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To cite this version:

Jean-Pierre Vila. Nonparametric multi-step prediction in nonlinear state space dynamic systems. Statistics and Probability Letters, 2010, 81 (1), pp.71. 10.1016/j.spl.2010.09.020 . hal-00698852

HAL Id: hal-00698852

https://hal.science/hal-00698852

Submitted on 18 May 2012

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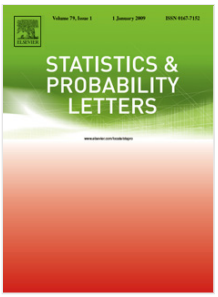

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PII: S0167-7152(10)00270-1
DOI: 10.1016/j.spl.2010.09.020
Reference: STAPRO 5806

To appear in: *Statistics and Probability Letters*

Received date: 24 March 2010
Revised date: 23 September 2010
Accepted date: 24 September 2010

Please cite this article as: Vila, J.-P., Nonparametric multi-step prediction in nonlinear state space dynamic systems. *Statistics and Probability Letters* (2010), doi:10.1016/j.spl.2010.09.020

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Nonparametric multi-step prediction in nonlinear state space dynamic systems

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Abstract

Filtering and smoothing of stochastic state space dynamic systems have benefited from several generations of estimation approaches since the seminal works ol Kalman in the sixties. A set of global analytical or numerical methods are now available, as the well known sequential Monte Carlo particle methods which offer some theoretical convergence results for both types of problem. However save in the case of linear Gaussian systems, objectives of the third kind *i.e. prediction* objectives, which aim at estimating k time steps ahead the anticipated probability density function of the system state variables, conditional on past and present system output observations, still raise theoretical and practical difficulties. The aim of this paper is to propose a nonparametric particle multi-step prediction method able to consistently estimate such anticipated conditional pdf of the state variables as well as their expectations.

Keywords: state space dynamic systems; prediction; filtering; smoothing; kernel density estimators.

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1 Introduction

Given a discrete-time dynamic system with unobserved state variables x_t and observed output variables y_t, one often wants to estimate when it exists, the conditional probability density function (pdf) $p(x_{t+k}|y_1, \ldots, y_t)$, from the knowledge of the system model and some initial distribution of the state variables. When $-t < k < 0$ the problem is known as *smoothing*. When $k = 0$, it is known as *filtering*, and it is known as *prediction* when $k > 0$. The theoretical general solution of this estimation problem is given by the so-called *Bayesian Recursive Relations* (BRR). However it can be solved exactly only in the linear Gaussian case (Anderson and Moore,1979) and corresponds to the well-known Kalman filter/predictor/smoother (K-FPS). See Lewis (1986). In the general case one has to resort to some approximation approaches of the Bayesian Recursive Relations solutions. The first ones have been local approaches, in which the nonlinear state model and/or observation model are approximated by Taylor series. They have given rise to the famous and widely used Extended K-FPS and its refinements, as the Second Order K-FPS, the Iterative K-FPS, and some derivative-free versions, and also to a large amount of literature (Jazwinski 1970, Tanizaki 1993, Nørgaard *et al.* 2000, Duník *et al.* 2005, to cite just a few). Other local approaches rely on approximations of the state variables pdf rather than the model equations, leading for example to the so-called Unscented Kalman filter (Wan and Van der Merwe 2000, Julier and Uhlmann 2004). The local validity of these approximations does not ensure convergence of the corresponding pdf estimates and the main interest of these approaches is their relative simplicity when approximating the BRR solutions. Global approximation approaches to the state FPS problem, with validity in the full state space, have also been de-

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veloped. A first global, analytical approach, is represented by the Gaussian Sum method which involves multiple linearizations of the state space and approximations of the conditional state variables pdf by sums of Gaussian densities, providing weighted averages of collections of Extended K-FPS (Sorenson and Alspach 1971, Šimandl and Královec 2000). More accurate but also more computer-intensive, global approximation methods, are numerical methods which approximate the state space by a system of numerous discrete points. For example, the Point Mass method (Kramer and Sorenson 1988, Šimandl *et al.* 2006, Královec and Šimandl 2004) approximates the state space by an orthonormal grid. Other and now famous numerical global approaches are the Monte Carlo approaches in which the state space is approximated by randomly distributed particles (Liu and Chen 1998, Doucet *et al.* 2001).They benefited from theoretical convergence results (Del Moral 1998, 2004, Del Moral *et al.* 2001). Several convergence improvements starting from the discrete nature of the probability distribution approximation provided by the first sequential importance sampling and resampling Monte Carlo approaches, were performed, as probability distribution regularizations (Musso *et al.* 2001). But in spite of their acknowledged efficiency in smoothing and especially filtering estimation problems (Doucet and Johansen 2009, Briers *et al.* 2009), the theoretical and practical application of the particle methods to *prediction problems* seems to be not so advanced. The issue is however of great concern and deserves special attention: an efficient multi-step prediction facility is of crucial importance in several applications of the dynamic systems state space modelling approach (*e.g.* radio guidance, economics, predictive miocrobiology, etc) an especially in predictive control context (Magni *et al.* 2009).

The aim of this note is to propose such a convergent multi-step prediction

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method, relying on sequential recursive random particle simulations and non-parametric density estimation procedures. This prediction method can be seen as an extension of a new generation of convergent filtering methods based on convolution kernel density estimation and implicit regularization of both state and output variables probability distribution estimates (Rossi 2004, Rossi and Vila 2005, 2006, Hilgert *et al.* §3.2, 2007). Moreover this approach allows to deal with the frequent situation in which the probability distributions of both state and output variables are analytically unknown but can be simulated.

The paper is organized as follows. Section 2 presents the general structure of stochastic state space models to be considered. The multi-step prediction problem and the corresponding Bayesian recursive relations are introduced in Section 3. Section 4 is devoted to the construction of the proposed nonparametric particle multi-step predictor. Its convergence properties are presented in Section 5.

2 The modelling context

The systems of interest are supposed to obey general state space models of the form:

$$\begin{cases} x_t &= f_t(x_{t-1}, \theta^x, \varepsilon_t) \\ y_t &\backsim g_t(.|x_t, \theta^y) \end{cases} \tag{1}$$

in which $x_t \in I\!R^d$ is the vector of the unobserved state variables, $y_t \in I\!R^q$ that of the observed output variables. $\theta = (\theta^{xT}, \theta^{yT})^T \in \Theta \subset I\!R^p$ is a vector of p unknown fixed parameters. ε_t is a vector of random variables (possibly noises),

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the $\{\varepsilon_t\}$ being independent from each other. f_t is a known Borel measurable function. g_t is an absolutely continuous probability distribution function with bounded density. f_t and g_t can both be possibly time-varying. The probability distribution function g_t and that of ε_t are not necessarily known but supposed to be at least simulatable. As a particular case the output variables model can be given by a regression equation $y_t = r_t(x_t, \theta^y, \eta_t)$ in which r_t is a known Borel measurable function, where η_t is a vector of random variables (possibly noises) supposed to be at least simulatable.

Remark 1 In predictive control context (Magni et al. *2009), some control variables u_t are present in the state model function f_t, in order to allow the optimization over a chosen sliding horizon, of a given criterion function of the predicted state variables values. The principles of the prediction algorithm to be presented in the following are unchanged and easily adapted to that case.*

2.1 Assumptions and notations

Let

- p_0^x : the known probability density of the state variables x at time $t = 0$.
- p_0^θ : a given prior density for $\theta \in \Theta$, non zero for θ^* the true values of the parameters.
- $\mathcal{L}_{\varepsilon_t}$: the probability distribution function of ε_t, not necessarily analytically known but at least simulatable whatever t.
- $y_{1:t} := (y_1, \ldots, y_t)$, observed values of the output variables up to time t (notation).

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3 The multi-step prediction problem

Given a positive time shift k, the objective as told previously is to estimate at time t, $p(x_{t+k}|y_{1:t})$, the k-step-ahead probability density of the state vector x_{t+k}, conditional on the observed values up to time t of the output variables. One can also wish to estimate the corresponding conditional expectation $\mathbb{E}[x_{t+k}|y_{1:t}]$. The pdf of interest $p(x_{t+k}|y_{1:t})$ satisfies the following obvious Bayesian recursive relation:

$$\begin{aligned} p(x_{t+k}|y_{1:t}) &= \int p(x_{t+k}, x_{t+k-1}|y_{1:t})\mathrm{d}x_{t+k-1} \\ &= \int p(x_{t+k}|x_{t+k-1}, y_{1:t})p(x_{t+k-1}|y_{1:t})\mathrm{d}x_{t+k-1} \\ &= \int p(x_{t+k}|x_{t+k-1})p(x_{t+k-1}|y_{1:t})\mathrm{d}x_{t+k-1} \end{aligned} \tag{2}$$

Only in few special cases (as linear systems with Gaussian noises) can this recursive equation be solved analytically, starting from the filtering pdf $p(x_t|y_{1:t})$. The next section is devoted to a convergent nonparametric particle estimation of the solution of this equation.

4 A nonparametric approach

4.1 A reformulation of the problem

At time t:

Let us consider the state vector x at the k next future times:

$$\begin{aligned} x_{t+1} &= f_{t+1}(x_t, \theta, \varepsilon_{t+1}) = f_{t+1}(f_t(x_{t-1}, \theta, \varepsilon_t), \theta, \varepsilon_{t+1}) := F_{t+1}(x_{t-1}, \theta, \varepsilon_t, \varepsilon_{t+1}) \\ x_{t+2} &= f_{t+2}(x_{t+1}, \theta, \varepsilon_{t+2}) = \ldots := F_{t+2}(x_{t-1}, \theta, \varepsilon_t, \varepsilon_{t+1}, \varepsilon_{t+2}) \\ &\vdots \\ x_{t+k} &= f_{t+k}(x_{t+k-1}, \theta, \varepsilon_{t+k}) = \ldots := F_{t+k}(x_{t-1}, \theta, \varepsilon_t, \varepsilon_{t+1}, \ldots, \varepsilon_{t+k}) \end{aligned} \tag{3}$$

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Let us consider the following k random variables:

$\nu_t^1 \sim \mathcal{L}_{\varepsilon_{t+1}}, \quad \nu_t^2 \sim \mathcal{L}_{\varepsilon_{t+2}}, \quad \ldots, \quad \nu_t^k \sim \mathcal{L}_{\varepsilon_{t+k}}.$

Let us then define k new variables of dimension d, $z_t^i, i = 1, \ldots, k$, such that: $z_t^i = F_{t+i}(x_{t-1}, \theta, \varepsilon_t, \nu_t^1, \ldots, \nu_t^i)$.

The variables $\{z_t^i\}$ are jointly distributed as the corresponding variables x_{t+i}, $i = 1, \ldots, k$, and the recursive relation (2) applies to the z_t^i's as well, particularly to z_t^k:

$$p(z_t^k|y_{1:t}) \;=\; \int p(z_t^k|z_t^{k-1})p(z_t^{k-1}|y_{1:t})\mathrm{d}z_t^{k-1} \tag{4}$$

Estimating the conditional pdf $p(z_t^k|y_{1:t})$ is then equivalent to estimating the pdf of interest $p(x_{t+k}|y_{1:t})$.

The remaining of the paper is devoted to a convergent approximation of (4).

4.2 Nonparametric particle estimation of $p(z_t^k|y_{1:t})$

Let us introduce z_t^k as a new state variable of dimension d into the state equations of model (1), and let us also introduce as state equation the parameter invariance equality $\theta_t = \theta_{t-1}$. Model (1) is unchanged by these additions but it writes now:

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$$\begin{cases} x_t &= f_t(x_{t-1}, \theta^x_{t-1}, \varepsilon_t) \\ z^k_t &= F_{t+k}(x_{t-1}, \theta^x_{t-1}, \varepsilon_t, \nu^1_t, \ldots, \nu^k_t) \\ \theta_t = \theta_{t-1} \\ y_t &\backsim g_t(.|x_t, \theta^y_{t-1}) \end{cases} \tag{5}$$

The estimation of the joint conditional pdf $p(x_t, z^k_t, \theta_t|y_{1:t})$ and its marginals $p(x_t|y_{1:t})$, $p(z^k_t|y_{1:t})$, $p(\theta_t|y_{1:t})$, is now a filtering problem. A convergent non-parametric particle filtering approach has been recently proposed to solve filtering problems under the mild assumptions of Section 2 (Rossi 2004, Rossi and Vila 2006, 2005, Hilgert *et al.* §3.2, 2007). In the following this approach is adapted to the estimation of the pdf $p(z^k_t|y_{1:t})$.

The approach relies on the simulation of n particles $(\tilde{x}^i_t, \tilde{z}^{k,i}_t, \tilde{\theta}^i_t, \tilde{y}^i_t)$, $i = 1, \ldots, n$, at each time step t.

Let:

- $K^y_{\Delta_n}(v) = \Pi^q_{j=1} \frac{1}{\delta^y_{n,j}} K^y(\frac{v_j}{\delta^y_{n,j}})$, where $K^y(.)$ is a positive bounded Parzen-Rosenblatt kernel (Parzen 1962) of dimension 1, and v_j is the jth component of the vector v of dimension q. $\delta^y_{n,j}$ is the kernel window width parameter, chosen empirically. In the present case, a relevant choice can be derived from recommendations of Silverman (1986):
  At time t: $\delta^y_{n,j} = 1.06 \times \min\left(\sqrt{\mathrm{var}(\tilde{y}_{t,j})}, \frac{\mathrm{iqr}(\tilde{y}_{t,j})}{1.34}\right) \times n^{-\frac{1}{4+q}}$, where $\tilde{y}_{t,j}$ is the vector of the n particles $(\tilde{y}^i_{t,j},\ i = 1, \ldots, n\ )$ and $\mathrm{iqr}(\tilde{y}_{t,j})$ is the inter-quartile range of the $\tilde{y}^i_{t,j},\ i = 1, \ldots, n$.
  we shall denote: $\Delta^q_n = \Pi^q_{j=1} \delta^y_{n,j}$.

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- $K^x_{\Delta_n}(.), K^z_{\Delta_n}(.), K^\theta_{\Delta_n}(.)$: positive bounded Parzen-Rosenblatt kernels of dimension d, d and p, corresponding to x, z^k, and θ respectively, defined like $K^y_{\Delta_n}(.)$ for the output vector y, and with window width parameters analog to that of the kernel $K^y_{\Delta_n}(.)$ and collectively denoted as δ_n, vector of dimension $q+2d+p$.

  we shall denote: $\Delta_n^{q+2d+p} = \Pi_{j=1}^q \delta^y_{n,j} \cdot \Pi_{j=1}^d \delta^x_{n,j} \cdot \Pi_{j=1}^d \delta^z_{n,j} \cdot \Pi_{j=1}^p \delta^\theta_{n,j}$.

Algorithm:

- Step $t=0$: For $i=1,\dots,n$: $\bar{x}_0^i \sim p_0^x$, $\bar{\theta}_0^i \sim p_0^\theta$, $t=t+1$.
- Step $t>0$: For $i=1,\dots,n$
  - if $t=1$: $\tilde{\varepsilon}_1^i \sim \mathcal{L}_{\varepsilon_1}$, $\tilde{\nu}_1^{1,i} \sim \mathcal{L}_{\varepsilon_2}$, $\dots$, $\tilde{\nu}_1^{k,i} \sim \mathcal{L}_{\varepsilon_{1+k}}$, $\tilde{x}_1^i = f_1(\bar{x}_0^i, \bar{\theta}_0^{x,i}, \tilde{\varepsilon}_1^i)$, $\tilde{z}_1^{k,i} = F_{1+k}(\bar{x}_0^i, \bar{\theta}_0^{x,i}, \tilde{\varepsilon}_1^i, \tilde{\nu}_1^{1,i}, \dots, \tilde{\nu}_1^{k,i})$, $\tilde{\theta}_1^i = \bar{\theta}_0^i$, $\tilde{y}_1^i \sim g_1(.|\tilde{x}_1^i, \tilde{\theta}_1^{y,i})$.
  - if $t>1$: $(\bar{x}_{t-1}^i, \bar{z}_{t-1}^{k,i}, \bar{\theta}_{t-1}^i) \sim p^n(x, z^k, \theta | y_{1:t-1})$, $\tilde{\varepsilon}_t^i \sim \mathcal{L}_{\varepsilon_t}$, $\tilde{\nu}_t^{1,i} \sim \mathcal{L}_{\varepsilon_{t+1}}$, $\tilde{\nu}_t^{2,i} \sim \mathcal{L}_{\varepsilon_{t+2}}$, $\dots$, $\tilde{\nu}_t^{k,i} \sim \mathcal{L}_{\varepsilon_{t+k}}$, $\tilde{x}_t^i = f_t(\bar{x}_{t-1}^i, \bar{\theta}_{t-1}^{x,i}, \tilde{\varepsilon}_t^i)$, $\tilde{z}_t^{k,i} = F_{t+k}(\bar{x}_{t-1}^i, \bar{\theta}_{t-1}^{x,i}, \tilde{\varepsilon}_t^i, \tilde{\nu}_t^{1,i}, \dots, \tilde{\nu}_t^{k,i})$, $\tilde{\theta}_t^i = \bar{\theta}_{t-1}^i$, $\tilde{y}_t^i \sim g_t(.|\tilde{x}_t^i, \tilde{\theta}_t^{y,i})$.

  Let

$$p^n(x, z^k, \theta | y_{1:t}) := \frac{\sum_{i=1}^n K^y_{\Delta_n}(\tilde{y}_t^i - y_t) \times K^x_{\Delta_n}(\tilde{x}_t^i - x) \times K^z_{\Delta_n}(\tilde{z}_t^{k,i} - z^k) \times K^\theta_{\Delta_n}(\tilde{\theta}_t^i - \theta)}{\sum_{i=1}^n K^y_{\Delta_n}(\tilde{y}_t^i - y_t)} \quad (6)$$

$$p^n(z^k | y_{1:t}) := \frac{\sum_{i=1}^n K^y_{\Delta_n}(\tilde{y}_t^i - y_t) \times K^z_{\Delta_n}(\tilde{z}_t^{k,i} - z^k)}{\sum_{i=1}^n K^y_{\Delta_n}(\tilde{y}_t^i - y_t)} \quad (7)$$

  $t = t+1$, go back to Step t.

$p^n(x, z^k, \theta | y_{1:t})$ and $p^n(z^k | y_{1:t})$ are nonparametric particle estimators of the conditional joint and marginal pdf $p(x, z^k, \theta | y_{1:t})$ and $p(z^k | y_{1:t})$ of (x_t, z_t^k, θ_t) and z_t^k, respectively. $p^n(z^k | y_{1:t})$ is then also a nonparametric

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particle estimator of the conditional pdf of x_{t+k} at time t, *i.e* a predictor at time t of the k-step ahead conditional pdf of the x variables. Similar estimators can be proposed for the conditional pdf's of x_t and θ_t.

The following presentation of convergence results is restricted to $p^n(z^k|y_{1:t})$ the estimator of the conditional pdf of z_t^k, *i.e.* of x_{t+k} (similar convergence results have been established for the estimators at time t of the conditional pdf's of x_t and θ_t. See Rossi and Vila 2005, 2006).

Remark 2 It can be checked that (7) is a recursive kernel approximation of (4) for $z^k = z_t^k$.

5 Convergence properties of the particle multi-step predictor

5.1 Almost sure L_1-convergence of the predictor $p^n(z^k|y_{1:t})$ of the conditional pdf of x_{t+k} at time t.

Theorem 5.1 *If the pdf $p(y|y_{1:t-1})$ is continuous and strictly positive at y_t whatever t, then*

$$\begin{cases} \lim_{n\to\infty} \frac{n\Delta_n^{q+2d+p}}{\log n} = \infty \\ \lim_{n\to\infty} \delta_n = 0 \\ \Delta_n^q = o(n^{-\alpha/2}),\ 0 < \alpha < 1 \end{cases} \Longrightarrow \begin{array}{l} \lim_{n\to\infty} \|p^n(x, z^k, \theta|y_{1:t}) - p(x, z^k, \theta|y_{1:t})\|_{L1} = 0 \quad a.s. \\ \lim_{n\to\infty} \|p^n(z^k|y_{1:t}) - p(z^k|y_{1:t})\|_{L1} = 0 \quad a.s. \end{array}$$

Proof. It is a straightforward application to the extra state variable z_t^k, of the a.s. L_1 convergence result of the convolution particle filter (Rossi 2004, Rossi and Vila 2006).

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Convergence speed results as the number of particles n grows to infinity, of $p^n(z^k|y_{1:t})$ to $p(z^k|y_{1:t})$ the true conditional pdf of x_{t+k} at time t, can also be obtained in the same way.

5.2 Punctual multi-step prediction

Let $\bar{z}_t^{k,i} \sim p^n(z^k|y_{1:t}),\ i = 1, \ldots, n,$ and $\hat{z}_t^{k,n} = \frac{1}{n}\sum_{i=1}^n \bar{z}_t^{k,i}$.

Theorem 5.2 *If $Var[x, z^k, \theta|y_{1:t}]$ according to $p(x, z^k, \theta|y_{1:t})$ exists, then $\forall\ t$*

$$\begin{cases} \lim_{n\to\infty} \frac{n\Delta_n^{q+2d+p}}{\log n} = \infty \\ \lim_{n\to\infty} \delta_n = 0 \\ \Delta_n^q = o(n^{-\alpha/2}),\ 0 < \alpha < 1 \end{cases} \quad \Longrightarrow \quad \lim_{n\to\infty} \left|\hat{z}_t^{k,n} - \mathbb{E}[x_{t+k}|y_{1:t}]\right| = 0 \quad a.s.$$

Proof: application to the extra state variable z_t^k of the punctual convergence results of the convolution particle filter (Rossi and Vila 2005).

Remark 3 As in most particle sequential methods, for a given application, there is at present no definitive rule to guess the minimum value of the particle number n to be chosen, which depends on the system complexity and problem setting. If the cinetic of the process is rather slow (e.g. biotechnological processes), one can rely on empirical run comparisons with different values of n: in convolution filtering one can start with $n = 10000$. Sometimes $n = 1000$ may be acceptable to stabilize convergence of the estimations, but one has to go much more beyond quite often. This practical issue will be considered more

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deeply in applications of the algorithm to real and simulated case studies in another paper to come.

6 Conclusion

A nonparametric particle k-step ahead predictor of the state vector pdf conditional on the past and present output variables values of a state space dynamic system has been proposed, as well as a predictor of the k-step ahead conditional expectations of the state variables. Convergence results of these predictors to their true counterparts when the number of particles used grows to infinity, have been provided. These nonparametric particle predictors can be considered as generalizations of corresponding nonparametric particle filtering estimators recently developed. Under rather mild assumptions these nonparametric particle predictors provide a theoretical and practical solution to the prediction problem in general nonlinear state space dynamic systems, still rather neglected by the existing particle estimation methods. Applications of this particle multi-step prediction approach to real and simulated case studies will be presented in a more practically oriented paper to come, with discussion on practical implementation of the proposed algorithm.

Acknowledgments. *The author would like to thank the Co-Editor-in-Chief and a Reviewer for their helpful comments and suggestions.*

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