Fast Continuous-Discrete DAF-Filters

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Abstract

This paper introduces a new method for nonlinear continuous-discrete filtering. It is shown that the Fokker-Planck-Equation can be solved numerically by using distributed approximating functionals (DAFs). The approximation is very accurate and resolves the time interval between observations in one calculation step. Additionally, the operator matrix has to be evaluated only once and not necessarily online. Therefore the method is very efficient.

Keywords: Fokker-Planck-Equation; Distributed Approximating Functionals; Continuous-Discrete Nonlinear Filter.

1. Introduction

Continuous-discrete nonlinear filters are an active field of research in engineering and applied statistics. They are extremely useful in describing diffusion processes with discrete noisy observations. Since the pioneering contributions of Kalman (1960) and Schmidt (1966), tremendous progress has been achieved. Modern filter designs are highly diversified in their strategies of state propagation and handling of nonlinearities of the measurement model.

Historically, the first applicable continuous-discrete nonlinear filter was derived as generalization of the the classical extended Kalman-Filter (EKF, Jazwinski, 1970, chap. 6 & 9). The generalization of discrete time filters to continuous time is a concept, which has proven both fruitful and universal in subsequent, more sophisticated filtering schemes. Many modifications have been suggested to improve the quality of the nonlinear filter approximation. An incomplete list includes sum filter approaches (Sorenson and Alspach, 1971; Ito and Xiong, 2000), local linearization techniques (Shoji and Ozaki, 1997; Shoji, 1998), quadrature methods (Julier and Uhlmann, 1997; 2004; Julier et al., 2000; Ito and Xiong, 2000), multigrid methods and point-mass approximations (Kitagawa, 1987; Kramer and Sorenson, 1988; Simandl et al., 2006). Remarkably, Daum (1986) was able to derive an exact nonlinear filter for a small class of diffusion problems, extending the work of Beneš (1981) (1985).

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An approach more tailored to the continuous time evolution of the state involves the immediate manipulation of the Fokker-Planck-operator, or the corresponding backward-operator, respectively. This strategy was first suggested for pure diffusions by Aït-Sahalia (2002), in order to obtain closed equations for higher moments (see also Jensen and Poulsen, 2002). These moments were used in a series expansion around the normal density, involving Hermite-polynomials. The approach was later modified and generalized by Singer (2006, 2008). Such methods suffer from problems of a particular kind; due to finite series expansion they can generate locally negative density approximations.

After the seminal paper of Gordon et al. (1993), a promising new class of stochastic particle filters became a rapidly evolving field of research. A few important cornerstones are the bootstrap-/SIR filter (Gordon et al., 1993; Liu and Chen, 1998; Liu et al., 1998), the auxiliary particle filter (Pitt and Shephard, 1999), the Rao-Blackwellized- or mixture Kalman-Filter (Chen and Liu, 2000; Andrieu and Doucet, 2002), the rejection particle filter Tanizaki (1999a,b, 2001) and the MCMC particle filter of Berzuini et al. (1997). An excellent review of recent advances in sequential Monte-Carlo-filtering is provided in Arulampalam et al. (2002) and Cappé et al. (2007). Particle filters are incredibly successful in estimating latent states in nonlinear problems and they can partially beat the curse of dimensionality, but they suffer from a major drawback: resampling steps are necessary to avoid sample degeneration and thus the likelihood function becomes fuzzy (see for example Singer, 2003). Recent approaches try to overcome this problem (Pitt, 2002; Beskos et al., 2006), but they are only valid for a limited class of problems.

In this article a new nonlinear filter is suggested, which is capable of solving the nonlinear filtering problem with predefined accuracy, generating a perfectly smooth likelihood surface. Furthermore, the continuous state evolution is calculated in one step, without introducing a discrete skeleton of intermediate time intervals. This is accomplished by representing the Fokker-Planck-operator in matrix form with help of distributed approximating functionals (Hoffman et al., 1991; Hoffman and Kouri, 1992; Wei et al., 1997; Zhang et al., 1997a,b). As a result, the method is very efficient and extremely fast. Even though it is best suited for stationary processes, because it operates on a discrete spatial grid, it is not limited to a particular class of diffusions.

The remainder of the paper is organized as follows: Section 2 introduces distributed approximating functionals and the necessary formalism to operate them. In sections 3 and 4 a moment based- and an exact version of the DAF-Filter is derived in one dimension. Both algorithms are compared in section 5 by reference to a bimodal diffusion problem due to Ginzburg and Landau (1950). This problem is known to be a challenging benchmark for nonlinear filters. Both, state- and parameter estimation via maximum likelihood are surveyed with simulated data. In section 6 the formalism is extended to cover higher dimensional problems. The procedure is exercised on a simple but instructive example, which demonstrates the advantages of a density based filter over a moment based one. In section 7 the full potential of the method is demonstrated in a bivariate limit cycle diffusion with full nonlinear observation model. Section 8 closes the paper with a brief discussion of the advantages, weaknesses and
2. Distributed Approximating Functionals

In this section a brief review of the distributed approximating functional (DAF) formalism is presented. For a more elaborate treatment on this subject see Hoffman et al. (1991); Hoffman and Kouri (1992) and Zhang et al. (1997a,b).

Formally, DAFs are characterized as approximate mapping of a certain set of continuous $L^2$ functions to itself (Zhang et al., 1997a,b). Consider the definition of Dirac $\delta$-function

$$ f(x) = \int \delta(x-x') f(x') dx'. \quad (1) $$

Now a particular class of DAF-functions, the Hermite-DAFs, can be used to approximate the $\delta$-function in a very convenient way

$$ f(x) \approx \int \delta_M(x-x';\sigma) f(x') dx', \quad (2a) $$

with

$$ \delta_M(x;\sigma) = \frac{1}{\sigma} \phi\left(\frac{x}{\sigma}\right) \sum_{m=0}^{M/2} \frac{1}{m!} \left(-\frac{1}{4}\right)^m H_{2m}\left(\frac{x}{\sqrt{2}\sigma}\right). \quad (2b) $$

In (2b), $\phi(x)$ denotes the standard normal probability density function and $H_n(x)$ is the $n$-th Hermite-polynomial, orthogonal with respect to the weight function $e^{-x^2}$. Notice that only even Hermite-polynomials are used because the $\delta$-function is symmetric in its argument. Furthermore, $M$ is the highest degree polynomial involved in the construction of the DAF and $\sigma$ is its bandwidth. Obviously, the mapping is exact for polynomials of degree less or equal to $M+1$, but polynomials are clearly not $L^2$. This emphasizes the character of the DAFs as approximate, rather than exact, mapping on the Hilbert-space of $L^2$ functions (Zhang et al., 1997b).

The parameters $M$ and $\sigma$ of the Hermite-DAF control the accuracy of the approximation. By fixing one or the other, one obtains

$$ \lim_{M \to \infty} \int \delta_M(x-x';\sigma) f(x') dx' = \lim_{\sigma \to 0} \int \delta_M(x-x';\sigma) f(x') dx' = f(x), \quad (3) $$

which is an alternative way of defining the $\delta$-function (Lighthill, 1966, chap. 2.2). Detailed numerical analysis about the optimal choice of $M$ and $\sigma$ is provided in Wei et al. (1997) and Zhang et al. (1997b).

The DAF mapping can be used to sample the function of interest only at discrete points. If these quadrature points form an equispaced grid, equation (2a) can be approximated by

$$ f(x) \approx \Delta x \sum_{j=1}^{N} \delta_M(x-x_j;\sigma) f(x_j), \quad (4) $$

further research perspectives of the method.
with $\Delta x = x_j - x_{j-1}$. Equation (4) suggests that DAFs are particularly suited for interpolation purposes (Hoffman et al., 1998). But the potential of the DAF-approach extends far beyond interpolation. Consider the definition of the $l$-th derivative of Dirac’s $\delta$-function

$$
\delta^{(l)}(x) = \int \delta^{(l)}(x-x')f(x')dx'.
$$

(5)

Usually, this relation cannot be exploited for numerical purposes, because the derivative of the $\delta$-function is not defined directly in the class of distributions. The operation of differentiation has to be rolled over to $f(x)$ by partial integration first. But if a differentiating Hermite-DAF is defined by

$$
\delta_M^{(l)}(x;\sigma) = \frac{(-1)^l}{2^l/2\sigma^{l+1}}\phi \left( \frac{x}{\sigma} \right) \sum_{m=0}^{M/2} \frac{1}{m!} \left( \frac{-1}{4} \right)^m H_{2m+1} \left( \frac{x}{\sqrt{2}\sigma} \right),
$$

(6)

the derivative (5) can be approximated by

$$
f^{(l)}(x) \approx \Delta x \sum_{j=1}^{N} \delta_M^{(l)}(x-x_j;\sigma) f(x_j).
$$

(7)

Thus, the operation of differentiation has turned into an algebraic operation. Furthermore, the derivative is approximated at the same level of approximation as the function itself. The expression that DAFs are always well tempered refers to this property (Zhang et al., 1997a,b). These important features make the DAFs a powerful tool in representing differential operators.

By discretizing the left hand side of (7) on the same spatial grid, one obtains

$$
f^{(l)}(x_i) \approx \Delta x \sum_{j=1}^{N} \delta_M^{(l)}(x_i-x_j;\sigma) f(x_j).
$$

(8)

Obviously (8) can be written most conveniently in matrix/vector form, $f^{(l)} = Lf$, by identifying the components of the operator matrix $L(x_i, x_j) = \Delta x \delta_M^{(l)}(x_i-x_j;\sigma)$. Thus, an arbitrary differential operator of the form

$$
L(x) = f(x) \frac{\partial}{\partial x} + g(x) \frac{\partial^2}{\partial x^2}
$$

(9a)

has the Hermite-DAF matrix representation

$$
L(x_i, x_j) = \Delta x f(x_i) \delta_M^{(1)}(x_i-x_j;\sigma) + \Delta x g(x_i) \delta_M^{(2)}(x_i-x_j;\sigma).
$$

(9b)

This is exactly the form of the Kolmogoroff-Backward operator. Analogously, a forward operator can be defined by

$$
L^1(x) = -\frac{\partial}{\partial x} f(x) + \frac{\partial^2}{\partial x^2} g(x),
$$

(10a)

which has the matrix representation

$$
L^1(x_i, x_j) = -\Delta x f(x_j) \delta_M^{(1)}(x_i-x_j;\sigma) + \Delta x g(x_j) \delta_M^{(2)}(x_i-x_j;\sigma).
$$

(10b)
This is the structure of the Fokker-Planck operator. Notice that the subscript of the argument in the functions $f$ and $g$ has turned from $i$ into $j$, indicating the differential operator acting now on $f$ and $g$. The operator matrices (9b) and (10b) can be computed most efficiently, because the differentiating DAF matrices have Toeplitz-structure.

Remark: there are two approximations involved in computing the matrix representation of the differential operator. First, the delta function is approximated by an even Hermite-series with leading Gaussian term (2b), which is sufficiently smooth everywhere. Second, the integral in (5) is evaluated by rectangular approximation (7). Discretizing the left hand side of equation (7) on the same spatial grid results in a matrix/vector product with the general operator matrix representation (9b) or (10b), respectively.

3. One-Dimensional Moment Filter

In this section the approximative moment filter in one dimension is derived. This filter is the first step beyond the classical Kalman-Filter, with continuous state and linear observation model, disturbed by Gaussian noise. The remaining assumptions of linearity and normality are abandoned in the exact DAF-Filter, derived in the next section.

Every filter algorithm has to perform three primary tasks: the time evolution of the probability density between observations, the incorporation of new information due to observation, and the calculation of the likelihood contribution of each observation, in order to successfully conduct parameter estimation via maximum-likelihood. Formally, these tasks can be summarized in their most general form

\[
p(x_t|\mathcal{F}_{t-1}) = \int p(x_t|x_{t-1})p(x_{t-1}|\mathcal{F}_{t-1})dx_{t-1} \quad (11a)
\]

\[
p(x_t|\mathcal{F}_t) = \frac{p(y_t|x_t,\mathcal{F}_{t-1})p(x_t|\mathcal{F}_{t-1})}{L_t} \quad (11b)
\]

\[
L_t = \int p(y_t|x_t,\mathcal{F}_{t-1})p(x_t|\mathcal{F}_{t-1})dx_t. \quad (11c)
\]

Equation (11a) is the Chapman-Kolmogoroff equation with the Markov-kernel $p(x_t|x_{t-1})$ and the $\sigma$-algebra $\mathcal{F}_{t-1}$, generated by the observation process $y_1, \ldots, y_{t-1}$, (11b) is the Bayes-formula and (11c) the likelihood contribution associated with the new observation $y_t$. Generally, these quantities cannot be evaluated analytically, except in rare cases, and have to be approximated. The necessary steps are detailed below.

3.1. Time Evolution of Moments

Let $x(t)$ be a standard Itô- or generalized Wiener-process with

\[
dx(t) = f(x,t)dt + g(x,t)dW(t), \quad (12)
\]
where $W(t)$ is a Brownian motion. Then the evolution of the corresponding probability density is governed by the Fokker-Planck equation

$$\frac{\partial}{\partial t} p(x,t) = -\frac{\partial}{\partial x} f(x,t) p(x,t) + \frac{1}{2} \frac{\partial^2}{\partial x^2} g^2(x,t) p(x,t)$$

(13a)

with the Fokker-Planck operator

$$L_{FP}(x,t) = -\frac{\partial}{\partial x} f(x,t) + \frac{1}{2} \frac{\partial^2}{\partial x^2} g^2(x,t).$$

(13b)

If the drift- and diffusion functions $f$ and $g$ are autonomous, which is assumed in what follows, the Fokker-Planck operator does not depend on $t$ explicitly, and the solution can be written formally

$$p(x,t + \Delta t) = e^{L_{FP}(x)\Delta t} p(x,t).$$

(14)

Now the $k$-th moment is given by

$$M_k(t + \Delta t) = \int x^k e^{L_{FP}(x)\Delta t} p(x,t) dx$$

$$= \int \left( e^{L_{FP}(x)\Delta t} x^k \right) p(x,t) dx,$$

(15a)

with the adjoined Fokker-Planck operator

$$L_{FP}^\dagger(x) = f(x) \frac{\partial}{\partial x} + \frac{1}{2} g^2(x) \frac{\partial^2}{\partial x^2},$$

(15b)

which is also known as Kolmogoroff-Backward operator. Expression (15a) can be approximated most conveniently using the DAF formalism of section 2. Suppose a discrete support, which covers $p(x,t)$ and $p(x,t + \Delta t)$ with an equispaced grid $x_1, \ldots, x_N$. Let $\Delta x = x_i - x_{i-1}$ be the grid spacing for $i = 2, \ldots, N$. Then the $k$-th moment is approximately

$$M_k(t + \Delta t) \approx \Delta x \sum_{i=1}^{N} \sum_{j=1}^{N} \left( e^{L_{FP}^\dagger\Delta t} \right)_{ij} x_j^k p(x_i,t),$$

(16a)

with the operator matrix

$$L(x_i, x_j) = \Delta x f(x_i) \delta_M^{(1)}(x_i - x_j; \sigma) + \frac{\Delta x}{2} g^2(x_i) \delta_M^{(2)}(x_i - x_j; \sigma).$$

(16b)

Notice that (16a) contains a matrix-exponential. There are several methods to calculate a matrix exponential (see Moer and van Loan 2003, for an excellent

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If the Fokker-Planck operator is not autonomous, the time order of the infinitesimal intervals has to be preserved. Formally this can be expressed with help of the Dyson time ordering operator

$$p(x,t + \Delta t) = T \exp \left[ \int_t^{t+\Delta t} L_{FP}(x,s) ds \right] p(x,t).$$
treatment on this subject). To simplify further discussions, equation (16a) is
reformulated in vector/matrix form. Let \( \mathbf{p}(t) \) be the column vector composed
of \( p(x_i, t) \) for \( i = 1, \ldots, N \), \( \mathbf{L} \) the operator matrix and \( \mathbf{x}^k \) the vector of the \( k \)-th
powers of \( x_1, \ldots, x_N \). Then the moment approximation reads
\[
M_k(t + \Delta t) \approx \Delta \mathbf{x} \mathbf{p}'(t) \exp[\mathbf{L} \Delta t] \mathbf{x}^k,
\]
where \( \mathbf{p}' \) is the transposed vector of \( \mathbf{p} \). For numerical purposes it can be as-
sumed that \( \mathbf{L} \) is not defective, which means that it has linearly independent
eigenvectors. However, problems occur, if \( \mathbf{L} \) is nearly defective. This compli-
cation will be addressed in the next paragraph, for the moment it is assumed
that the eigenvalue decomposition of \( \mathbf{L} \) can be calculated without numerical
problems. One obtains
\[
\exp[\mathbf{L} \Delta t] = \mathbf{V} \exp[\mathbf{\Lambda} \Delta t] \mathbf{V}^{-1},
\]
where \( \mathbf{V}^{-1} \) is the inverse matrix of \( \mathbf{V} \) and \( \mathbf{\Lambda} \) is the diagonal matrix of eigenvalues
of \( \mathbf{L} \) and hence \( \exp[\mathbf{\Lambda} \Delta t]_{ij} = e^{\lambda_i \Delta t} \), for \( i = j \) and 0 elsewhere. Therefore, the
moment approximation can be computed as
\[
M_k(t + \Delta t) \approx \Delta \mathbf{x} \mathbf{p}'(t) \mathbf{V} \exp[\mathbf{\Lambda} \Delta t] \mathbf{V}^{-1} \mathbf{x}^k.
\]
A more stable and efficient method to calculate the eigensystem of \( \mathbf{L} \) is to
initially compute a Schur-Decomposition
\[
\mathbf{LQ} = \mathbf{QT},
\]
where \( \mathbf{T} \) is an upper triangular matrix. Representation (20) was chosen to em-
phasize that no matrix inversion is involved. The next step is to calculate the
eigenvalue decomposition of \( \mathbf{T} \), which is particularly easy, because the eigenval-
ues are already available as diagonal elements of \( \mathbf{T} \), due to its upper triangular
structure. One obtains
\[
\mathbf{LQR} = \mathbf{QRA}.
\]
By identifying terms, the desired matrix of eigenvectors can be calculated from
matrix multiplication \( \mathbf{V} = \mathbf{QR} \). Furthermore, owing to the properties of the
Schur-Decomposition, the relation \( \mathbf{Q}^{-1} = \mathbf{Q}^* \) holds, where \( \mathbf{Q}^* \) is the transposed
conjugate matrix to \( \mathbf{Q} \). Hence, the inverse \( \mathbf{V}^{-1} \) can be calculated most efficiently
by solving the linear system \( \mathbf{RY} = \mathbf{Q}^* \) for \( \mathbf{Y} \), and identifying \( \mathbf{Y} = \mathbf{V}^{-1} \).

The classical Kalman-Filter uses only the first two moments for time- and
observation update, because a Gaussian system is completely specified by these
quantities. The moments can be calculated easily from (19). To simplify no-
tation, assume that the observations are equispaced in time \( t_0, \ldots, t_T \) with
\( \Delta t = t_i - t_{i-1} \) for \( i = 1, \ldots, T \). This is not a necessary requirement, because the Kalman-Filter can easily handle unbalanced designs. The time-update equa-
tions are
\[
\Phi'(t_i, \Delta t) = \Delta \mathbf{x} \mathbf{p}'(t_i) \mathbf{V} \exp[\mathbf{\Lambda} \Delta t] \mathbf{V}^{-1}
\]
\[
\mu(t_{i+1}|t_i) = \Phi'(t_i, \Delta t) \mathbf{x}
\]
\[
\Sigma(t_{i+1}|t_i) = \Phi'(t_i, \Delta t) \mathbf{x}^2 - \mu^2.
\]
Notice that the eigensystem $V \exp[\Lambda \Delta t]V^{-1}$ has to be calculated only once and not necessarily online, which makes the time update algorithm very efficient. If the observation design is unbalanced, only the exponential diagonal matrix has to be recomputed. However, if the underlying process is not stationary, or the discrete grid, supporting initial- and prior density has to be recalculated for any reason, the operator matrix, and hence its eigensystem, has to be recomputed too. Thus, the algorithm is best suited for weak stationary processes.

### 3.2. Observation Update and Likelihood Contribution

In this first extension of the linear filter, the observation model remains linear (or at least nearly linear so that Taylor-linearization applies). This assumption will be dropped for the exact nonlinear filter derived in the next section. But for now the observation equation is

$$y_i = hx(t_i) + \epsilon_i,$$

with observation $y_i$ at time $t_i$ and $\epsilon_i \sim N(0, R)$. Thus, the ordinary Kalman-Filter observation update is

$$K_i = \frac{h}{\Gamma_i} \Sigma(t_i|t_{i-1})$$

$$\mu(t_i|t_i) = \mu(t_i|t_{i-1}) + K_i \nu_i$$

$$\Sigma(t_i|t_i) = (1 - hK_i) \Sigma(t_i|t_{i-1})$$

with the prediction error decomposition

$$\nu_i = y_i - h\mu(t_i|t_{i-1})$$

$$\Gamma_i = h^2 \Sigma(t_i|t_{i-1}) + R.$$  

Remark: the conditional notation used here is incomplete. Because the state estimates are conditioned on the $\sigma$-algebra generated by the observation process, the quantities are conditioned on the whole history of observations. For example, the conditional state expectation at $i < t < i + 1$ correctly reads $\mu(t|t_i, t_{i-1}, \ldots, t_0)$. Since the Kalman-Filter is a recursive scheme, this dependence evolves as natural consequence of its application. Hence, the simpler but slightly abusive notation $\mu(t|t_i)$ is used.

Because the posterior density is also Gaussian, the vector $p(t_i)$ in (22a) contains the probability density at the quadrature points $x_i$, with respect to a Gaussian density with expectation $\mu(t_i|t_i)$ and variance $\Sigma(t_i|t_i)$.

The log-likelihood contribution of the $i$-th observation results from the prediction error decomposition theorem of Schwerpe (1965). Using (24d) and (24e) one obtains

$$l_i = -\frac{1}{2} \left( \log[2\pi \Gamma_i] + \frac{\nu_i^2}{\Gamma_i} \right).$$

The entire log-likelihood function is calculated as sum over all contributions $l_i$ for $i = 0, \ldots, T$, after the filtering cycle is complete.
The whole procedure is summarized in algorithm 1. The matrix exponential of $L$ should be computed by matrix decomposition methods (18) to (21). If not suitable, other procedures like power series expansion or Padé-approximation, not detailed in this paper, are available (see Moler and van Loan, 2003). Notice that when an initial observation $y_0$ is available, the recursion starts with the observation update.

**Algorithm 1: Approximative Moment Filter**

Define a grid $x_1, \ldots, x_N$ and calculate $L$

\[\text{Initialization} \quad \text{for } i = 1, \ldots, T \text{ do} \]

- **Time update**
  \[\Phi'(t_{i-1}, \Delta t) = \Delta x \Phi'(t_{i-1}) \exp[L \Delta t]\]
  \[\mu(t_i|t_{i-1}) = \Phi'(t_{i-1}, \Delta t)x\]
  \[\Sigma(t_i|t_{i-1}) = \Phi'(t_{i-1}, \Delta t)x^2 - \mu^2\]

- **Observation update**
  \[K_i = \frac{h}{\Gamma_i} \Sigma(t_i|t_{i-1}) \quad \text{▷ Kalman-Gain}\]
  \[\mu(t_i|t_i) = \mu(t_i|t_{i-1}) + K_i \nu_i\]
  \[\Sigma(t_i|t_i) = (1 - hK_i)\Sigma(t_i|t_{i-1})\]

- **Prediction error decomposition**
  \[\nu_i = y_i - h \mu(t_i|t_{i-1}) \quad \text{▷ Innovation}\]
  \[\Gamma_i = h^2\Sigma(t_i|t_{i-1}) + R\]

\end{for}

**4. Exact One-Dimensional DAF-Filter**

In this section the exact DAF-Filter in one dimension is derived. This filter overcomes the limits of the approximate moment filter in that the full prior density is obtained within the time update step. Furthermore, restrictions of the observation model are relaxed to full nonlinear, non-Gaussian measurements.

In order to achieve these generalizations, the whole filter design has to be located on a discrete grid. The grid $x_1, \ldots, x_N$ now supports prior-, observation- and posterior densities. The prior density is obtained from an initial density, or the previous posterior density, respectively, by the solution (14) of the Fokker-Planck-equation. This formal solution is approximated by

\[
p(x_i, t + \Delta t) \approx \sum_{j=1}^{N} \left( e^{L \Delta t} \right)_{ij} p(x_j, t), \quad (26a)
\]
with the operator matrix

\[ L(x_i, x_j) = -\Delta x f(x_j) \delta_M^{(1)}(x_i - x_j; \sigma) + \frac{\Delta x}{2} g^2(x_j) \delta_M^{(2)}(x_i - x_j; \sigma). \]  

(26b)

Obviously, (26a) is a linear matrix/vector equation. The matrix exponential should again be evaluated following the outlined procedures (18) to (21).

The observation model (23) in the previous section was a linear function of the unobserved state, \( hx(t_i) \), with an additional Gaussian error with variance \( R \). Hence, the observation density, conditioned on the unobserved state, could have been written

\[ p(y_i|x(t_i)) = \varphi(y_i; hx(t_i), R), \]

where \( \varphi \) is the normal density function. In the exact filter setup it is only required that the conditional observation density is known. It neither has to be Gaussian, nor linear in the system state argument. It not even has to be differentiable. If the conditional observation density is known, the posterior density is obtained by evaluating the Bayes-formula on the discrete grid \( x_1, \ldots, x_N \). Suppressing the time argument to simplify notation one obtains

\[ p(x_i|y) = \frac{p(y|x_i)p(x_i)}{\Delta x \sum_{j=1}^{N} p(y|x_j)p(x_j)}. \]  

(27)

The denominator in (27) is the likelihood contribution of the observation \( y \). The observation update on a discrete grid degenerates to a reweighting process, which is known from particle filtering.

Let \( p(t_i|t_j) \) be the column vector of state probability density on the discrete grid \( x_1, \ldots, x_N \) at time \( t_i \), conditioned on the information available at \( t_j \). Analogously, let \( p(y_i|t_j) \) be the column vector of observation density on the discrete grid at time \( t_i \), conditioned on the system state density at time \( t_j \). Then algorithm 2 summarizes the results. Again, if an initial observation \( y_0 \) is available, the recursion starts with the reweighting step.

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**Algorithm 2: Exact DAF-Filter**

Define a grid \( x_1, \ldots, x_N \) and calculate \( L \)  \( \triangleright \) Initialization

for \( i = 1, \ldots, T \) do

Time update

\[ p(t_i|t_{i-1}) = \exp[L\Delta t]p(t_{i-1}|t_{i-1}) \]

Reweighting

\[ l_i = \Delta x p'(y_i|t_i)p(t_i|t_{i-1}) \quad \triangleright \text{Likelihood} \]

\[ p_j(t_i|t_{i-1}) = \frac{p_j(y_i|t_i)p_j(t_i|t_{i-1})}{l_i} \]

end for

---

The exact filter algorithm 2 is more compact than the approximate moment filter algorithm 1. On the other hand, the discrete grid has to cover prior-,
observation- and posterior density, which requires a slightly larger discrete support. However, considering the fact that the operator matrix and its eigenvalue decomposition has not to be computed in every step of the recursion, the exact filter seems already more efficient.

5. Inference in a Bimodal Potential

To assess the performance of the derived DAF-Filters, the algorithms are tested in a bimodal diffusion problem. First, the accuracy of the time update step is investigated. Subsequently, maximum-likelihood inference is conducted with both algorithms. This comparative analysis should not only assess the quality of the filters, but should answer the generic question whether or not an exact density filter is required to generate trustworthy parameter estimates.

5.1. The Ginzburg-Landau Model

The bimodal potential model of Ginzburg and Landau [1950] is a challenging benchmark for nonlinear filters (cf. Miller et al., 1994; Singer, 2002, 2008), due to its massive deviation from normality. It was originally designed to describe phase transitions in superconductors. If the fourth-order potential \( \Phi(x) = \frac{\alpha}{2}x^2 + \frac{\beta}{4}x^4 \) passes through a transition from \( \alpha > 0 \) to \( \alpha < 0 \), a bifurcation occurs and the stable system becomes bistable. Figure 1 left illustrates the phase transition. A diffusion in the Ginzburg-Landau- (GL) potential is described by the Itô-process

\[
dx(t) = -\frac{\partial}{\partial x}\Phi(x)dt + g(x)dW(t) \\
= -(\alpha x + \beta x^3)dt + g(x)dW(t).
\]

(28)

For fixed diffusion coefficient \( g(x) = g \), the stationary probability density can be calculated \( p_{\text{st.}}(x) \propto \exp\left[ -\frac{\beta}{2} \Phi(x) \right] \). This allows for verification of the precision
of the DAF-Filter time update. In particular, for large $\Delta t$, the moments should coincide with the stationary moments of the GL-distribution. This is not a trivial task, in which most established non-stochastic filtering schemes, like first and second order extended Kalman-Filter and unscented Kalman-filter of Julier and Uhlmann (1997, 2004), fail. For a detailed analysis see Mazzoni (2007, chap. 4.10). Only filters based on Gauss-Hermite-Quadrature (for example Ito and Xiong 2000; Singer 2008) seem to work properly.

In the following analysis the parameter configuration $\beta = g = 1$ and $\alpha = -1$ is chosen. Both, the approximate moment filter and the exact filter are operated on a grid $[x_1, x_N] = [-3, 3]$ with $\Delta x = 0.1$. Throughout the rest of this paper, the Hermite-DAF parameters are chosen $M = 54$ and $\sigma = 2.36 \Delta x$ in agreement with Zhang et al. (1997b). The initial density is assumed Gaussian, with expectation $\mu = 0.5$ and variance $\Sigma = 0.25$. The stochastic differential equation (28) was simulated using an Euler-Maruyama-scheme (Kloeden and Platen 1992, chap. 9.1) with time discretization $\Delta \tau = 0.01$. Subsequently, an observation series $y_0, \ldots, y_T$ with $T = 100$ and $\Delta t = 1$ was generated from the linear observation model (23) with $h = 1$ and Gaussian noise $\epsilon_i \sim N(0, 0.1)$, in order to make the two filters comparable.

Figure 1 right shows a small section of the simulated trajectory. Obviously, the process bounces between the two potential floors at $x = \pm 1$ from time to time, if its stochastic energy is sufficient to break through the potential barrier. This property makes it very difficult for analytic filters to keep proper track of the system state, whereas stochastic algorithms, like sequential Monte-Carlo filters, manage this task easily, if a sufficient number of particles is simulated. The observations at integer times are indicated by dots. They are clearly dislocated sometimes due to noisy measurement.

stationary probability density is given by

$$p_{st.}(x) = \frac{2}{\pi} \left( J_{-1/4} \left[ \frac{1}{2} \right] + J_{1/4} \left[ \frac{1}{2} \right] \right) e^{-\frac{1}{2} \left( x^4 - 2x^2 + \frac{1}{2} \right)}.$$

For a detailed numerical analysis of preferable choices see Hoffman et al. (1991); Hoffman and Kouri (1992); Wei et al. (1997); Zhang et al. (1997b).
5.2. Accuracy of Time Updates

The moment evolution for the specified initial distribution is illustrated in figure 2 (left) for $t = [0, 10]$. Obviously, the moments relax rapidly to their stationary values $\mu = 0$ and $\Sigma = 0.893$. The absolute differences between the approximate DAF-Filter solutions at $t = 100$ and the correct moments, calculated from the stationary Ginzburg-Landau-distribution, are $\Delta \mu = 0$ and $\Delta \Sigma = 1.289 \times 10^{-7}$. This is a fairly good result, because it is very accurate and it is obtained in a one step calculation.

The exact density evolution is shown in figure 2 (right). It is easily seen that the unimodal initial density becomes bimodal, because the probability to break through the potential barrier increases over time. With help of the stationary distribution, a measure for the quality of the density evolution, similar to the moment differences, can be established. Let $\Delta p$ be the vector of differences between the stationary distribution and the exact filter solution on the discrete grid $x_1, \ldots, x_N$ at $t = 100$. Then the root mean square error is $\|\Delta p\|/\sqrt{N} = 3.277 \times 10^{-8}$. This is although a very accurate result which is obtained in one single calculation step. The time update mechanism of the suggested filters seems to work very precise and efficient.

5.3. Maximum-Likelihood Inference

To verify the ability of the suggested filters to generate suitable maximum-likelihood parameter estimates, the known parameters $\alpha$ and $\beta$ are estimated from the simulated observation series. Figure 3 shows the log-likelihood surfaces generated by the approximate moment filter (left) and the exact DAF-Filter (right). There is a qualitative difference between the log-likelihood functions. The surface generated by the approximate moment filter contains a rift, which is not present in the likelihood surface of the exact filter. Remember that the observation model is linear and Gaussian, and therefore exact, which means that a moment filter generates a likelihood with wrong surface attributes. This is true, even if the filter is able to track the moments of the underlying process exactly.

Because the GL-process is ergodic, the asymptotical behavior of the ML-
estimates can be explored by simply extending the observation series. Table 1 reports the results of several estimation procedures with different numbers of observations. A secant method, assembling an approximate Hesse-matrix without calculating derivatives, was used for numerical maximization (cf. Dennis and Schnabel 1983, chap. 9). Figure 4 illustrates the maximization steps for both filters with $T = 100$ observations in the relevant area of the likelihood surface. The total number of iterations is indicated in the respective initial columns in Table 1. Asymptotic standard deviations, calculated from the Hesse-matrix of the log-likelihood function, are given parenthesized below the corresponding estimates.

Both algorithms seem to provide estimates, which cover the true parameter value well within an interval of two standard deviations. However, in larger samples the exact filter generates estimates with roughly half the variability of the moment filter estimates. It is fair to say that the approximate moment filter, despite of a wrong likelihood, is not totally insufficient for parameter estimation in this problem.

Table 1: Maximum-Likelihood estimation of simulated observation series

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<td>(0.492)</td>
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<td>(0.365)</td>
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<td></td>
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<td>1</td>
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Figure 4: ML-estimation – Approximative moment filter (left) and exact filter (right)
6. Higher Dimensional DAF-Filter

In this section, the exact one-dimensional DAF-filter of section 4 is extended to cover higher dimensional problems. This is done by switching to tensor notation. The procedure is demonstrated in an instructive example.

6.1. Tensorial Eigenvalue Decomposition

The time update equation in algorithm 2 involved the computation of a matrix exponential. This was done with help of a preceding eigenvalue decomposition. For higher dimensional forms, neither an exponential, nor an eigenvalue decomposition is defined. But a higher dimensional problem of this kind can be reduced to an ordinary matrix decomposition problem.

The following preliminaries are valid for arbitrary $n$-dimensional vector spaces in which an inner product is defined. Let $y^i$ be the elements of a contravariant vector, i.e. a vector with respect to an arbitrary basis, preferably an orthonormal basis. Then $x_j$ are the components of a covector or covariant vector, which means a vector with respect to the corresponding dual basis. Roughly spoken, a contravariant vector appears as column vector, whereas a covariant vector appears as row vector. Now suppose $y$ is the result of an operator $L$, acting on a vector $x$. In tensor notation this is written as

$$ y^i = L^i_j x^j. \quad (29) $$

In (29) Einsteins sum-convention was used. By this convention a summation has to be performed, if the same index appears twice in one term. Indices are not allowed to appear more than once in upper and lower position. In (29) the sum of all components with index $j$ of $L$ and $x$ has to be taken, which makes the operation a simple matrix/vector product. Notice that each index runs over the full number of dimensions $i,j = 1, \ldots, n$. For the sake of simplicity, objects like $y$ and $L$ are called tensors of rank one and two, respectively, without verifying their transformation properties under a change of coordinates. Notice that (29) is a componentwise notation, so the order in which the tensors are arranged is arbitrary.

The eigenvalue decomposition of $L$ can also be written in tensorial notation. One obtains

$$ y^i = V^i_k \Lambda_k^l V_l j x^j. \quad (30) $$

Equation (30) needs some explanation. Even if $A$ has diagonal structure, double indexing is prohibited. The summation is therefore to be taken over $k$ and $l$. The expression $\Lambda_k^k$ would mean trace of $A$. The indices are positioned one above the other to emphasize that $A$ is symmetric. The matrix $V_{ij}$ is the inverse matrix of $V^{ij}$, which means $V^{ij} V_{jk} = \delta^i_k$, with the identity matrix $\delta^i_k$ in tensor notation. Generally, this property is only valid for the metric tensor. However, this is consistent, because a certain kind of spectral metric is induced by $V$.

\footnote{See McCullagh (1987) for an excellent treatment of tensor methods in statistics.}
The original time update equation of algorithm 2 reads in tensorial notation

\[ p^i(t + \Delta t) = \exp[\mathbf{L}\Delta t]_{ij}^i p^j(t) = V^{ik} \exp[\Lambda^l_{k,l} \Delta t] V^j_{kl} p^j(t). \]  

(31)

This equation can be extended to multivariate problems by index splitting. In order to keep the notation simple, (31) is reformulated for the bivariate case

\[ P^{i_1i_2}(t + \Delta t) = V^{i_1i_2k_1k_2} \exp[\Lambda^l_{k_1l_1k_2} \Delta t] V^l_{i_1l_2j_1j_2} P^{j_1j_2}(t). \]  

(32)

Now \( i_1, \ldots, l_1 \) and \( i_2, \ldots, l_2 \) have dimensions \( n_1 \) and \( n_2 \), respectively. \( P \) is a tensor of rank 2, \( \mathbf{V} \) and \( \Lambda \) are tensors of rank 4. They correspond to a rank 4 tensor \( L^{i_1i_2j_1j_2} \) in the following way: Define index functions \( I = n_2(i_1 - 1) + i_2 \) for all indices \( i,j,k,l \). Then

\[ L^I_{J} = V^{IK} \Lambda^K_{LJ} \]  

(33)

is the eigenvalue decomposition of the \((n_1 n_2 \times n_1 n_2)\)-matrix \( L^I_{J} \). Equation (33) relates the higher rank tensor expressions in (32) to a simple matrix decomposition problem. The rank four tensors are literally flattened out into tensors of rank two. This works for arbitrary \( d \)-variate problems by defining index functions

\[ I = 1 + \sum_{k=1}^{d} \prod_{l=k}^{d-1} n_{l+1}(i_k - 1), \]  

(34)

for all indices involved. For computational purposes it is difficult to extend this scheme beyond moderately \( d \)-variate problems, because the size of the matrices involved in the eigenvalue decomposition grows exponentially.

6.2. Bivariate Diffusion example

In order to apply the concepts of the previous subsection, a very easy, but instructive example is now introduced. First let’s generalize the differentiating DAF of section 2 to the bivariate case

\[ \frac{\partial^{k+l}}{\partial x^k \partial y^l} f(x, y) = \int \int \delta^{(k)}(x - x') \delta^{(l)}(y - y') f(x', y') dx' dy' \approx \Delta x \Delta y \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} \delta^{(k)}(x - x_i; \sigma) \delta^{(l)}(y - y_j; \sigma) f(x_i, y_j). \]  

(35)

The corresponding bivariate Fokker-Planck-operator with \( x_1 = x \) and \( x_2 = y \) reads

\[ L_{FP}(x_1, x_2) = -\sum_{i=1}^{2} \frac{\partial}{\partial x_i} f_i(x_1, x_2) + \frac{1}{2} \sum_{i=1}^{2} \sum_{j=1}^{2} \frac{\partial^2}{\partial x_i \partial x_j} g_{ij}(x_1, x_2). \]  

(36)

An extension to higher variate problems is obvious.

A very simple, but instructive example is based on the geometrical Brownian motion (GBB)

\[ dy(t) = \mu y dt + \gamma y dW(t), \]  

(37)
which is a popular model for stock asset prices in finance (e.g. Black and Scholes, 1973). In its original form, the GBB is a univariate instationary process and hence, two modifications are made. First, the model is transformed into the corresponding return-process and second, the diffusion coefficient is made endogenous as (extended) state variable without individual dynamics. The latter is proposed in several approaches for online parameter estimation (for example Mazzoni, 2009). Applying Itô’s lemma to the relation $x(t) = \log[y(t)]$ and extending the state space yields

$$d\begin{pmatrix} x(t) \\ \gamma(t) \end{pmatrix} = \begin{pmatrix} \mu - \gamma^2/2 \\ 0 \end{pmatrix} dt + \begin{pmatrix} \gamma \\ 0 \end{pmatrix} dW(t).$$  \hfill (38)

The second components of drift and diffusion function $f$ and $g$ are identically zero. If the constant expected return is also set to zero, $\mu = 0$, the corresponding Fokker-Planck-operator has a particularly simple form

$$L_{\text{FP}}(x, \gamma) = \gamma^2/2 \left( \frac{\partial}{\partial x} + \frac{\partial^2}{\partial x^2} \right).$$  \hfill (39)

Defining a two dimensional discrete grid $x_1, \ldots, x_N$, and $\gamma_1, \ldots, \gamma_N$, with grid spacing $\Delta x$ and $\Delta \gamma$, respectively, the Fokker-Planck-operator (39) has a rank four tensor representation

$$L(x_i, \gamma_i, x_j, \gamma_j) = \Delta x \Delta \gamma \delta_{\gamma_i \gamma_j} \gamma_i^2/2 \left( \delta_M^{(1)}(x_i - x_j; \sigma) + \delta_M^{(2)}(x_i - x_j; \sigma) \right).$$  \hfill (40)

The Kronecker-Delta results from the differentiating DAF of degree zero $\delta_M^{(0)}(\gamma_i - \gamma_j; \sigma) = \delta_{\gamma_i \gamma_j}$, according to (35). The rank four operator tensor (40) is related to the matrix eigenvalue decomposition (33) by the appropriate index functions (34), and hence to the time update equation (32).

In the present example the cartesian grid $[-5, 5]^2$ was chosen, with grid spacing $\Delta x = \Delta \gamma = 0.25$. A linear observation model

$$y_i = x(t_i) + \epsilon_i,$$  \hfill (41)

with $\epsilon_i \sim N(0, 0.25)$ was used, where only the returns $x(t)$ were observed. This is a typical situation in financial applications because the volatility is assumed an unobserved latent quantity. Now algorithm 2 applies with minor obvious modifications. Figure 5 gives a sequence of three succeeding measurements. In all cases, the prior density is indicated by the left contour plot, the observation density at the center and the posterior to the right.

The initial density is Gaussian, and remains Gaussian throughout the initial measurement. But the first time update causes a symmetry breaking with respect to the $x$-component (center-left in figure 5). Notice that the $\gamma$-symmetry remains intact at all times because the Fokker-Planck-operator (39) contains only terms quadratic in $\gamma$. This $x$-asymmetry is amplified by subsequent measurements and finally the probability density becomes completely bimodal (bottom-right in figure 5).

The symmetry in $\gamma$ is the reason for the incapability of Gaussian filters to track unobserved volatility. It is easy to see that the linear correlation and hence
the covariance between $x$ and $\gamma$ is zero. Therefore, no information about $\gamma$ is obtained by observing $x$, if the information is processed only by the covariance matrix. This problem can only be fixed by filters, involving higher moments, and therefore nonlinear correlations, or by approximately exact density filters like the DAF-filter.

7. Stochastic Limit Cycle Model

In this section a stochastic version of the Van der Pol-oscillator is investigated. This problem is more elaborate because it contains a limit cycle. Furthermore, it is analyzed within a highly nonlinear observation model in order to test the suggested method under most adverse conditions.

The Van der Pol-oscillator is a popular benchmark for nonlinear filtering.
schemes (e.g., Sitz et al., 2002; Mazzoni, 2008). It is also an example for a very stiff set of nonlinear ODEs (see the famous STIFF-DETEST set, introduced by Enright et al., 1975). Thus, it is often used to verify the quality of numerical computations (Hairer and Wanner, 1996, chap. 4.10). The original second order oscillator equation reads

\[ \ddot{x} - \varepsilon (1 - x^2) \dot{x} + x = 0, \tag{42} \]

with \( \varepsilon > 0 \) and dots indicating derivatives with respect to time. Without detailed analysis, some properties of the Van der Pol-equation are summarized. When \( x \) is small, the quadratic term \( x^2 \) can be neglected and the system (42) becomes repulsive to the origin, due to a negative dampening term \(-\varepsilon \dot{x}\). For large \( x \), the quadratic term becomes dominant and the origin now acts as attractor. Hence, the system can be expected to remain in a certain area around the origin. Actually it satisfies Liénards theorem, guaranteeing the existence of a stable limit cycle in phase space.

For the present analysis, the oscillator is decomposed into its phase components with the substitution \( \dot{x} = v \), and augmented by a state independent stochastic inhomogeneity. The resulting bivariate SDE reads

\[ d \begin{pmatrix} x(t) \\ v(t) \end{pmatrix} = \begin{pmatrix} v \\ \varepsilon (1 - x^2) v - x \end{pmatrix} dt + \begin{pmatrix} 0 \\ g \end{pmatrix} dW(t). \tag{43} \]

Further, assuming that only the radial distance of the phase state with respect to the origin can be observed and that the measurement is affected by noise, the highly nonlinear observation model is

\[ y_i = \sqrt{x^2(t_i) + v^2(t_i)} + \epsilon_i. \tag{44} \]

In the present setup the parameter vector \((\varepsilon, g) = (0.5, 1)\) is chosen and the measurement error is assumed \(\epsilon_i \sim N(0, 0.25)\). Figure 6 left shows a streaming plot of the phase space and a simulated trajectory of the SDE (43) for \( t = [0, 20] \). The initial distribution is Gaussian with \( \mu = 0 \) and \( \Sigma = I \). The initial state is indicated by an empty triangle, whereas the final state is marked by a filled triangle. The simulation of the stochastic differential equation was again conducted with an Euler-Maruyama-scheme with time discretization \( \Delta \tau = 0.01 \).

Figure 6 right gives a density plot of the nonlinear observation density for a hypothetical observation \( y = 2 \) in the phase space. It clearly indicates that local linearization techniques are inadequate for this kind of problem. Altogether, (43) and (44) represents a state space model, which is very difficult to process by conventional filters, especially by filters based on local linearizations. On the other hand, the DAF-filter can easily handle this problem.

Figure 7 shows the first 12 posterior densities calculated by the DAF-filter, with observations at all integer times \( t_i \) with \( i = 0, \ldots, 20 \). Again a cartesian grid of \([-5, 5]^2\), with grid spacing \( \Delta x = \Delta v = 0.25 \) was used. Because the phase state position cannot be observed directly, the probability mass is distributed orbital around the origin. Some areas on this orbit are more likely than others at different times, because the limit cycle is not quite circular as seen from figure
Notice that the orbital distribution of probability mass is symmetric with respect to the origin. This means that a calculation of the posterior expectation yields \( E[x] = E[v] = 0 \) for all times. Because \( x = v = 0 \) is an unstable equilibrium, the probability of finding the system in the vicinity of this state is zero. Thus, the posterior expectation is a very poor indicator for the system state and moment based filters are doomed to fail. The DAF-filter on the other hand draws a very clear and precise picture of the true local conditions.

8. Conclusions

Two new continuous-discrete filtering schemes, based on matrix representation of the Fokker-Planck-operator with distributed approximating functionals, were introduced. It has been shown that these filters are capable of high precision time evolution of the Fokker-Planck-equation in one step, once an adequate discrete grid is established and the corresponding operator matrix and its eigenvalue decomposition is calculated. These matrices can be computed offline, and once available, the time update reduces to a simple matrix/vector multiplication.

The potential of the method was surveyed in univariate and bivariate examples. Particularly difficult benchmark problems have been addressed and the DAF-Filter has proven capable of handling nonlinearities of every kind. Furthermore, the adequacy with respect to maximum-likelihood parameter estimation was investigated, which is the weak spot of most sequential Monte-Carlo-filters. Even in this regard, the DAF-Filter has proven useful and efficient.

A general problem of filters, designed to work on a discrete grid, is their extension to multivariate problems. The DAF-Filter also suffers from this drawback. Even in the bivariate case, the operator matrix becomes very high dimen-
Figure 7: Posterior densities of the limit cycle oscillator

sional. Hence, at this time the method seems to be restricted to moderately high $k$-variate problems. Here is potential for future research. Another inconvenience is caused by the necessity of recalculation of the operator matrix, once the supporting discrete grid is changed. Recomputation seems unavoidable if the grid support is no longer sufficient. These kinds of defects generally occur in nonstationary problems or in case of observation outliers. They can be fixed by transforming the model to a stationary type or by broaden the discrete support. In the context of ML-estimation, the recalculation of the operator matrix is absolutely unavoidable, even if the grid support is sufficient and the grid is unaltered. But this is considered a minor inconvenience by the author, because non differentiable likelihood surfaces, like usually generated by sequential Monte-Carlo-filters, are causing far more serious problems in parameter estimation.
References


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