PARAMETRIC AND NONPARAMETRIC APPROACHES TO DETECTION IN MAGNETIC RESONANCE FORCE MICROSCOPY

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ABSTRACT

We address signal detection in magnetic resonance force microscopy (MRFM) and single spin microscopy (SESM). MRFM and SESM are considered as a promising technology to provide nondestructive and atomic-scale imaging. From a signal processing point of view, the main challenge is to extract very weak signals from measurements with a signal to noise ratio (SNR) typically less than -15 dB. We investigate two detection schemes based different features of the underlying system. The parametric approach is derived from the generalized likelihood ratio test (GLRT). The nonparametric approach exploits the spectral property of the observation. Numerical experiments show that both detectors provide excellent results at very low SNRs.

1. INTRODUCTION

Signal detection in magnetic resonance force microscopy (MRFM), [4], and single spin microscopy (SESM) [3] have become an active research area recently [1]. MRFM and SESM's potential to observe molecules, protein and chemicals in their environment at nanoscales is considered as a promising technology to provide nondestructive and atomic-scale imaging.

The signal of interest in MRFM and SESM is generated by interaction of a spin-spin system-one spin in the magnetic tip of the cantilever (the sensor), the other spin in the sample of material being microscoped. From a signal processing point of view, the main challenge lies in the very low signal to noise ratio, typically smaller than -15 dB.

In [1], the desired spin signal is modeled as a telegraph signal. Despite its simplicity, this model captures the most important aspect of quantum mechanical effects. Based on this model, a straightforward approach to construct the test statistic is the generalized likelihood ratio test (GLRT). In many cases, the GLRT has optimal properties. However, due to unknown distribution of the test statistic, a bootstrap procedure is applied to determine the test threshold. In order to obtain bootstrap samples, the data set is divided into several blocks. Each data block has a reduced data length. Furthermore, we need to know the physical parameters in advance. These values may not be readily available in practice.

To overcome these difficulties, we suggest a nonparametric approach based on the spectral property of the observations. Since the power spectrum of a white noise is constant, detecting a signal is equivalent to testing whether the power spectrum of the observation process is constant or not. The threshold for a given test level α can be accurately calculated by the formulae in [7].

In the following section, we give a short description of the signal and noise model. The parametric and nonparametric approaches are outlined in section 3 and 4, respectively. We discuss simulation results in section 5. Concluding remarks are given in section 6.

2. PROBLEM FORMULATION

The MRFM signal is modeled as a sinusoidal wave of known frequency modulated by a phase switching process

$$s(t) = \tilde{A}x(t)\cos(\omega t + \phi), \tag{1}$$

where $\tilde{A}$, ω, ϕ denote the amplitude, frequency and initial phase, respectively. The phase switching process $x(t)$ is modeled as a telegraph process. By definition, $x(t) = \mathbf{a}e^{j\mathbf{k}(t)\pi}$, where $\mathbf{a}$ is a random variable taking values $+1$ and -1 with equal probability and $\mathbf{k}(t)$ is a Poisson process with parameter ν.

As the frequency ω is known, the data can be down shifted to baseband, lowpass filtered and sampled with frequency f_s. The pre–processed data is expressed as

$$s_t = Ax_t, \;\; x_t \in \{1, -1\} \tag{2}$$

where $A = \tilde{A}\cos\phi$ and the switching process x_t is a first order discrete–time Markov process with transition probabilities

$$\begin{aligned} q &= p(x_t = 1|x_{t-1} = 1) = p(x_t = -1|x_{t-1} = -1) \\ &= \frac{1}{2} + \frac{1}{2}\exp(-\frac{2\nu}{f_s}), \qquad (3) \\ \bar{q} &= p(x_t = -1|x_{t-1} = 1) = p(x_t = 1|x_{t-1} = -1) \\ &= 1 - q. \qquad (4) \end{aligned}$$

From the physical point of view, q is the probability that the spin stays in the same state from the current sample to the next sample. With properly selected f_s, q usually lies between 0.90 and 0.99.

Let n_t denote a white Gaussian noise process with zero mean and known variance σ^2. Our problem is to detect the signal s_t based on the observation $y_t, (t = 1, \dots, T)$.

3. PARAMETRIC APPROACH

In the parametric approach, detecting the discrete signal s_t is formulated as a hypothesis test

$$\begin{aligned} H_0 &: \quad y_t = n_t \qquad 1 \le t \le T \\ H_1 &: \quad y_t = s_t + n_t \qquad 1 \le t \le T. \end{aligned} \tag{5}$$

Let $f_0(\cdot)$ and $f_1(\cdot)$ denote the likelihood function under H_0 and H_1, respectively. Applying the generalized likelihood ratio test (GLRT) [5], we construct the test statistic as follows

$$\lambda = \max_{A,\boldsymbol{x}} \log f_1(\boldsymbol{y}; A\boldsymbol{x}) - \log f_0(\boldsymbol{y}), \tag{6}$$

where $\boldsymbol{x} = [x_1, \dots, x_T]$ represents the phase sequence and $\boldsymbol{y} = [y_1, \dots, y_T]$ collects the observations from $t = 1$ to T. Note that both A and $\boldsymbol{x}$ are unknown. According to the signal and noise model defined previously, (6) can be expressed as [1]

$$\lambda = \sum_{t=1}^{T} \left[\frac{1}{\sigma^2}(\hat{A}\hat{x}_t)y_t - \frac{1}{2\sigma^2}(\hat{A}\hat{x}_t)^2 + \log p(\hat{x}_t|\hat{x}_{t-1}) \right] \tag{7}$$

where $\hat{A}$, $\hat{\boldsymbol{x}} = [\hat{x}_1, \dots, \hat{x}_T]$ denote the maximum likelihood estimate of A, $\boldsymbol{x}$, respectively. Let α, t_α denote the test level and corresponding threshold, respectively. The signal is detected when $\lambda > t_\alpha$. Otherwise no signal is detected.

Maximizing the log–likelihood $\log f_1(\boldsymbol{y}; A\boldsymbol{x})$ is greatly simplified by applying the well known Viterbi algorithm [8]. To apply the Viterbi algorithm to maximize $\log f_1(\boldsymbol{y}; A\boldsymbol{x})$, we need to know A, which is unknown. We address this problem by dividing the parameter space of A into discrete points $A_1, \dots, A_M$ and running a bank of M Viterbi algorithms with each tuned to one of these values. This provides an efficient way of finding the most likely amplitude and state sequence in the maximum *a posteriori* probability sense of a process assumed to be a finite–state discrete time Markov process.

One difficulty encountered in this approach is that the distribution of the test statistic under H_0 can not be determined analytically. To solve this problem, we apply the bootstrap test which requires little knowledge about the distribution of the test statistic.

3.1. Bootstrap Test

The key idea behind the bootstrap is that, rather than repeating the experiment, one obtains the "samples" by reassignment of the original data samples. We outline the basic concept and the test procedure. For more details, the reader is referred to [9] and references therein.

Let $\mathcal{Z} = \{z_1, z_2, \dots, z_M\}$ be an i.i.d. sample set from a completely unspecified distribution F. Let ϑ denote an unknown parameter, such as the mean or variance, of F. The goal of the following procedure is to construct the distribution of an estimator $\hat{\vartheta}$ derived from $\mathcal{Z}$.

The bootstrap principle

1. Given a sample set $\mathcal{Z} = \{z_1, z_2, \dots, z_M\}$
2. Draw a bootstrap sample $\mathcal{Z}^* = \{z_1^*, z_2^*, \dots, z_M^*\}$ from $\mathcal{Z}$ by resampling with replacement.
3. Compute the bootstrap estimate $\hat{\vartheta}^*$ from $\mathcal{Z}^*$.
4. Repeat 2. and 3. to obtain B bootstrap estimates $\hat{\vartheta}_1^*, \hat{\vartheta}_2^*, \dots, \hat{\vartheta}_B^*$.
5. Approximate the distribution of $\hat{\vartheta}$ by that of $\hat{\vartheta}^*$.

In step 2., a pseudo random number generator is used to draw a random sample of M values, with replacement, from $\mathcal{Z}$. A possible bootstrap sample might look like $\mathcal{Z}^* = \{z_{10}, z_8, z_8, \dots, z_2\}$.

For the problem testing the hypothesis $H_0 : \vartheta = \vartheta_0$ against $H_0 : \vartheta \neq \vartheta_0$, we define the test statistic as

$$\hat{\mathcal{T}} = \frac{|\hat{\vartheta} - \vartheta_0|}{\hat{\sigma}} \tag{8}$$

where $\hat{\sigma}^2$ is an estimator of the variance of $\hat{\vartheta}$. The inclusion of $\hat{\sigma}$ guarantees $\hat{\mathcal{T}}$ is asymptotically pivotal. The following procedure solves the problem when the distribution of the test statistic can not be determined analytically.

Bootstrap test

1. *Resampling*: Draw a bootstrap sample $\mathcal{Z}^*$.
2. Compute the bootstrap statistic $\hat{\mathcal{T}}^* = \frac{|\hat{\vartheta}^* - \vartheta_0|}{\hat{\sigma}}$.
3. Repeat 1. and 2. to obtain B bootstrap statistics.
4. *Ranking*: $\hat{\mathcal{T}}_{(1)}^* \le \hat{\mathcal{T}}_{(2)}^* \le \dots \le \hat{\mathcal{T}}_{(B)}^*$
5. *Testing*: Reject H_0 if $\hat{\mathcal{T}} \ge \hat{\mathcal{T}}_{(L)}^*$ where L is chosen such that $L = \lfloor (1-\alpha)(B+1) \rfloor$.

3.2. Detection of the phase process

As i.i.d. samples are assumed in the bootstrap procedure, the detection scheme presented previously is modified. We divide the observation $\boldsymbol{y}$ into M non–overlapping data blocks of length T/M

$$\boldsymbol{y}_1, \boldsymbol{y}_2, \dots, \boldsymbol{y}_M.$$

To ensure independence between data blocks, one can drop the last sample of each block. The statistic (7) is computed independently for each data block

$$\lambda_1, \lambda_2, \dots, \lambda_M.$$

We consider these as i.i.d. samples from a random variable Λ. For computational simplicity, we estimate the mean of Λ in the bootstrap test.

More precisely, the hypothesis testing specified by (5) is reformulated as

$$\begin{aligned} H_0 &: \quad \vartheta = \mu_0, \\ H_1 &: \quad \vartheta \neq \mu_0, \end{aligned} \tag{9}$$

where $\vartheta = E\Lambda$ is the mean of Λ and $\mu_0 = E[\Lambda|y_t = n_t, 1 \leq t \leq T]$ is the mean of Λ when the data contains only noise. The sample mean $1/M \sum_{m=1}^{M} \lambda_m$ is used as the estimator $\hat{\vartheta}$. In this particular case, $\hat{\sigma}$ is given by the estimate of the standard deviation $\sqrt{\frac{1}{M-1}\sum_{m=1}^{M}(\lambda_m - \hat{\vartheta})^2}$. As the distribution of Λ can not be determined analytically, μ_0 needs to be estimated by using training data that contains only noise.

The proposed detection scheme is summarized as follows.

Bootstrap detector

Input: $\boldsymbol{y} = [\boldsymbol{y}_1, \boldsymbol{y}_2, \ldots, \boldsymbol{y}_M]$, μ_0

1. Maximizing log–likelihood of $\boldsymbol{y}_m$ over A,$\boldsymbol{x}$, to obtain $\hat{A}_m, \hat{\boldsymbol{x}}_m, m = 1, \ldots, M$.
2. Compute $\lambda_m, m = 1, \ldots, M$.
3. Bootstrap test.

Output: signal detected or not

In order to the reduce computational cost, we suggest an approximation to the above procedure. Instead of maximizing the log–likelihood of $\boldsymbol{y}_m$ over A_m and $\boldsymbol{x}_m$, we estimate A from the first data block $\boldsymbol{y}_1$ by maximizing the corresponding log–likelihood $f_1(\boldsymbol{y}_1; A\boldsymbol{x}_1)$. We assume that the estimate $\hat{A}_1$ from a data block is a good estimate for $A_2, \ldots, A_M$. In the subsequent data blocks $\boldsymbol{y}_2, \ldots, \boldsymbol{y}_M$, the log–likelihood is maximized over the state sequence using a fixed value of $\hat{A}_1$ in the Viterbi algorithm. Steps 2. and 3. remain the same.

4. NONPARAMETRIC APPROACH

In the nonparametric approach, we exploit the spectral property of the observation y_t. According to the signal model described in section 2, the signal s_t is a discrete process sampled from a telegraph process with amplitude A. The correlation function and the power spectrum of such a process are given by [6]

$$c(\tau) = 4A^2 \exp(-2\nu|\tau|) \tag{10}$$

and

$$C(\omega) = \frac{4A^2\nu}{4\nu^2 + \omega^2}\ , \tag{11}$$

respectively. The power spectrum of s_t can be expressed by eq. (11) as

$$C_{ss}(\omega) = \frac{1}{T_s}\sum_{m=-\infty}^{\infty} C(\frac{\omega - 2\pi m}{T_s}) \tag{12}$$

where T_s is the sampling interval. When a signal is present, the observation process y_t has a non-constant power spectrum

$$C_{yy}(\omega) = C_{ss}(\omega) + \sigma^2. \tag{13}$$

Otherwise, $C_{yy}(\omega)$ is equal the constant noise spectrum σ^2. Therefore, to decide whether a signal is present or not, we can test whether the spectrum $C_{yy}(\omega)$ is constant or not. More precisely, the detection problem is formulated as the following hypothesis test.

$$\begin{aligned} H_0 &: C_{yy}(\omega) \text{ is constant.} \\ H_1 &: C_{yy}(\omega) \text{ is not constant.} \end{aligned} \tag{14}$$

The test statistic is constructed from the periodogram values

$$Y_r = I_{yy}(\frac{2\pi r}{T}) = \frac{1}{T}|\sum_{t=1}^{T} y_t e^{-j\frac{2\pi r}{T}t}|^2, (r=1,\ldots,R), R=[\frac{T-1}{2}]$$

based on the observations $y_t, (t = 1, \ldots, T)$. Let

$$V = \sum_{r=1}^{R} Y_r \quad \text{and} \quad V_s = \sum_{r=1}^{s} Y_r/V. \tag{15}$$

Then when the null hypothesis H_0 is true, V_s $(s = 1, R-1)$ are uniformly distributed over the interval [0, 1] [7]. However, it is considered more natural to consider the ith order statistic of the V_s set and to base a test on the maximum deviation of V_s from its expected value s/R [2]. Thus the test statistic is given by

$$U = \max_{s=1,\ldots,R-1} |V_s - \frac{s}{R}|. \tag{16}$$

From [7] we know that the threshold for a given test level α, the threshold $t_{R,\alpha}$ can be accurately approximated by

$$t_{R,\alpha} = \frac{\sqrt{-\frac{1}{2}\ln\frac{\alpha}{2}}}{\sqrt{R-1} + 0.2 + \frac{0.68}{\sqrt{R-1}}} - \frac{0.4}{R-1}. \tag{17}$$

For $R \geq 6$ and $\alpha \leq 0.62$, the error is less than 0.01.

The ”constant spectrum detector” is summarized as follows.

Constant spectrum detector

Input: $\boldsymbol{y}$

1. Compute periodogram values Y_r, $(r = 1, \ldots, R), R = [\frac{T-1}{2}]$.
2. Compute $V_s, (s = 1, \ldots, R-1)$.
3. Obtain the test statistic U and threshold $t_{R,\alpha}$.

Output: signal detected or not

Compared to the parametric approach discussed previously, the constant spectrum detector requires no prior knowledge about the model parameter, such as the transition probability q and noise variance σ^2. The only assumption we made is that n_t is a white noise. The proposed nonparametric detector is a good alternative to the parametric one when these physical parameters are not available.

5. NUMERICAL EXPERIMENTS

We test the proposed detectors by simulated baseband data. The SNR, defined as $10\log(A^2/\sigma^2)$, varies from -35 dB to -5 dB in 2.5 dB steps. In the first experiment, we consider a transition probability of $q = 0.95$, false alarm rate $\alpha = 0.05$. In the second experiment, the transition probability q is 0.99. The number of trials in each experiment is 100. The bootstrap detector uses a data set of length $T = 10^5$. The number of data blocks $M = 20$. Thus the effective data length is $\bar{T} = T/M = 5000$. For a fair comparison, the constant spectrum detector uses a data set of length $\bar{T} = 5000$.

Fig. 1 shows that the probability of detection increases with growing SNR. For $q = 0.95$, both detectors behave similarly. At

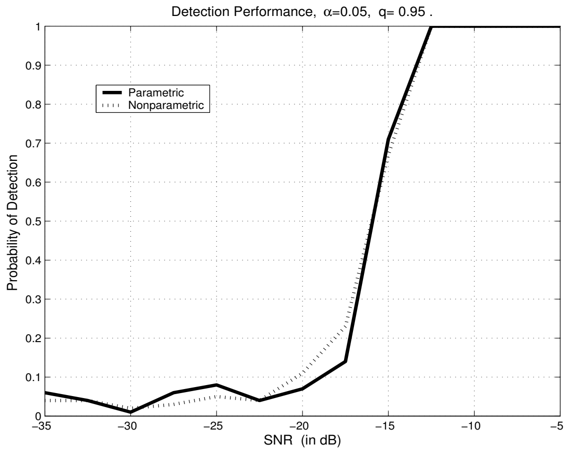

Fig. 1. Probability of detection vs. SNR. SNR= $[-35 : 2.5 : -5]$ dB, $\alpha = 0.05$, $q = 0.95$, data length of the bootstrap detector: $T = 10^5$, data length of the constant spectrum detector: $\bar{T} = 5000$.

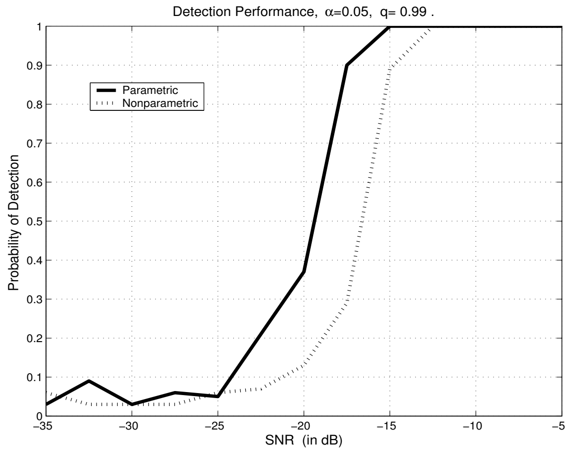

Fig. 2. Probability of detection vs. SNR. SNR= $[-35 : 2.5 : -5]$ dB, $\alpha = 0.05$, $q = 0.99$, data length of the bootstrap detector: $T = 10^5$, data length of the constant spectrum detector: $\bar{T} = 5000$.

SNR < -17.5 dB, there is little chance to detect the signal. In the threshold region -17.5 to -12.5 dB, the probability of detection increases drastically from 0.1 to 1. For SNR > -15 dB, the presence of the signal can always be detected.

Fig. 2 presents results of the second experiment with $q = 0.99$. The overall probability of detection is larger than that in the previous experiment. While both detectors have the same SNR threshold in fig. 1, the bootstrap detector has a lower SNR threshold than the constant spectrum detector in this setting. When $q = 0.99$, the estimate for the phase sequence $\hat{x}$ is more accurate than that at $q = 0.95$. Obviously, the parametric approach is more sensitive to change in the model parameter than the nonparametric approach. The bootstrap detector has a probability of detection of 0.9 at -17.5 dB and the constant spectrum detector achieves the same performance at -15 dB. This is a encouraging result for the MRFM application.

In the simulation we also observe that both methods have a better performance when a larger data set is used. It implies that we can further improve detection performance by increasing the observation time. Fig. 1 shows that the constant spectrum detector needs significantly less data than the bootstrap detector for the same performance. The relation between data length and detection performance is still under investigation.

6. CONCLUSION

We considered the problem of detecting a weak sinusoidal signal with random phase. Signals of this type are particularly important in MRFM. Main challenges associated with this application include signal incoherence, low SNRs and limited observation time. We studied two totally different methods. The parametric approach is based on the GLRT and the bootstrap technique. The test procedure requires prior knowledge about the underlying model parameters. The nonparametric approach exploits the spectral property of the observation. The detector decides whether the power spectrum of the observation process is constant or not. A nonconstant spectrum indicates presence of a signal. Numerical experiments showed that both methods provide satisfying results at low SNRs. The bootstrap detector is more sensitive to parameter change than the constant spectrum detector. The spectral detector requires fewer data than the bootstrap detector to achieve the same performance. Thus the nonparametric approach may be preferable to the parametric approach in some settings.

7. REFERENCES

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