A GLRT AND BOOTSTRAP APPROACH TO DETECTION IN MAGNETIC RESONANCE FORCE MICROSCOPY

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ABSTRACT

Magnetic resonance force microscopy (MRFM) is a technology that will potentially enable microscopy of molecules and proteins at atomic–scale detail. Physicists are pursuing MRFM and single electron spin microscopy (SESM). Many technological challenges exist for MRFM and SESM to deliver on the promise of "visualizing" a single electron spin. The forces of interest are in the subattoneNewton and attoneNewton range (10^{-18} N). In this paper we consider the problem in MRFM and SESM of detecting extremely weak signals buried in noise with SNR in the range of -15 dB to -40 dB. We describe a model that, although simplistic, captures the features of the problem. We present a GLRT and bootstrap approach that incorporates a bank of Viterbi algorithms, and show by simulations that, with physically realistic parameter values, the detector can achieve probability of detection $\beta = 0.9$ with false alarm rate $\alpha = 0.05$, at SNR$= -20$ dB.

1. MOTIVATION

Magnetic resonance force microscopy (MRFM), [3], and single spin microscopy, [2], are being actively researched as an enabling technology for non–invasive, non–destructive atomic–scale imaging. MRFM's goal is to provide the ability of current optical microscopes but at nanoscales– to be able to observe in their environment, with chemical specificity, molecules and protein with atomic scale details. MRFM borrows from magnetic resonance imaging (MRI), but, MRI is a bulk phenomena, ruled by Boltzman statistics, and involving averaging effects over millions of spins, while MRFM and SESM aim at sensing isolated and individual spins.

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The basic principle of MRFM and SESM is simple. The spin signal of interest is measured from the deflection of a cantilever. The cantilever deflects due to the interaction between 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. The sample and sensor are placed in a rapidly oscilating magnetic field (RF) that flips the magnetic moment of the spin, which induces a forced vibration on the cantilever. By shining light on the cantilever, a laser based optical inferferometer transduces the mechanical deflection into an optical and finally electrical signals.

MRFM and SESM face many challenges, from design and fabrication of cantilevers, to detection of extremely weak signals that detect the presence of the desired spin. The forces of interest are very small, in the $10^{-15} \sim 10^{-20}$ Newton range, as are the mechanical displacements. From a signal processing point of view, the problem lies with the very low signal to ratios (SNR), in ranges of -15 to -40 dB.

We consider in this paper a very simplistic version of the problem. We introduce a simplistic model that still captures some of its very significant aspects namely, the phase switching typical of spin systems in quantum mechanics. We then develop for this model detectors based on the generalized likelihood ratio test (GLRT), and bootstrap. The GLRT is used because besides the unknown phase switching process, for the model to be realistic for MRFM and SESM, parameters like the amplitude of the signal component should be assumed unknown. Bootstrap is needed because the distribution of the test statistic under the null hypothesis is unknown.

The GLRT incorporates a bank of Viterbi algorithms, where each Viterbi assumes a particular value of the amplitude of the switching process. Simulation results are very encouraging, showing that at probability of false alarm $\alpha = 0.05$ the probability of detection $\beta = 0.9$ at SNR$= -20$ dB.

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. We assume A and $\underline{x}$ unknown.

Let y_t denote the noise corrupted observation of s_t. Detecting the discrete signal s_t is formulated as the hypothesis test

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

where n_t is a white Gaussian noise process with zero mean and known variance σ^2.

In the following section, we shall derive a likelihood ratio (LR) test statistic.

3. GENERALIZED LIKELIHOOD RATIO TEST

Our detection scheme is based on the generalized likelihood ratio test (GLRT) [4]. Let $f_0(\cdot)$, $f_1(\cdot)$ denote the likelihood function under H_0 and H_1, respectively. The logarithm of the likelihood ratio is given by

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

where A represents the signal amplitude, $\underline{x} = [x_1, \ldots, x_T]$ is the state sequence and $\underline{y} = [y_1, \ldots, y_T]$ collects the observations from $t = 1$ to T. According to the signal and noise model defined previously, (6) can be expressed as

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

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

Maximizing the log–likelihood $\log f_1(\underline{y}; A\underline{x})$ is greatly simplified by applying the well known Viterbi algorithm [5]. To apply the Viterbi algorithm to maximize $\log f_1(\underline{y}; A\underline{x})$, we need to know A, which is unknown. We address this problem by dividing the parameter space of A into discrete points $A_1, \ldots, A_M$ 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 the proposed approach is that the distribution of the test statistic under H_0 can not be determined analytically. Thus we can not find the value of the threshold directly. To solve this problem, we apply the bootstrap test that requires little knowledge about the distribution of the test statistic.

4. BOOTSTRAP TEST

The bootstrap [1], [6] requires little prior knowledge on the data model. The key idea of bootstrap is that, rather than repeating the experiment, one obtains the "samples" by reassignment of the original data samples. We give a brief description of the basic concept and then introduce our test procedure. For more details, the reader is referred to [6] and references therein.

Basic concept Let $\mathcal{Z} = \{z_1, z_2, \ldots, z_M\}$ be an i.i.d. sample eset 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 $\mathcal{Z} = \{z_1, z_2, \ldots, z_M\}$
2. Draw a bootstrap sample $\mathcal{Z}^* = \{z_1^*, z_2^*, \ldots, z_M^*\}$ 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 $$\hat{\vartheta}_1^*,\ \hat{\vartheta}_2^*, \ldots,\ \hat{\vartheta}_B^*.$$
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 $\mathcal{Z}^* = \{z_{10}, z_8, z_8, \ldots, z_2\}$. Given the sample set $\mathcal{Z}$, the bootstrap procedure can be easily adapted to calculate a confidence interval of $\hat{\vartheta}$ or construct a hypothesis test.

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 $$\hat{\mathcal{T}}^* = \tfrac{|\hat{\vartheta}^* - \vartheta_0|}{\hat{\sigma}^*}.$$
3. Repeat 1. and 2. to obtain B bootstrap statistics.
4. *Ranking*: $\hat{\mathcal{T}}_{(1)}^* \leq \hat{\mathcal{T}}_{(2)}^* \leq \ldots \leq \hat{\mathcal{T}}_{(B)}^*$
5. *Testing*: Reject H_0 if $\hat{\mathcal{T}} \geq \hat{\mathcal{T}}_{(L)}^*$ where L is chosen such that $L = \lfloor (1-\alpha)(B+1) \rfloor$.

Detection of the phase process As i.i.d. samples are assumed in the bootstrap procedure, the detection scheme in section 3 is modified. We divide the observation $\underline{y}$ into M non–overlapping data blocks of length T/M

$$\underline{y}_1, \underline{y}_2, \ldots, \underline{y}_M. \tag{9}$$

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

$$\lambda_1, \lambda_2, \ldots, \lambda_M. \tag{10}$$

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

$$\begin{aligned} H_0 &: \vartheta = \mu_0, \\ H_1 &: \vartheta \neq \mu_0, \end{aligned} \tag{11}$$

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: $\underline{y} = [\underline{y}_1, \underline{y}_2, \ldots, \underline{y}_M], \mu_0$

1. Maximizing log–likelihood of $\underline{y}_m$ over A,$\underline{x}$, to obtain $\hat{A}_m, \hat{\underline{x}}_m$, $m = 1, \ldots, M$.
2. Compute λ_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 $\underline{y}_m$ over A_m and $\underline{x}_m$, we estimate A from the first data block $\underline{y}_1$ by maximizing the corresponding log–likelihood $f_1(\underline{y}_1; A\underline{x}_1)$. 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 $\underline{y}_2, \ldots, \underline{y}_M$, 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.

5. SIMULATION RESULTS

The detector in sections 3 and 4 is applied to simulated baseband data. As the signal of interest is very weak compared to noise, the SNR varies from -35 dB to -5 dB in 2.5 dB steps. The SNR is defined as $10\log(A^2/\sigma^2)$. In the first experiment, we consider the data length $T = 10^5$ or 8×10^5, false alarm rate $\alpha = 0.05$, and a transition probability of $q = 0.95$. In the second experiment, the transition probability q is given by 0.99. The number of trials in each experiment is 100.

Fig. 1 shows that the probability of detection increases with growing SNR. The longer data length $T = 8 \times 10^5$ leads to a better performance than that of $T = 10^5$. For SNR

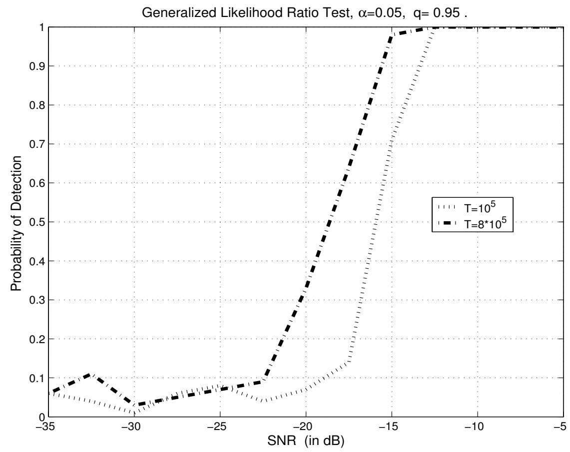

Fig. 1. Probability of detection vs. SNR. SNR= $[-35 : 2.5 : -5]$ dB, $\alpha = 0.05$, $q = 0.95$, $T = 10^5,\ 8 \times 10^5$, $M = 20$.

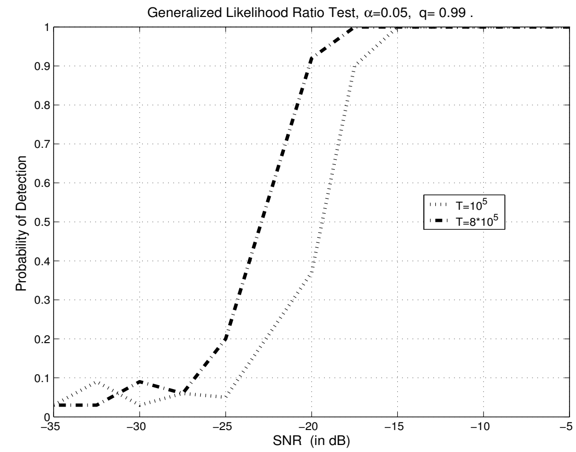

Fig. 2. Probability of detection vs. SNR. SNR= $[-35 : 2.5 : -5]$ dB, $\alpha = 0.05$, $q = 0.99$, $T = 10^5,\ 8 \times 10^5$, $M = 20$.

< -22.5 dB, the chance of detecting a signal is less than 0.1. For SNR > -15 dB, the probability of detection is very close to 1. Comparing the behavior of both curves between -22.5 and -15 dB, it is easy to see that the threshold is lowered by 2.5 dB by using a longer observation.

Fig. 2 presents simulation results from the second experiment with $q = 0.99$. Both curves look similar to those in Fig. 1. However, the threshold region is 2.5 dB lower than when $q = 0.95$. The transition probability $q = 0.99$ corresponds to a lower rate of phase jump than $q = 0.95$. In this case, the estimate for the state sequence $\underline{x}$ is more accurate when a signal is present. This should lead to a higher degree of correlation between the observation and the estimated signal. Hence, the detector performs better.

From Fig. 2 we see that at probability of false alarm $\alpha = 0.05$ the detector provides a probability of detection $\beta = 0.9$ at SNR$= -20$ dB. This is a promising result that bodes well for MRFM.

6. CONCLUSION

Detection of a weak sinusoidal signal with random phase is studied and tested. A telegraph signal is used to model the random phase. Signals of this kind are of particular importance in MRFM and single electron spin microscopy. Due to signal incoherence, conventional methods designed for coherent waves are no longer applicable. Additional challenges include low SNRs and limited observation time. To achieve best performance, we developed a detector based on a GLRT. As the threshold can not be determined analytically, bootstrap is applied to the detection procedure. Simulations show that the GLRT detector provides satisfying results at very low SNRs. Moreover, the detection performance improves as the data length increases.

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