu_n}{2}]$. To account for this the average under $\sigma(\nu_n)$ over a few frequency bins can be taken as a test statistic. Whether this is useful depends, among other things, on the magnitude of the width of the spectral line with the highest intensity relative to the width of the frequency bins. Moreover, as NQR spectra are generally a function of the temperature of the sample and because this parameter is difficult to estimate in demining applications within a range of 5 to 10 Kelvin, the value of $\nu_{\max}$ will depend on the temperature too. To make sure we do not miss the peak one can then take the area over a region in the frequency domain where one expects the peak. We will later briefly elaborate on the inclusion of temperature. All our experimental samples are taken at the same temperature. As expected, we see little change in the efficiency of the method, whether we use $\sigma(\nu_{\max})$, or a sum of values $\sum \sigma(\nu_{\max})$ for a tiny region surrounding the relevant frequency bin. Obviously, knowledge of the location of multiple peaks does offer a considerable improvement upon which we reported elsewhere [13]. The results that we present here employ the single peak value $\sigma(\nu_{\max})$ of the frequency bin containing the mean excitation frequency 841.5 kHz.

B. Matched filter approach

If we know exactly which signal we are looking for, we can apply a matched filter approach [19] to the problem. In [10] such an approach was presented for NQR detection with multiple antennae, and the results for a single antenna are a special case. The method starts from the binary decision problem 4. The test statistic is the given by the correlation

$$\theta = \langle V(t), V_{TNT}(t) \rangle$$

If the value of θ exceeds a given threshold value, H_1 is adopted, otherwise, we assume H_0 to hold. The method is readily extended to incorporate dependency of the spectrum on a parameter vector (such as temperature, or a mixture of explosives) in the following way. We model the noise-free NQR echo $V^{\alpha}_{TNT}(t)$ as function of an unknown parameter vector α. Different values of α then correspond to different spectra as a result of temperature dependency or mixtures. The test statistic is the maximal value of the correlation

$$\theta = \max_{\alpha} \{\theta_\alpha = \langle V(t), V^{\alpha}_{TNT}(t) \rangle\}$$

Under the assumption that H_1 holds, θ_α obtains its maximal value for the value α that corresponds to the noise-free signal $V^{\alpha}_{TNT}(t)$. If $V_{noise}(t)$ represents zero-mean Gaussian white noise, the maximal value of θ_α can still be shown to be the proper estimate, and the corresponding $V^{\alpha}_{TNT}(t)$ the most likely estimate for the true signal [19].

C. The entropic detector

The use of registration, detection and similarity measures based on mutual information has drastically increased over the last decade. To illustrate this fact, [20] gives a list of over 160 references, gathered between 1994 and 2002 and mainly restricted to medical applications. To apply the rich and well-developed theory of information to the problem of landmine detection, we conceive of the NQR active compound as the transmitter, and the coil of the NQR detector as receiver. The echo emitted by the NQR compound after the pulse was initiated, is treated as a message that is to be communicated through a “communication channel” (the soil and environment) to the receiver. The amount of discrete information that can be reliably transmitted over a channel, is called the channel capacity and is known to be bound by the mutual information. Hence we can use the mutual information as a measure of how good the channel was in transmitting the message. Regular soil will, in absence of TNT, not contain the searched for NQR echo and will classify as a very bad communication channel for transmitting this signal, whereas the TNT containing soil will contain a faint, noisy replica of the signal, and will turn out to be a better communication channel. As mentioned before, the (almost) noise-free echoes emitted by the NQR compound of a specific landmine is obtained by recording and adding the signal for many repetitions of the experiment. Mutual information is classically defined for probability distributions, whereas the data obtained in the experiment are the quadrature components $V(t)$. There are two ways of approaching the problem. The first method consists of considering the histogram of the sampled values $V(t)$, regard these values as estimates for the probability of each digitized value and apply the mutual information to this probability distribution. As the quadrature signal is complex, this has to be done for each component separately. A theoretically better founded approach consists of taking a quantum mechanical perspective on the problem and model the complex signal received from the spectrometer as a quantum operation[2] acting on the electromagnetic field of the echo. It is well-known that inefficient and incomplete measurements can be modelled very well by quantum operations [21], [22], [23]. The precise form

[2]A quantum operation offers the most general possible description of an evolution [21], and is defined as a mapping ε that transforms an initial state ρ_0 to a final state ρ by $\rho = \varepsilon(\rho_0)$ such that there exists a set $\mathcal{O} = \{E_k : \sum_k E_k E_k^\dagger = I, \forall \rho : Tr(E_k \rho) \geq 0\}$, called *operation elements*, for which ε can be written as $\varepsilon(\rho_0) = \sum_k E_k \rho_0 E_k^\dagger$.

the quantum operation takes in this case is of no concern to us. What is of importance here is that the famous Holevo bound for quantum channels can be generalized to such measurements [24], [25], [26], [27], [28]. The Holevo theorem [29] applied for two states says that, if a system is in either one of two density operators $\hat{\rho}_0$ or $\hat{\rho}_1$, with equal probability equal to 1/2, then the information that can be gathered about the identity of the state in a single measurement never exceeds

$$I \leq \frac{1}{2}(S(\sum_{i=0,1} \hat{\rho}_i) - \sum_{i=0,1} S(\hat{\rho}_i)), \quad (5)$$

where $S(\hat{\rho})$ is the Von Neumann entropy defined as:

$$S(\hat{\rho}) = -Tr(\hat{\rho} \ln \hat{\rho}). \quad (6)$$

To calculate the last two expressions we take the complex time dependent echo $V(t)$, normalize it $\tilde{V}(t) = V(t)/||V(t)||$, and take the exterior product with its dual. Writing, as is customary in quantum physics, the vectors in the Dirac bra-ket notation, we have:

$$\hat{\rho}_V = |\tilde{V}(t)\rangle\langle\tilde{V}(t)|.$$

To evaluate the operator expression (6) we calculate the eigenvalues of the operator $\hat{\rho}_V$, call them λ_i, and evaluate

$$S(\hat{\rho}_V) = -Tr(\sum \lambda_i \ln \lambda_i). \quad (7)$$

The base of logarithm in (7) is in information theory 2 by convention. Using (7) one can straightforwardly calculate the Holevo bound 5 as

$$I \leq \frac{1}{2}(S(\hat{\rho}_V + \hat{\rho}_{ref}) - S(\hat{\rho}_V) - S(\hat{\rho}_{ref})). \quad (8)$$

It is the information bound of the quantum channel on the right-hand side of expression (8) that we will use as a test statistic for a mutual information based detector. Here $\hat{\rho}_{ref}$ is the operator obtained by taking the normalized outer product of the signal averaged over a great many measurements. The entropic method we propose here replaces the correlation function of the matched filter approach by the Holevo bound.

$$\theta = \frac{1}{2}(S(\hat{\rho}_V + \hat{\rho}_{ref}) - S(\hat{\rho}_V) - S(\hat{\rho}_{ref}))$$

If the spectrum is a function of an unknown parameter α, the density operator $\hat{\rho}^{\alpha}_{ref}$ is also a function of α, and we calculate

$$\theta_\alpha = \frac{1}{2}(S(\hat{\rho}_V + \hat{\rho}^{\alpha}_{ref}) - S(\hat{\rho}_V) - S(\hat{\rho}^{\alpha}_{ref}))$$

and the value of θ is then given as the maximal value of the bound as a function of α :

$$\theta = \max_{\alpha} \theta_\alpha$$

IV. Experimental results

A. Set up and data acquisition

The data employed for our analysis was kindly provided by the NQR group of King's College, London, under supervision of Professor J.A.S. Smith. In the experimental set up employed, a pure monoclinic TNT sample with a weight typical of that found in an anti-personnel mine, is placed inside a solenoidal coil. The solenoid is used both for the emission of the RF-pulse, as well as for the reception of the subsequent NQR echo. The returned echo signal is routed through a hardware band-pass filter with a bandwidth of approximately 50 kHz and subsequently sent to a Tecmag Libra spectrometer that splits the signal in two signals which are then mixed with two quadrature components, yielding a complex discrete time series. Because of the close to ideal laboratory conditions under which the signal has been obtained, the results will compare unrealistically optimistic with respect to those obtained under field conditions. In particular the absence of RF interference and the use of a coil that contains the sample in its entirety must be taken into account when attempting to compare the results of our analysis with those of data obtained under more realistic conditions. The emitted RF signals are pulsed, spin-locked echo signals with a mean excitation frequency of 841.5 kHz. The mean and width of the excitation are such that 4 spectral lines of TNT can be detected within the frequency range of the band pass filter. Because the same coil is used for the emission of the RF signal (which has a mean power of several kilo watts) as for the reception of the echo (which is extremely weak), the returned echo contains so-called antenna ringing effects. To cancel the effect of the antenna ringing a phase cycling technique, popular in the more established field of NMR, is employed. The phase cycling technique requires forming an appropriate sum of four signals. The signals used for the analysis are the sum of 5 such phase-cycled sums and hence consist of 20 repeated data acquisitions, averaged to improve SNR. The sampling time is 5μS. and each set has 8192 data points, which consists of 32 sequential echo signals, each containing 256 data points. The pulse sequence is of the type

$$\pi/2 - \tau - \pi - 2\tau - \pi - 2\tau - \pi - 2\tau - ...$$

Here π denotes the RF pulses and the 1280 μs of data (256 times 5 μs) for each echo signal is acquired during the 2τ periods between the pulses. All algorithms are programmed in MATLAB 7 on a 2,2 GHz PC with 512 MB RAM. All methods we present here are fast: the determination of whether a given signal was obtained in the presence of TNT or not, requires a calculation time less than a second, more than one order of magnitude below the necessary data acquisition time.

B. Detector performance

The statistical assessment of detector performance is based on the sensitivity, specificity and ultimately on the functional relationship which exists between these two as expressed in the receiver operating characteristic (ROC). The data used to calculate the ROC curves consists of 100 data samples with TNT, and 100 data samples without TNT. Because of spin-lattice relaxation, we expect the signal quality to decrease as a function of the echo number, a behavior we see reflected in the ROC curves and in the line intensities of the three most visible resonances as a function of the echo number, as depicted in figure 1.

In figures 2, 3 and 4 we have depicted ROC curves for the three detection methods.The comparison between the methods is further facilitated using the area under a ROC curve, which

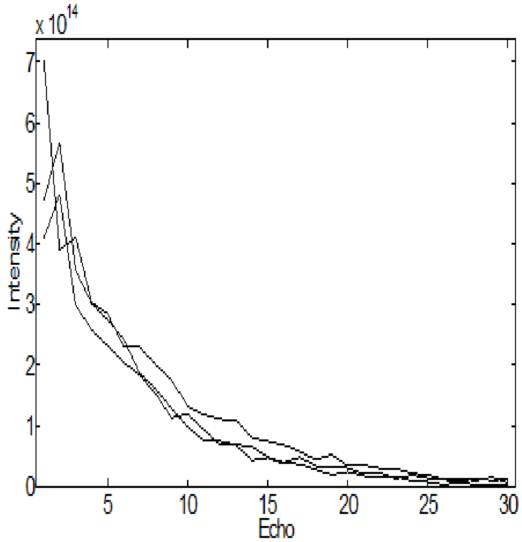

Fig. 1. The intensity of the three TNT quadrupole resonances within experimental reach, for a sum of 100 signals, as a function of the echonumber. The decrease in intensity is in good approximation exponential with approximately the same relaxation constant for the three resonances.

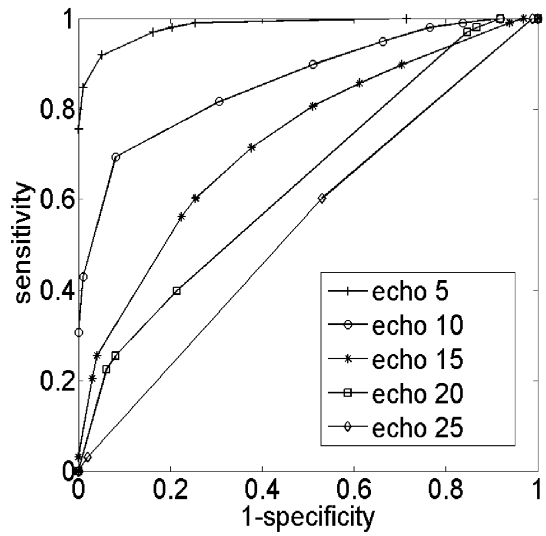

Fig. 2. ROC curves for the demodulation detector. Depicted are ROC curves for echo numbers 5, 10, 15, 20 and 25 in decreasing order of performance respectively. The first four echoes are not shown as they yield close to ideal detectors.

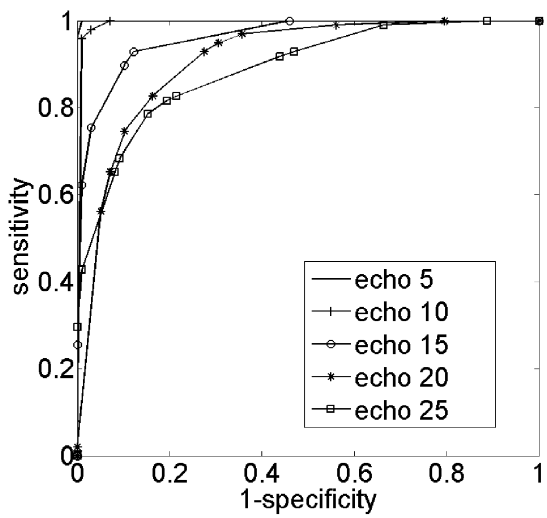

Fig. 3. ROC curves for the matched filter detector. Depicted are ROC curves for echo numbers 5, 10, 15, 20 and 25, in decreasing order of performance respectively. The first ten echoes yield close to ideal detectors.

can be taken as a measure of the overall performance of the detection scheme. The ideal case corresponds to an area of one, the completely ignorant detector scores one half. The results of this analysis for the three methods, is presented in 5.

One can see from that for the first 5 echoes, all three detectors yield close to ideal results. After echo 5, the performance of the demodulation technique degrades. In contrast, the matched filter detector allows to use any of the first 10 echo numbers to obtain a detector that is very close to ideal, and for the mutual information detector, even echo 19 delivers a close to ideal detector. For echo numbers above 20, the area under the ROC for the demodulation technique remains under 0.6, indicating no reliable information can be drawn from the results. The matched filter performs somewhat better, but the mutual information detector still has a very respectable area between 0.96 and 0.85. As explained above, the SNR decreases exponentially as a function of the echo number. From figure 1 we see that the average intensity of the peaks at echo number 20 is about 3.10^{13}, approximately one tenth of the average intensity at echo number 5, which is 3.10^{14}. Hence a rough estimate learns that for this data set the mutual information detector delivers a close to ideal detector for an SNR that is one order of magnitude lower as when similar performance is required from the demodulation technique.

V. Concluding remarks

As the first few echoes already yield a perfect detector for all three methods it seemingly makes little sense to further improve the detection capabilities. However, the spin-lattice relaxation for TNT constrains the time between the spin-locked pulses to a minimum of the order of 10s. Each data point consists of the sum of 20 individual measurements, giving a data acquisition time for each data sample of the order of 20.10s = 200s. Although an acquisition time of more than 3 minutes for every single location may seem quite long, when used as a confirmation sensor it is both much safer and far less time consuming than the extremely careful digging that is required without it. It should however be kept in mind that the data used for this analysis was obtained under laboratory conditions. In actual demining applications, the necessary acquisition time will further increase as a result of unknown sample temperature, mixtures of explosives, RF interference, other interfering soil constituents such as piezo-electric ceramics, and the fact that in field applications only single sided (as opposed to the sample being within the coil) remote acquisition is possible. As our results are calculated

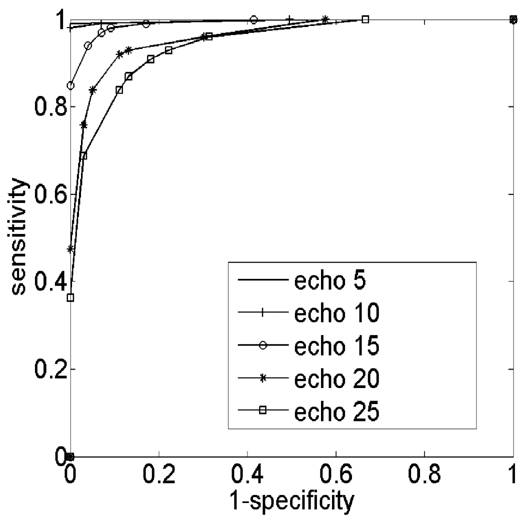

Fig. 4. ROC curves for the mutual information detector. Depicted are ROC curves for echo numbers 5, 10, 15, 20 and 25. We clearly see even higher echo numbers still deliver quite reliable detectors.

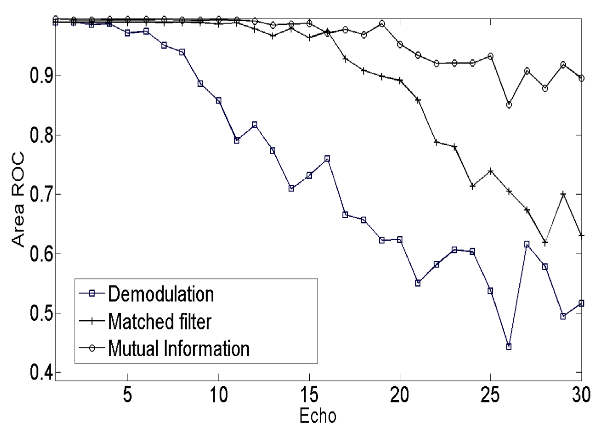

Fig. 5. Comparison of the three methods using the area under the ROC curve as a function of the echonumber. The upper diamond marked line represents the mutual information method, the middle circle marked line is the matched detector, the lower star marked line is the demodulation technique. We see that especially for higher echo numbers only the mutual information detector delivers reasonbly reliable information.

as a function of single echoes, an obvious way to drastically increase the performance of any of the proposed detectors, is to combine the results obtained for individual echoes, for example by making a weighted sum of the threshold values obtained for individual echoes. It is hence of vital importance to improve the detector performance for *all* the echoes in the pulse sequence. The proposed detector succeeds in doing just that. Needless to say, it remains to be seen how much merit of the mutual information technique remains in the field, and extensive field testing is always required before a final verdict can be made on any detection method. It is nevertheless promising that the mutual information results indicate an improvement over the two other approaches which becomes more pronounced as the echo number increases and the SNR decreases.

VI. Acknowledgements

This work was done as part of Flemish Fund for Scientific Research (FWO) research project G.0362.03N. We gratefully acknowledge J.A.S. Smith and M. Rowe for supplying us their NQR data.

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