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Estimating the State of a Quantum System in Real Time from Noisy Schrodinger Dynamics using Extended Kalman Filter

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Abstract—*In this paper we propose to apply the extended Kalman filter (EKF) algorithm to the problem of estimating dynamically the pure state of a quantum system evolving under the Schrodinger dynamics in the presence of white Gaussian noise (WGN). Noisy measurements of an observable in the randomly evolving state are taken. This leads to the proposed measurement model to which the EKF is applied to obtain the conditional expectation of the state at a time given observation up to that time. First we apply this to one free quantum particle in a cuboid and then to the truncated harmonic oscillator. MATLAB programs for implementing the noisy Schrodinger dynamics, the noisy measurements, the EKF and the riccati equation for the state estimation error covariance matrix are set up. Excellent noise to signal ratios (NSRs) are obtained.*

1. INTRODUCTION

In 1960 when Kalman filter came into existence it was for linear systems only. For nonlinear continuous time systems EKF [1] was designed in late 60s which linearizes an estimate of the mean and covariance in discrete time. To start with the system dynamics, its measurement model are presented as

$$x_k = f(x_{k-1}, v_k) + w_k \ (1)$$

$$z_k = h(x_k) + v_k \ (2)$$

where, $x_k \ \varepsilon \ R^n$ and $z_k \ \varepsilon \ R^m$ are the state vector and measurement vector, respectively; $w_k \sim N(0,Q)$ and $v_k \sim N(0,R)$ are the process noise and observation noise, respectively, both of these are assumed to be zero mean Gaussian noise. $Q \geq 0$ and $R>0$ are the covariances matrices for $w_k \sim N(0,Q)$ and $v_k \sim N(0,R)$, respectively. For any estimator of the current state based on measurements up to the current time, we need $P(t,x|z_t)$ i.e. the conditional probability density function of the current state given the measurements z_t up to the current time. Using this conditional probability density function, we can implement maximum likelihood, mmse, map, minimum L^P-norm estimator etc. Kushner's equation [2] is a stochastic pde for $P(t,x|z_t)$ which tells us how to compute this pdf recursively in time as we collect more and more measurements. However, since Kushner's equation is an infinite dimensional filter and hence it is not implementable. The EKF is an implementable finite dimensional approximate estimation to Kushner's equation and rather than giving the entire conditional pdf, it gives the approximate conditional mean and conditional covariance of the current state based on measurements up to the current time. Conditional mean is the same as the mmse. The EKF gives the conditional mean and covariance on a real time basis.

2. BRIEF REVIEW OF KUSHNER'S EQUATION

In 1964, Kushner presented an equation for the conditional probability density of the state of a stochastic non-linear system and a noisy measurement of the system state. Let us assume the state of the system and noisy measurements of that system state are

$$dX_t = f(t, X_t)dt + g(t, X_t)dB_t \ (3)$$

$$dZ_t = h(t, X_t)dt + \sigma dv_t \ (4)$$

where, $X_t \ \varepsilon \ R^n$ is the process state and $Z_t(t) \ \varepsilon \ R^q$ is the noisy observation process. $B_t \ \varepsilon \ R^m$ and $v_t \ \varepsilon \ R^q$ are the brownian motions [3] representing the process noise and obsevation noise respectively. Let $Z_t=\{Z(s):s\leq t\}$ i.e. the set of measurements up to time t. We have to find $p(X_t|Z_t)$; first we will find $p(X_{t+}dt|Zt_{+dt})$

$$p(X_{t+dt}|\, Z_{t+dt}) = \frac{p(X_{t+dt}, Z_t, dz_t)}{p(\, Z_t, dz_t)} \ (5)$$

$$p(X_{t+dt}|\, Z_{t+dt}) = \frac{\int p(dz_t|X_t)p(X_{t+dt}|\, X_t)p(X_t|\, z_t)dX_t}{\int p(dz_t|X_t)p(X_{t+dt}|\, X_t)p(X_t|\, z_t)dX_{t+dt}} \ (6)$$

Using the state and noisy measurement equations and applying quantum ito's formula [4] to it kushner's equation is obtained.

$$dp(x,t) = L\big(p(x,t)\big)dt + \big(h(x,t) - E_t h(x,t)\big)^T R^{-1}(t)(\, dz_t - E_t h(x,t)dt)p(x,t) \ (7)$$

where, p(x,t) is conditional probability density, L is the Kolmogorov forward operator. Here E_t denotes conditional expectation of a random variable given Z_t

3. SCHRODINGER'S EQUATION NOISE, COMPLEX AND REAL

First we will transform the complex Shrodinger's equation [5] of dimension N into a real Shrodinger's equation of dimension 2N. Noisy measurements of an observable X is randomly evolving state |ψ(t)> are taken. This leads to the measurement model.

$\dot{z}(t) =< \psi(t)|X|\psi(t) > +\dot{V}(t)$ (8)

where $\dot{V}(t)$ is white gaussian noise. The EKF is applied to this model to obtain the conditional expectation of the state. First, we apply this to a 2X2 Hamilton matrix.

$$d\begin{bmatrix}\psi_R(t)\\ \psi_I(t)\end{bmatrix} = K(t)\begin{bmatrix}\psi_R(t)\\ \psi_I(t)\end{bmatrix}\psi_R(t)dt + \begin{bmatrix}V_I\psi_R + V_R\psi_I\\ V_R\psi_R - V_I\psi_I\end{bmatrix} dB(t) \quad (9)$$

where, ψ_R and ψ_I both are 2X2 matrix; then (9) can be seen to be the same as the noisy Schrodinger equation [6]

$$d\underline{\psi}(t) = \left(-(iH + V^2/2)dt + VdB(t)\right)\underline{\psi}(t) \quad (10)$$

where, the non-skew Hamilton term $V^2/2dt$ is a consequence of using Ito's formula $(dB(t))^2=dt$ to guarantee evolution, i.e.

$$d\left(\underline{\psi}(t)\underline{\psi}^*(t)\right) = 0 \quad (11)$$

and hence $\underline{\psi}(t)\underline{\psi}^*(t)=1$ ∀ t≥0 if $\underline{\psi}(0)\underline{\psi}^*(0)==1$. K(t) is Kalman filter gain which is defined for the above equation as

$$K(t) = \begin{bmatrix} H_I - 1/2(V^2)_R & H_R + 1/2(V^2)_I\\ -H_R + 1/2(V^2)_I & H_I + 1/2(V^2)_R\end{bmatrix} \quad (12)$$

where, H_I and H_R both are 2X2 Hamilton matrices. If we define

$\psi(t) = \psi_R(t) + j\psi_I(t)$ (13)

$H = H_R + jH_I$ (14)

$V = V_R + jV_I$ (15)

$V^2 = (V^2)_R + j(V^2)_I$ (16)

${V_R}^2 - {V_I}^2 = (V^2)_R$ (17)

$2V_RV_I = (V^2)_I$ (18)

The measurement equation for the proposed model is given by

$dZ(t) =< \psi \mid X \mid \psi > dt + \sigma_v dv(t)$ (19)

Thus,

$h(\psi_R,\psi_I) = Re[({\psi_R}^T - i{\psi_I}^T)(X_R - iX_I)(\psi_R + i\psi_I)]$ (20)

where, σ_v is the spectral strength. Since ${X_R}^T=X_R$ and ${X_I}^T=-X_I$ so on expanding equation 20, we get

$h = {\psi_R}^T X_R\psi_R + {\psi_I}^T X_R\psi_I - {\psi_R}^T X_I\psi_I + {\psi_I}^T X_I\psi_R$ (21)

$$\widehat{H}_t^{\,T} = \begin{bmatrix}\left(\frac{\delta h}{\delta\psi_I}\right)^T\\ \left(\frac{\delta h}{\delta\psi_R}\right)^T\end{bmatrix} = 2\begin{bmatrix}X_R\psi_R - X_I\psi_I\\ X_R\psi_I + X_I\psi_R\end{bmatrix} \quad (22)$$

The EKF obtained by approximating the Kushner filter has it's error covariance P(t) satisfying the Riccati equation [7]

$$\frac{dP_t}{dt} = K(t)P(t) + P(t)K(t)^T - {\sigma_v}^{-2}P(t)\widehat{H}_t^{\,T}\widehat{H}_tP(t) + \widehat{G}_t\widehat{G}_t^{\,T} \quad (23)$$

Where

$$\widehat{H}_t^{\,T} = 2\begin{bmatrix}X_R\widehat{\psi}_R(t) - X_I\widehat{\psi}_I(t)\\ X_R\widehat{\psi}_I(t) - X_I\widehat{\psi}_R(t)\end{bmatrix} \quad (24)$$

and

$$\widehat{G}_t = \begin{bmatrix}V_I\widehat{\psi}_R(t) - V_R\widehat{\psi}_I(t)\\ V_R\widehat{\psi}_R(t) - V_I\widehat{\psi}_I(t)\end{bmatrix} \quad (25)$$

We define

$$\widehat{E}(t) = \begin{bmatrix}\widehat{\psi}_R(t)\\ \widehat{\psi}_I(t)\end{bmatrix} = E[\begin{bmatrix}\psi_R(t)\\ \psi_I(t)\end{bmatrix} |Z_s, s \le t] \quad (26)$$

Then

$$\widehat{H}_t^{\,T} = 2\begin{bmatrix}X_R & -X_I\\ X_I & X_R\end{bmatrix}\widehat{E}(t) = X_0\widehat{E}(t) \quad (27)$$

Also,

$$h(\widehat{\psi}_R,\widehat{\psi}_I) = [{\psi_R}^T\ {\psi_I}^T]\begin{bmatrix}X_R & -X_I\\ X_I & X_R\end{bmatrix}\begin{bmatrix}\widehat{\psi}_R(t)\\ \widehat{\psi}_I(t)\end{bmatrix} = \widehat{E}(t)^T X_0\widehat{E}(t) \quad (28)$$

So equation 23 can be expressed as

$$\frac{dP_t}{dt} = K(t)P(t) + P(t)K(t)^T - {\sigma_v}^{-2}P(t)X_0\widehat{E}(t)\widehat{E}(t)^T X_0P(t) + V_0\widehat{E}(t)\widehat{E}(t)^T V_0 \quad (29)$$

where

$$V_0 = \begin{bmatrix}V_I & V_R\\ V_R & -V_I\end{bmatrix} \quad (30)$$

The EKF state estimate evolution is given by

$$d\widehat{E}(t) = K(t)\widehat{E}(t)dt + {\sigma_v}^{-2}P(t)\widehat{H}_t^{\,T}\left(dZ(t) - h\left(\widehat{E}(t)\right)dt\right) \quad (31)$$

with $h(\widehat{E}(t))= \widehat{E}(t)^T X_0\widehat{E}(t)$. After applying EKF to one cuboid and obtaining the desired results; We will apply the same to the truncated harmonic oscillator. Equations for Schrodinger dynamics, the noisy measurements, the EKF and the Riccati equation for the state estimator error covariance matrix are derived. C matrix is created which is derived using quantum filtering [8] and applying creation and annhilation operators. The noisy Schrodinger dynamics the state vector $[C_m(t)]_m$ in the eigen basis of the harmonic oscillator taking into account it's corrections is given by m+1/2 is the m[th] executive state of the unperturbed oscillator.

$$dC_m(t) = [-i(m+1/2)C_m(t) - 1/2\sum_n < m|L^2|n > C_n(t)]dt - idB(t)\sum_n < m|L|n > C_n(t) \quad (32)$$

where, L= $\alpha a+\bar{\alpha}a^+$ in which a nd a^+ are annhilation and creation operator respectively; a|n>=$\sqrt{n}$|n-1> and a^+|n> =$\sqrt{n+1}$|n+1> are defined in this way and similarly

$$< m|L|n = \alpha < n|a|n > +\bar{\alpha} < m|a^+|n > \quad (33)$$

Equation 32 can be expressed in matrix notation as

$$dC_R = (A_R C_R - A_I C_I)dt + (Q_R C_R - Q_I C_I)dB \quad (34)$$

$$dC_I = (A_R C_I - A_I C_R)dt + (Q_R C_I - Q_I C_R)dB \quad (35)$$

where, A_R, A_I are constructed out of the energy levels m+1/2, m=0,1,... and the matrix elements <m|L[2]| n> of L^2. On combining equation 34 and 35, it can be written in matrix form.

$$d\begin{bmatrix}\underline{C_R}\\ \underline{C_I}\end{bmatrix} = \begin{bmatrix}A_R & -A_I\\ A_I & A_R\end{bmatrix}\begin{bmatrix}C_R\\ C_I\end{bmatrix}dt + \begin{bmatrix}Q_R & -Q_I\\ Q_I & Q_R\end{bmatrix}\begin{bmatrix}C_R\\ C_I\end{bmatrix}dB(t) \quad (36)$$

where, A is interpreted as the gain factor, $\underline{C}(t) = \underline{C_R}(t) + j\underline{C_I}(t)$ is the predicted state matrix. The measuerment state for a truncated harmonic osscilator using EKF could be defined as

$$dz(t) = ({C_R}^T - j{C_I}^T)(X_R + jX_I)(C_R + jC_I)dt + \sigma_v dv(t) \quad (37)$$

On solving, equation 37 and considering the real part only; It can be defined in matrix form as follows

$$dz(t) = [{C_R}^T \quad {C_I}^T]\begin{bmatrix}X_R & -X_I\\ X_I & X_R\end{bmatrix}\begin{bmatrix}C_R\\ C_I\end{bmatrix} + \sigma_v dv(t) \quad (38)$$

where, $\sigma_v dv(t)$ is the noisy term. Now the estimated state is derived and is expressed in the matrix form.

$$d\begin{bmatrix}\hat{C}_R\\ \hat{C}_I\end{bmatrix} = \begin{bmatrix}A_R & -A_I\\ A_I & A_R\end{bmatrix}\begin{bmatrix}\hat{C}_R\\ \hat{C}_I\end{bmatrix}d + P(t)\begin{bmatrix}X_R & -X_I\\ X_I & X_R\end{bmatrix}\begin{bmatrix}\hat{C}_R\\ \hat{C}_I\end{bmatrix}(dz(t) - [\hat{C}_R^T \quad \hat{C}_I^T]\begin{bmatrix}X_R & -X_I\\ X_I & X_R\end{bmatrix}\begin{bmatrix}\hat{C}_R\\ \hat{C}_I\end{bmatrix}dt) \quad (39)$$

where, P(t) is the covariance matrix of dimension 4X4. After updating the state and measurement estimates let us update the covariance estimate, using the Riccati equation:

$$\frac{dP(t)}{dt} = P(t)\left(\begin{bmatrix}A_R & -A_I\\ A_I & A_R\end{bmatrix} + \begin{bmatrix}A_R & -A_I\\ A_I & A_R\end{bmatrix}^T\right) - {\sigma_v}^{-2}P(t)\begin{bmatrix}X_R & -X_I\\ X_I & X_R\end{bmatrix}\begin{bmatrix}\hat{C}_R\\ \hat{C}_I\end{bmatrix}[\hat{C}_R^T \quad \hat{C}_I^T]\begin{bmatrix}X_R & -X_I\\ X_I & X_R\end{bmatrix} + \begin{bmatrix}Q_R & -Q_I\\ Q_I & Q_R\end{bmatrix}\begin{bmatrix}\hat{C}_R\\ \hat{C}_I\end{bmatrix}[\hat{C}_R^T \quad \hat{C}_I^T]\begin{bmatrix}Q_R & -Q_I\\ Q_I & Q_R\end{bmatrix} \quad (40)$$

where Q_R, Q_I are constructed out of the matrix elements <m|L|n> of L. The NSR is calculated as follows:

$$NSR = \frac{\sum_t ||\psi(t) - \hat{\psi}(t)||^2}{\sum_t ||\psi(t)||^2} \quad (41)$$

4. SIMULATION RESULTS

Simulated noisy Schrodinger equation which generates the evolution of wave function. The wave function ψ is shown in fig. 1.

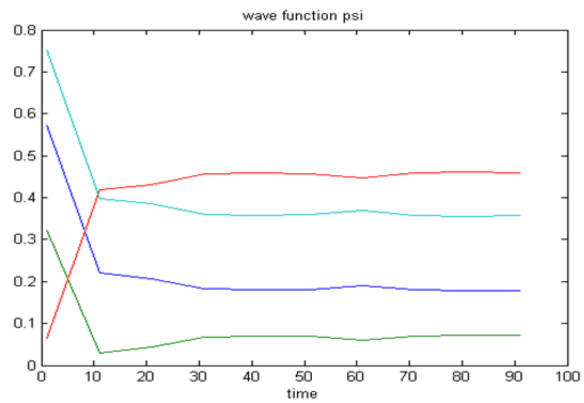

Fig. 1: Wave Function

The absolute square of difference between our wave function and $\hat{\psi}$ is given in fig. 2.

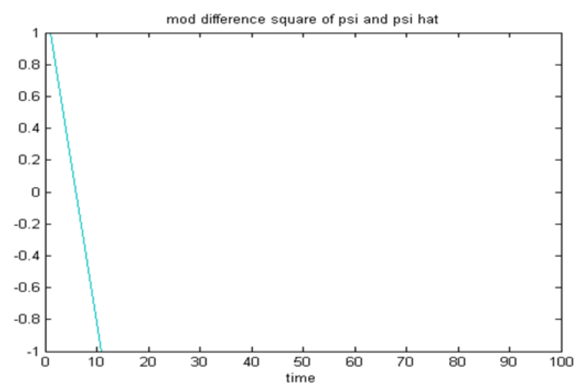

Fig. 2: $|\psi|^2$ - $|\hat{\psi}|^2$

Our graph show decrease of NSR with time and this implies that the EKF performs well. This is shown in fig. 3.

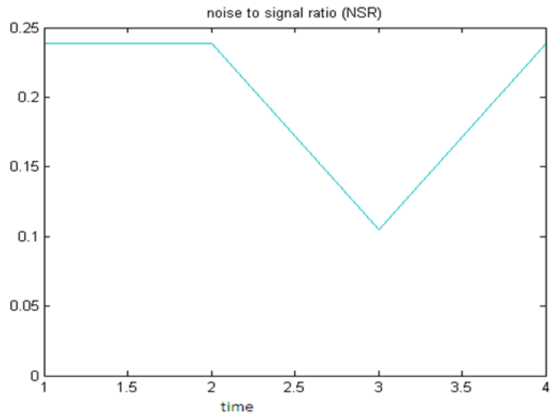

Fig. 3: Noise to Signal Ratio

5. CONCLUSION

In this paper, we first simulate noisy Schrodinger dynamics of a quantum system by taking into account the Ito correction term in the dynamics to preserve unitarity of the evolution (i.e. conservation of probability). We then simulate the measurement process which consists of measuring the average value of an observable X is the current state $|\psi_t\rangle$ taking into account additive white Gaussian noise. The measurement process is thus a quadratic function of the state ($\langle\psi_t|X|\psi_t\rangle$). We then simulate the EKF which computes the estimate of the current state $|\psi_t\rangle$ given noisy measurements of $\langle\psi_t|X|\psi_t\rangle$, upto time t ($s \leq t$). We plot the state evolution and its estimate based on the EKF with time. We also plot the probability error $|\psi_t|^2 - |\hat{\psi}_t|^2$ with time. The error remain constant for some time and then shows a gradual decrease followed by an increase. Simulations for further times are thus likely to show bounded oscillations of the error about a fixed value. It is noteworthy that the NSR remains bounded between 0.1 and 0.25, which implies that by measuring a single observable, we are able to get good estimates. Further improvement is possible if more than one observable is measured. However, in view of the Heisenberg uncertainty principle, the measured observables should commute with each other for simultaneous measurement to be possible.

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