TWO STATE MARKOV MODELLING AND DETECTION OF SINGLE ELECTRON SPIN SIGNALS

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ABSTRACT

The focus of this paper is the optimal detection of piecewise constant binary valued continuous-time (C-T) signals with Markovian state transitions. One example is the classic random telegraph signal for which the number of states is two and the transitions follow a Poisson process. This signal detection problem arises in many different areas of engineering and science, notably modulation classification in digital communications and detection of digital content in continuous signals or images with high noise contamination. Our motivation is single electron-spin detection in Magnetic Resonance Force Microscopy (MRFM), which is an emerging molecular scale imaging modality. We will obtain an optimal discrete time iterative detection algorithm and an associated upper bound on the Receiver Operating Characteristic (ROC) curve. These results will be used to show that the optimal detector reduces to a simple filtered energy detector when the state transition probabilities are symmetric, the signal-to-noise ratio (SNR) is low, and the time-bandwidth product is high. In the general case when the state transition probabilities can be either symmetric or asymmetric, the optimal detector reduces to a hybrid filtered energy/amplitude/energy detector when the SNR is low and there are a large number of samples per observation.

1. INTRODUCTION

The detection of piecewise constant binary valued C-T signals with Markovian state transitions occurs often in different areas of science and engineering. One of the most common examples of such Markovian C-T signals is the random telegraph signal whose transitions are governed by a Poisson process. In this paper, we propose optimal detectors for signals that can be approximated by two-state signals with Markov transitions. The prime motivation for our work is the detection of a single electron spin in a very sensitive physics (MRFM) experiment called interrupted Oscillating Cantilever-driven Adiabatic Reversal (iOSCAR) described below. Accordingly, while our optimal filter structures and bounds are more generally applicable, we present all of our results in this specific application domain.

A general MRFM experiment involves the detection of perturbations of a thin micrometer-scale cantilever whose tip incorporates a submicron ferromagnet. When no electron spins are present, the cantilever acts as a harmonic oscillator. Unpaired electron spins in the sample behave like magnetic dipoles, exerting perturbing forces on the cantilever. Thus, the presence of electron spins can be detected based on measuring the perturbation of the cantilever position from its normal oscillatory behaviour. The iOSCAR method considered here uses an externally modulated radio frequency (RF) field to manipulate the electron spins in such a way as to produce periodic forces on the oscillating cantilever [1, 2]. This results in small changes in the cantilever's natural frequency ω_0. A laser interferometer measures the cantilever displacement; detection of these frequency shifts in the cantilever displacement signal identifies the presence of electron spins.

One model for the cantilever-electron spin interaction is suggested by the Stern-Gerlach experiment [3]. The resultant signal model takes the form of the classic C-T random telegraph process. A finite-dimensional optimal detector does not exist; however, a hybrid Bayes/Generalized Likelihood Ratio (GLR) detector was developed [4, 5]. Unfortunately, it has a running time that makes a real-time implementation unfeasible at this point. Consequently, we have formulated a (generalized) discrete-time (D-T) analog of the C-T random telegraph process. The optimal Likelihood Ratio Test (LRT) for the D-T random telegraph can be derived, with a complexity of $\mathcal{O}(N)$. Here, N is the number of samples per observation. Surprisingly, it can be shown that there exist simpler detectors, all with $\mathcal{O}(N)$ complexity, that approximate the LRT.

This paper describes two results. Firstly, the filtered energy detector is approximately asymptotically optimal for the D-T random telegraph model under the conditions of low SNR, high time-bandwidth product, and symmetric transition probabilities. Secondly, in the general D-T random telegraph model (which includes both symmetric and asymmetric transition probabilities), a hybrid filtered energy/amplitude/energy detector is approximately asymptotically optimal under the conditions of low SNR and long observation time. The MRFM single electron spin detection results described in this paper are more fully developed in [6], as are additional finite (non-binary) state Markov models and detectors.

The outline of this paper is as follows. In Section 2, we briefly review the iOSCAR experiment. Then, in Section 3, we describe the C-T and D-T random telegraph process. Section 4 develops the optimal LRT detector for the D-T random telegraph model and its approximately optimal forms. Simulation results are presented in Section 5.

2. DESCRIPTION OF THE IOSCAR EXPERIMENT

In the experiment, a submicron ferromagnet is placed on the tip of a cantilever that sits approximately 50 nanometers above a sample. In the presence of an applied RF field, the electron in the sample undergoes magnetic resonance if the RF field frequency matches the Larmor frequency. Only

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those spins that are within a thin resonant slice will satisfy the condition for magnetic resonance and interact with the cantilever. If the cantilever is forced into mechanical oscillation by positive feedback, the tip motion will cause the position of the resonant slice to oscillate. As the slice passes back and forth through an electron spin in the sample, the spin direction will be cyclically inverted due to an effect called adiabatic rapid passage [7]. The cyclic inversion is synchronous with the cantilever motion and affects the cantilever dynamics by changing the effective stiffness of the cantilever. Therefore, the spin-cantilever interaction can be detected by measuring small shifts in the period of the cantilever oscillation using a laser interferometer. This methodology has been used successfully to detect small ensembles of electron spins [1, 2].

Denote by $B_1(t)$ the amplitude of the RF magnetic field, $B_0(t)$ the amplitude of the tip magnetic field at the spin location, ω_{RF} the RF field frequency, and $\Delta B_0(t) = B_0(t) - \omega_{\mathrm{RF}}/\gamma$ the off-resonance field amplitude. The constant $\gamma = 5.6\pi \times 10^{10}\,\mathrm{s}^{-1}\mathrm{T}^{-1}$ is the gyromagnetic ratio. *If* $\Delta B_0(t)$ varies sufficiently slowly such that the adiabatic criterion $\mathrm{d}[\Delta B_0(t)]/\mathrm{dt} \ll \gamma B_1^2(t)$ is satisfied, the spin can be assumed to remain aligned with either $\vec{B}_{\mathrm{eff}}(t)$ or $-\vec{B}_{\mathrm{eff}}(t)$, where $\vec{B}_{\mathrm{eff}}$ is the effective magnetic field. These are the *spin-lock* and *anti-spin-lock* conditions, respectively.

3. MRFM SIGNAL MODELS

3.1 C-T random telegraph

Assume that the cyclic adiabatic criterion holds. In the iOSCAR protocol, $B_1(t)$ is turned off after every N_{skip} cycles over a half-cycle duration: this induces periodic transitions between the spin-lock and anti-spin-lock states. Let $\tilde{z}(t)$ be the result of frequency demodulating $z(t)$ to baseband. Using the perturbation analysis in [8], it can be shown that $\tilde{z}(t)$ is a square wave whose transitions coincide with those of $B_1(t)$ and is approximately periodic. Thus, spin detection can be accomplished by correlating $\tilde{z}(t)$ with a square wave reference derived from $B_1(t)$.

Unfortunately, the effects of random thermal noise and spin relaxation decorrelate $\tilde{z}(t)$ and the square wave signal reference. One model for this decoherence phenomenon is suggested by the Stern-Gerlach experiment [3]: the spins maintain either the spin-lock or anti-spin-lock states, but randomly change polarity during the course of the measurement. This leads to random transitions in $\tilde{z}(t)$, and we assume that their times are distributed according to a Poisson process with a rate of λ. Note that correlating $\tilde{z}(t)$ with the reference square wave, as was described in the previous paragraph, has the effect of cancelling out the deterministic transitions in $\tilde{z}(t)$. What remains after the correlation are the random transitions, and as the transition times are generated by a Poisson process, the resultant signal takes the form of a so-called random telegraph process [9].

Define $y(t)$ to be the result of correlating $\tilde{z}(t)$ with the reference square wave. Let $[0,T]$ be the total measurement time period over which the correlator integrates the measurements, and let $\vec{\tau} = \{\tau_i\}, i = 1,\ldots,\mathscr{K}$, be the time instants within this period at which random spin reversals occur. As $\vec{\tau}$ are the arrival times of a Poisson process with intensity λ, $\mathscr{K}$ is a Poisson random variable with rate λT. Thus, the random telegraph model is: $y(t) = s(t) + w(t)$ where $w(t)$ is Additive White Gaussian Noise (AWGN) with variance σ_w^2, and $s(t)$ is a random telegraph signal containing only the random transitions. The detection problem for this model is to design a test between the two hypotheses:

$$\begin{aligned} H_0 \text{ (spin absent)} &: \quad y(t) = w(t) \\ H_1 \text{ (spin present)} &: \quad y(t) = s(t) + w(t) \end{aligned} \tag{1}$$

for $t \in [0,T]$.

3.2 Generalized D-T Random Telegraph

Here, we treat $\vec{y} = [y_0,\ldots,y_{N-1}]'$ as samples of the baseband output of the frequency demodulator and correlator. The D-T random telegraph signal is a D-T Markov chain, and will be denoted by ζ_i, where $\zeta_i \in \{+A,-A\}, 0 \le i \le N-1$, and ζ_0 is equally likely to be either $\pm A$, where A can be computed from experimental parameters. The transition probabilities of $\zeta_i, i \ge 1$ are as follows:

$$P(\zeta_i|\zeta_{i-1}) = \begin{cases} p & \zeta_i = \zeta_{i-1} = A \\ 1-p & \zeta_i = -A, \zeta_{i-1} = A \\ q & \zeta_i = \zeta_{i-1} = -A \\ 1-q & \zeta_i = A, \zeta_{i-1} = -A \end{cases} \tag{2}$$

We restrict $0 < p,q < 1$. If $p = q$, we say that the transition probabilities are symmetric, and when $p \ne q$, we shall say that they are asymmetric. For the symmetric case, we can match the C-T model to the D-T model by equating the expected number of transitions of the Poisson process to that of the Markov chain. This results in $p = 1 - T_s\lambda$, where T_s is the sampling time interval and λ is the expected number of transitions per second. Define the signal vector $\vec{\zeta} = [\zeta_0,\ldots,\zeta_{N-1}]'$ and the noise vector $\vec{w} = [w_0,\ldots,w_{N-1}]'$. We shall model the w_i's as independent and identically distributed (i.i.d.) Gaussian random variables (r.v.s) with mean 0 and variance σ^2. The detection problem is then to decide between:

$$\begin{aligned} H_0 \text{ (spin absent)} &: \quad \vec{y} = \vec{w} \\ H_1 \text{ (spin present)} &: \quad \vec{y} = \vec{\zeta} + \vec{w} \end{aligned} \tag{3}$$

4. SIGNAL DETECTION STRATEGIES

We shall consider detectors for the D-T random telegraph. The detectors in this section operate on samples of $y(t)$, denoted by $\{y_i\}$. Define the SNR to be $\mathrm{SNR} = A^2/\sigma^2$ and its dB value to be $\mathrm{SNR_{dB}} = 10\log_{10}\mathrm{SNR}$.

One can derive the LRT for the D-T random telegraph. The LRT is a most powerful (MP) test that satisfies the Neyman-Pearson criterion: it maximizes the probability of detection (P_D) subject to a constraint on the probability of false alarm (P_F) [10], which is set by the user. This gives us a benchmark with which to compare other detectors tests. When the random transition times are known, the optimal LRT is the matched filter, called the omniscient matched filter (MF) in this paper. Although unimplementable in reality, the MF detector provides an absolute upper bound when comparing the various detectors' ROC curves.

Define $R_k(S) = P(\zeta_k = S|Y_{k-1},\ldots,Y_0)$, where $S \in \{\pm A\}$ and $k \ge 1$. Let $\gamma_{S_1,S_2} = P(S_1 \to S_2)$ be the probability that the signal ζ_i goes from S_1 in the current time step to S_2 in the next with $S_1, S_2 \in \{\pm A\}$. There exists a recursive formula for $R_k(S)$.

$$R_k(S) = \gamma_{A,S} \underbrace{\frac{e^{\frac{A}{\sigma^2}y_{k-1}}R_{k-1}(A)}{e^{\frac{A}{\sigma^2}y_{k-1}}R_{k-1}(A) + e^{-\frac{A}{\sigma^2}y_{k-1}}R_{k-1}(-A)}}_{\bigstar} + \gamma_{-A,S}(1-\bigstar) \quad (4)$$

for $k \geq 1$ and with initial conditions $R_0(A) = R_0(-A) = 1/2$. Note that $\bigstar = \exp(Ay_{k-1}/\sigma^2)R_{k-1}(A)/(\ldots)$. With this, one can derive the log LRT:

$$\ln \Lambda(\vec{y}) = \sum_{k=0}^{N-1} \ln \left[R_k(A)e^{\frac{A}{\sigma^2}y_k} + R_k(-A)e^{-\frac{A}{\sigma^2}y_k} \right] \underset{H_0}{\overset{H_1}{\gtrless}} \eta \quad (5)$$

The running time of the log LRT statistic is $\mathcal{O}(N)$, where N is the number of observations.

Under the regime of low SNR and long observation times ($N \gg 1$), the second-order expansion of (5) is approximately equal to the hybrid filtered energy/amplitude/energy detector:

$$\sum_k a_k^2 + \frac{1-\alpha^2}{2\alpha} C_{\mathrm{I}} \sum_k y_k + \frac{1-\alpha^2}{2\alpha} C_{\mathrm{II}} \sum_k y_k^2 \quad (6)$$

where $C_{\mathrm{I}} = (p-q)\sigma^2/[4qA(1-r)]$, $C_{\mathrm{II}} = r(1-q)/[2q(1-r)]$, and $r = p+q-1$. Here, $a_k = y_k * h_{\mathrm{LP}}[k]$, and $h_{\mathrm{LP}}[k]$ is the impulse response of the first-order, single-pole filter given by $H_{\mathrm{LP}}(z) = (1-\alpha)/2 \cdot (1+z^{-1})/(1-\alpha z^{-1})$, where we require $|\alpha| < 1$ for stability [11]. What this means is that in the aforementioned regime, we expect the hybrid detector to have performance similar to the optimal LRT test. When $p = q$, the second-order expansion of the LRT is approximately equal to the filtered energy detector for values of p close to 1. The filtered energy detector can be expressed as:

$$\sum_{i=0}^{N-1} a_i^2 \underset{H_0}{\overset{H_1}{\gtrless}} \eta \quad (7)$$

The complexity of the filtered energy and hybrid statistics is $\mathcal{O}(N)$.

5. SIMULATION RESULTS

The objective in this section is to compare the optimal LRT of the D-T random telegraph model (denoted by RT-LRT) with the filtered energy and hybrid detectors. Comparison of the various detectors is done using ROC curves, which is a plot of probability of detection (P_D) vs. probability of false alarm (P_F), and power curves, which is a plot of P_D vs. SNR at a fixed P_F. Some of the parameters used in the simulations are as follows: the natural frequency of the cantilever $\omega_0 = 2\pi \cdot 10^4$ rad s^{-1}; the sampling period $T_s = 1$ ms; and signal durations of $T = 60$ s and $T = 150$ s were used. The performance of the detectors varies as a function of T; in general, a larger T results in better performance. Realistic values of T are several orders of magnitude larger. Nevertheless, the comparative results obtained from using the two values of T above are representative of larger values. Indeed, our approximations to the optimal detectors improve with larger T.

Figure 1 depicts the simulated ROC curves at SNR = -35 dB, $\lambda = 0.5$ s^{-1}, and with symmetric transition probabilities ($p = q$). With $T_s = 1$ ms, this results in $p = q = 0.9995$. The RT-LRT, filtered energy, and hybrid detector curves are virtually identical, which confirms our previous analysis. The omniscient MF detector has the best performance, which is consistent with our expectations. We generated a power curve over a range of SNR under the same conditions as in Figure 2 with a fixed $P_F = 0.1$ The RT-LRT, filtered energy, and hybrid detector have similar performance from -30 dB to -45 dB. With this particular value of P_F and λ, the RT-LRT, filtered energy, and hybrid detector perform from 5 dB to 10 dB worse than the MF detector.

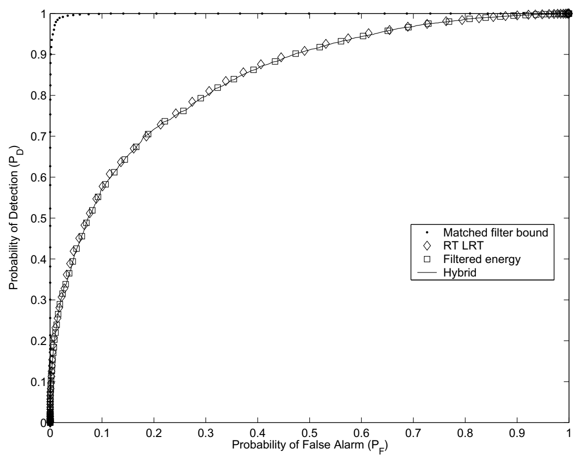

Figure 1: Simulated ROC curves for the D-T random telegraph model with symmetric transition probabilities at SNR = -35 dB, T = 60 s, and λ = 0.5 s^{-1} for the omniscient matched filter, D-T random telegraph LRT, filtered energy, and hybrid detectors. The RT-LRT is the optimal detector for this model.

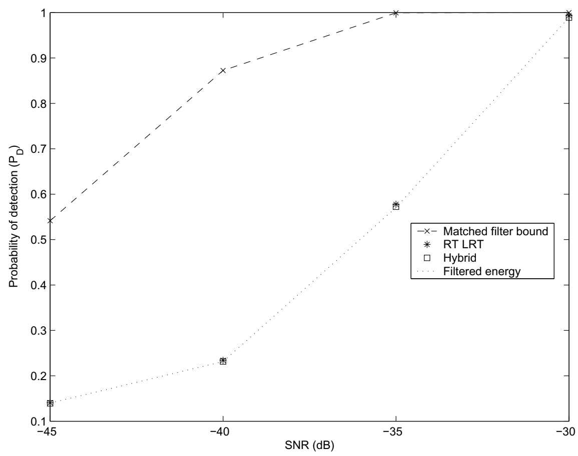

Figure 2: Simulated power curves (P_D vs. SNR) for the D-T random telegraph model with P_F fixed at 0.1 and $\lambda = 0.5$ s^{-1}, T = 60 s. The RT-LRT is the optimal detector for this model.

In the interest of space, ROC curves for a different value of λ will not be shown. However, performance degrades as

λ increases. In any case, the curves for the RT-LRT and filtered energy detector are similar. Before moving on, we would like to present an asymmetric case where $p \neq q$: set $p = 0.9998, q = 0.9992$. The ROC curves are presented in Figure 3. There is a noticeable difference between the curves of the RT-LRT and filtered energy detectors. The hybrid detector's curve is slightly below that of the LRT, and it is better than that of the filtered energy detector.

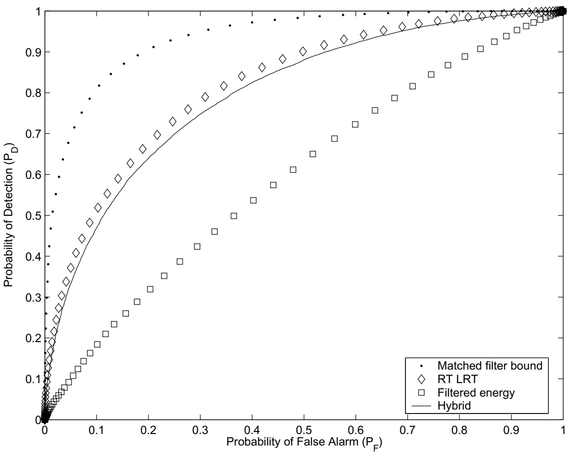

Figure 3: Simulated ROC curves for the D-T random telegraph model with asymmetric transition probabilities ($p = 0.9998, q = 0.9992$) at SNR = -45 dB, T = 150 s.

We generated a power curve from SNR = -55 dB to -35 dB for the asymmetric case in Figure 4. It seems that a larger value of T is required when $p \neq q$ for the hybrid filtered energy/amplitude/energy detector to approximate the optimal LRT, hence why we used $T = 150$ s for simulations of the asymmetric random telegraph model. The hybrid detector has better performance than the filtered energy detector, and has performance that is comparable to the RT-LRT for lower SNR values.

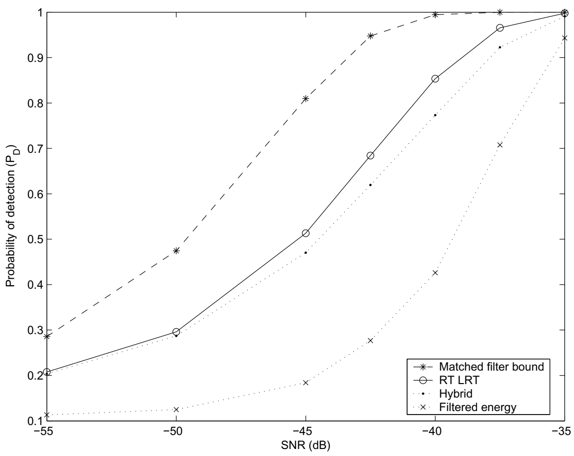

Figure 4: Simulated power curves (P_D vs. SNR) for the D-T random telegraph model with P_F fixed at 0.1, $p = 0.9998, q = 0.9992$, and T = 150 s. The RT-LRT is the optimal detector for this model.

6. CONCLUSION

We have developed the optimal LRT detector and two other approximately optimal detectors for the (generalized) D-T random telegraph model. We have shown that the filtered energy detector is approximately asymptotically optimal under the regime of low SNR, long observation times, and p close to 1 (the last two conditions imply a high time-bandwidth product). The last condition can be achieved by sampling at a sufficiently fast rate as compared to the rate of random transitions. In the case of the asymmetric D-T random telegraph model, we have shown that a hybrid filtered energy/amplitude/energy detector is an approximately asymptotically optimal detector under the regime of low SNR and long observation times.

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