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APPROXIMATIONS FOR THE NUMERICAL SOLUTION OF A
FOKKER-PLANCK EQUATION WITH REFLECTING BOUNDARY
CONDITIONS

K. J. Åström

Abstract

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1. INTRODUCTION

In TN 18.057 a first order non-linear system with stochastic disturbances was discussed. It was shown that under certain assumptions the problem could be reduced to the solution of the parabolic equation

$$(1.1.) \quad \frac{\partial f}{\partial t} = \frac{\partial}{\partial x} (gf) + A \frac{\partial^2 f}{\partial x^2}$$

with the initial condition

$$(1.2.) \quad f(t, x) \rightarrow f^0(x) \quad \text{as } t \downarrow 0$$

and the reflecting boundary condition

$$(1.3.) \quad g \cdot f + A \cdot \frac{\partial f}{\partial x} \rightarrow 0 \quad \text{as } \downarrow x \downarrow a$$

Some methods for the numerical solution of this problem will be discussed in this report.

By approximating the derivatives with respect to x by differences (1.1) is approximated by a set of ordinary differential equations with constant coefficients which can be solved on an analog computer.

For solutions on a digital computer we proceed by a straightforward difference approximation technique. To obtain an explicit difference formula special attention is given to the approximation of the boundary condition. It is shown that these are uniquely given by requiring that the approximated equations can be interpreted as the Kolmogorov equations for a Markov process with discrete states.

$$(2.1.7) \quad c_i = \begin{cases} \frac{A}{k^2} + \frac{g_{i+1}}{2k} & i = -m, \dots, m-1 \\ 0 & i = m \end{cases}$$

Initial condition

$$(2.1.8) \quad f_i(0) = f^0(ik) \quad i = -m, \dots, m$$

It is not obvious how the equations for $i = \pm m$ were obtained from the boundary conditions. This will, however, be discussed in section 2.2.

2.2. A physical interpretation of the approximations

The variables $k \cdot f_i(t)$ can be interpreted as the probability that the state variable x belongs to the set E_i

$$(2.2.1) \quad E_i = \left\{ x ; \left(i - \frac{1}{2}\right) k < x < \left(i + \frac{1}{2}\right) k \right\}$$

The approximation (2.1.4) of the Fokker-Planck equation can thus be interpreted physically as the Kolmogorov forward equation for a Markov process with the states E_i . This Markov process obviously has a finite number of states and continuous time. The transition probabilities

$$(2.2.2) \quad p_{ij} = P \left\{ \text{Transition } E_i \rightarrow E_j \text{ during } (t, t + \Delta t) \right\}$$

are given by

2. A DIFFERENCE - DIFFERENTIAL APPROXIMATION2.1. Introduction

Introduce the following difference approximations of the derivatives in the x- direction.

$$(2.1.1) \quad \frac{\Delta f}{\Delta x} \approx \frac{f_{i+1} - f_{i-1}}{2k}$$

$$(2.1.2) \quad \frac{\partial^2 f}{\partial x^2} \approx \frac{f_{i+1} - 2f_i + f_{i-1}}{k^2}$$

where

$$(2.1.3) \quad f_i = f(t, ik)$$

The equation (1.1) is then approximated by the following set of ordinary differential equations

$$(2.1.4) \quad \frac{df_i}{dt} = a_i f_{i-1} + b_i f_i + c_i f_{i+1}; \quad i = -m, \dots, 0, \dots, m$$

where

$$(2.1.5) \quad a_i = \begin{cases} 0 & i = -m \\ \frac{A}{k^2} - \frac{g_{i-1}}{2k} & i = -m+1, \dots, m \end{cases}$$

$$(2.1.6) \quad b_i = \begin{cases} - \left(\frac{A}{k^2} - \frac{g_{-m}}{2k} \right) & i = -m \\ - 2 \frac{A}{k^2} & i = -m+1, \dots, m-1 \\ - \left(\frac{A}{k^2} + \frac{g_m}{2k} \right) & i = m \end{cases}$$

$$P_{i(i+1)} = \left(\frac{A}{kZ} - \frac{g_i}{2k} \right) \Delta t + o(\Delta t) \quad i = -m+1, \dots, m-1$$

$$P_{i(i-1)} = \left(\frac{A}{kZ} + \frac{g_i}{2k} \right) \Delta t + o(\Delta t)$$

$$(2.2.3) \quad P_{ii} = \begin{cases} 1 - 2 \frac{A}{kZ} \Delta t + o(\Delta t) & i = -m+1, \dots, m-1 \\ 1 - \left(\frac{A}{kZ} + \frac{g_i}{2k} \right) \Delta t + o(\Delta t) & i = -m \text{ and } i = m \end{cases}$$

$$P_{ij} = o(\Delta t) \quad \text{all other indices}$$

If p should be a transition matrix it must be required that

$$(2.2.4) \quad 0 \leq p_{ij}(t) \leq 1$$

and

$$(2.2.5) \quad \sum_j p_{ij}(t) = 1$$

The first condition is satisfied if k is chosen sufficiently small.

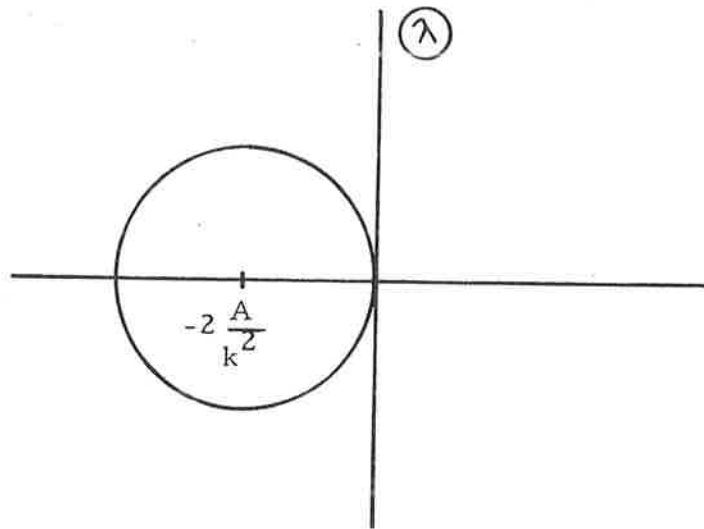
The second condition is satisfied due to the special approximation chosen for the boundary conditions. Conversely if the condition (2.2.5) is postulated the approximation for the reflecting boundary condition is uniquely given.

The equation (2.1.4) can be written as

$$(2.1.4') \quad \frac{df_i}{dt} = \sum_{j=-m}^m g_{ij} f_j$$

where $Q = \{g_{ij}\}$ is the matrix

Compare the Figure below



As one eigenvalue of Q is zero (2.2.8) the equation (2.1.4) has a nontrivial stationary solution which is proportional to the corresponding right eigenvector of Q^T . Due to the property 3 above this stationary solution to (2.1.4) converges exponentially to this independent of the initial conditions.

2.3. Check conditions

There are several identities which can be used to check the accuracy of the calculations.

The determination of the elements in the Q matrix can be tested by the identity (2.2.8) which also can be written as

$$(2.3.1) \quad a_{i+1} + b_i + c_{i-1} = 0$$

We also have the following identity

$$(2.3.2) \quad \int_{x_1}^{x_2} f(t, x) dx - \int_0^t \left\{ \left[gf + A \frac{\partial f}{\partial x} \right]_{x_1} + \left[gf + A \frac{\partial f}{\partial x} \right]_{x_2} \right\} dt = 1$$

which follows from (1.1) and which can be interpreted as an equation of continuity for the probability mass of the Markov process with continuous states, which says that the sum of the probability mass within (x_1, x_2) and the time integral of the probability flux over the boundaries x_1, x_2 equals unity. Using (2.2.3) we can write down the mathematical equivalence of this for the Markov process with discrete states and we obtain

$$(2.3.3) \quad k \sum_{i=i_1}^{i_2} f_i(t) - k \int_0^t \left[\frac{A}{k^2} (f_{i_1} + f_{i_2} - f_{i_1-1} - f_{i_2+1}) + \right. \\ \left. + \frac{1}{2k} (f_{i_1} g_{i_1} + f_{i_1-1} g_{i_1-1} - f_{i_2} g_{i_2} - f_{i_2+1} g_{i_2+1}) \right] dt = 1$$

which obviously is a formal difference approximation of (2.3.2).

2.4. An example

If $g(x)$ is an odd function and if the initial distribution $f^0(x)$ is an even function, the solutions to (2.1.4) will obviously have the property

$$(2.4.1) \quad f_i = f_{-i}$$

It is then sufficient to consider only nonnegative values of i .

The equation (2.1.4) then becomes

$$(2.4.2) \quad \frac{df_i}{dt} = a_i f_{i-1} + b_i f_i + c_i f_{i+1} \quad i = 0, \dots, m$$

where

$$(2.4.3) \quad a_i = \begin{cases} 0 & i = 0 \\ \frac{A}{k^2} - \frac{g_{i-1}}{2k} & i = 1, \dots, m \end{cases}$$

Compare the Example 5.2 of TN 18.057. Introducing the notations

$$T = \frac{a^2}{A}$$

$$s = \frac{ak'}{2A}$$

and

$$k \cdot m = 3a$$

the coefficients a_i , b_i and c_i become

$$(2.4.9) \quad a_i = \begin{cases} 0 & i = 0 \\ \frac{m^2}{9T} & i = 1 \\ \frac{m^2}{9T} \left(1 - 3 \frac{s}{m}\right) & i = 2, \dots, i_0 \\ \frac{m^2}{9T} & i = i_0 + 1 \\ \frac{m^2}{9T} \left(1 + 3 \frac{s}{m}\right) & i = i_0 + 2, \dots, m \end{cases}$$

$$(2.4.10) \quad b_i = \begin{cases} -2 \frac{m^2}{9T} & i = 0, \dots, m-1 \\ -\frac{m^2}{9T} \left(1 - 3 \frac{s}{m}\right) & i = m \end{cases}$$

$$(2.4.4) \quad b_i = \begin{cases} -2 \frac{A}{k^2} & i = 0, \dots, m-1 \\ -\left(\frac{A}{k^2} + \frac{g_m}{2k}\right) & i = m \end{cases}$$

$$(2.4.5) \quad c_i = \begin{cases} 2\left(\frac{A}{k^2} + \frac{g_1}{2k}\right) & i = 0 \\ \frac{A}{k^2} + \frac{g_{i+1}}{2k} & i = 1, \dots, m-1 \\ 0 & i = m \end{cases}$$

The initial condition is

$$(2.4.6) \quad f_i(0) = f^0(ik)$$

The equation (2.1.4) thus reduces to an equation of the order $m+1$, which means that a symmetric initial condition cannot excite all the eigenfunctions of (2.1.4). The eigenvalues of the system matrix of (2.4.2) obviously have the properties as those of the matrix Q of section 2.2. Especially one eigenvalue is zero which is highly undesirable from computational point of view. This can be avoided by deleting one of the equations in (2.4.2) and computing the corresponding function $f_i(t)$ from

$$(2.4.7) \quad f_0(t) - f_0(0) + 2 \sum_{i=1}^m [f_i(t) - f_i(0)] = 0$$

Assume that $g(x)$ is given by

$$(2.4.8) \quad g(x) = k' \operatorname{sgn}(x+a) - k' \operatorname{sgn} x + k \operatorname{sgn}(x-a), \quad |x| < 3a$$

and the initial condition by

$$f^0(x) = \delta(x)$$

$$(2.4.11) \quad c_i = \begin{cases} 2 \frac{m^2}{9T} \left(1 + 3 \frac{s}{m} \right) & i = 0 \\ \frac{m^2}{9T} \left(1 + 3 \frac{s}{m} \right) & i = 1, \dots, i_0 - 2 \\ \frac{m^2}{9T} & i = i_0 - 1 \\ \frac{m^2}{9T} \left(1 - 2 \frac{s}{m} \right) & i = i_0, \dots, m-1 \\ 0 & i = m \end{cases}$$

where i_0 is the smallest integer equal to or less than $\frac{1}{3} m$.

The check condition (2.3.3) runs

$$(2.4.12) \quad kf_0 + 2k \sum_{i=1}^{i_0-1} f_i - k \cdot \frac{m^2}{9T} \cdot \int_0^t \left[\left(1 - 3 \frac{s}{m} \right) f_{i_0-1} - f_{i_0} \right] dt = 1$$

where the interval (x_1, x_2) is chosen as $(- (i_0 + \frac{1}{2}) k, (i_0 + \frac{1}{2}) k)$.
Compare the equation (E.25) of TN 18.057.

3. FINITE DIFFERENCE APPROXIMATION3.1. Explicit formulas

Approximate the time derivative by the forward difference

$$(3.1.1) \quad \frac{\partial f}{\partial t} = \frac{f^{n+1} - f^n}{h}$$

where

$$(3.1.2) \quad f^n = f(nh, x)$$

and the space derivatives by (2.1.1) and (2.1.2).

The Fokker-Planck equation (1.1) with the reflecting boundary condition then reduces to

$$(3.1.3) \quad f_i^{n+1} = A_i f_{i-1}^n + B_i f_i^n + C_i f_i^n$$

$$n = 0, 1, 2, \dots$$

$$i = -m, \dots, m$$

where

$$(3.1.4) \quad f_i^n = f(nh, ik)$$

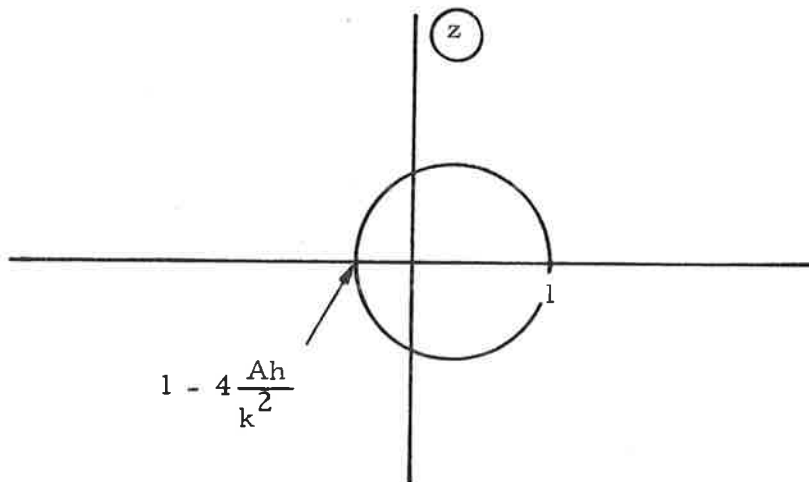
and

$$(3.1.5) \quad \left\{ \begin{array}{l} A_i = ha_i \\ B_i = (1 + hbi) \\ C_i = hc_i \end{array} \right.$$

The coefficients a_i , b_i and c_i are given by (2.1.5), (2.1.6) and (2.1.7).

The boundary conditions are handled in the same way as in section 2.
Compare also section 3.2.

Due to the properties of the coefficients a_i , b_i and c_i the characteristic roots of the difference equation (3.1.3) all lie within the circle.



The stability condition for the difference approximation is thus

$$(3.1.6) \quad \frac{Ah}{k^2} < \frac{1}{2}$$

3.2. Physical interpretations of the approximations

The equation (3.1.3) can be interpreted as the equation for the probabilities of a Markov process with finite states E_i and discrete time, whose transition probabilities

$$(3.2.1) \quad p_{ij} = P \left\{ x(n+1) \in E_j \mid x(n) \in E_i \right\}$$

are given by

$$\begin{aligned}
 p_{i(i+1)} &= h \left(\frac{\Lambda}{kZ} - \frac{\beta_i}{2k} \right) & i = -m+1, \dots, m-1 \\
 p_{i(i-1)} &= h \left(\frac{\Lambda}{kZ} + \frac{\beta_i}{2k} \right) \\
 (3.2.2) \quad p_{ii} &= \begin{cases} 1 - h \left(\frac{\Lambda}{kZ} - \frac{\beta_i}{kZ} \right) & i = -m \\ 1 - 2A \frac{h}{kZ} & i = -m+1, \dots, m-1 \\ 1 - h \left(\frac{\Lambda}{kZ} + \frac{\beta_i}{kZ} \right) & i = m \end{cases} \\
 p_{ij} &= 0 \quad \text{other indices}
 \end{aligned}$$

If P should be a probability matrix it must be required that

$$(3.2.3) \quad 0 \leq p_{ij} \leq 1$$

$$(3.2.4) \quad \sum_{j=-m}^m p_{ij} = 1$$

The first condition is satisfied if k and h are sufficiently small and if

$$(3.2.5) \quad 2A \frac{h}{kZ} \leq 1$$

which is the stability condition for the difference approximation.

The second condition is satisfied due to the special approximation chosen for the reflecting boundary condition. Compare section 2.2.

Thus if we choose a finite difference approximation of the Fokker-Planck equation which is the Kolmogorov equation of a Markov process, we obtain a unique way of approximating the reflecting boundary condition. The approximation is also a stable difference approximation.

This approximation may also be used to prove the existence of a stable stationary solution to the Fokker-Planck equation.

3.3. Check conditions

Using (3.1.5) the identity (2.3.1) runs

$$(3.3.1) \quad A_i + B_i + C_i = 1$$

Further, using (3.2.2) the identity (2.3.3) becomes

$$(3.3.2) \quad k \sum_{i=i_1}^{i_2} f_i^N - k \sum_{n=0}^{N-1} \left[\frac{A}{k^2} (f_{i_1}^n + f_{i_2}^n - f_{i_1-1}^n - f_{i_2-1}^n) + \right. \\ \left. + \frac{1}{2k} (f_{i_1}^n g_{i_1} + f_{i_1-1}^n g_{i_1-1} - f_{i_2}^n g_{i_2} - f_{i_2+1}^n g_{i_2+1}) \right] = 1$$

This approximation can also be obtained by approximating the integral in (2.3.3) by the tangent-formula.

3.4. An example

As an illustration we will analyse the problem of section 2.4.

An explicit finite difference approximation to this problem is

$$(3.4.1) \quad f_i^{n+1} = A_i f_{i-1}^n + B_i f_i^n + C_i f_{i+1}^n; \quad n = 0, 1, \dots; \quad i = 1, \dots, m$$

$$f_0^{n+1} = f_0^0 - 2 \sum_{i=1}^m (f_i^n - f_i^0)$$

where

$$(3.4.2) \quad A_i = \begin{cases} 0 & i = 0 \\ \frac{m^2}{9} \cdot \frac{h}{T} & i = 1 \\ \frac{m^2}{9} \cdot \frac{h}{T} \cdot \left(1 - 3 \frac{s}{m}\right) & i = 2, \dots, i_0 \\ \frac{m^2}{9} \cdot \frac{h}{T} & i = i_0 + 1 \\ \frac{m^2}{9} \cdot \frac{h}{T} \left(1 + 3 \frac{s}{m}\right) & i = i_0 + 2, \dots, m \end{cases}$$

$$(3.4.3) \quad B_i = \begin{cases} 1 - 2 \frac{m^2}{9} \cdot \frac{h}{T} & i = 0, \dots, m-1 \\ 1 - \frac{m^2}{9} \cdot \frac{h}{T} \cdot \left(1 - 3 \frac{s}{m}\right) & i = m \end{cases}$$

$$(3.4.4) \quad C_i = \begin{cases} 2 \frac{m^2}{9} \cdot \frac{h}{T} \cdot \left(1 + 3 \frac{s}{m}\right) & i = 0 \\ \frac{m^2}{9} \cdot \frac{h}{T} \cdot \left(1 + 3 \frac{s}{m}\right) & i = 1, \dots, i_0 - 2 \\ \frac{m^2}{9} \cdot \frac{h}{T} & i = i_0 - 1 \\ \frac{m^2}{9} \cdot \frac{h}{T} \cdot \left(1 - 3 \frac{s}{m}\right) & i = i_0, \dots, m-1 \\ 0 & i = m \end{cases}$$

The check condition (3.3.2) becomes

$$(3.4.5) \quad kf_0^N + 2k \sum_{i=1}^{i_0-1} f_i^N - k \frac{m^2}{9T} \sum_{n=0}^{N-1} \left[\left(1 - 3 \frac{s}{m}\right) f_{i_0-1}^n - f_{i_0}^n \right] = 1$$

The stability condition (3.2.5) runs

$$(3.4.6) \quad \frac{h}{T} < \frac{9}{2m^2}$$

According to the equation (E.24) of TN 18.057 the stationary values are approached exponentially with the time constant

$$(3.4.7) \quad T_1 = \frac{T}{s^2}$$

Using the maximum steplength required for stability (i. e. $h = \frac{k^2}{2A}$) we obtain a crude estimate on the number of steps required to reach the stationary values within 1% as follows

$$N \sim 4.6 \frac{T_1}{h} \sim \frac{m^2}{s^2}$$

4. CONCLUSIONS

The equation (1.1) is the Fokker-Planck equation for a Markov process with continuous time and continuous states. By approximating the derivatives by differences (1.1) can be approximated either by a set of ordinary differential equations or a set of difference equations. By approximating the boundary conditions (1.3) in a suitable way it can be achieved that the approximations can be interpreted as the Kolmogorov equations for a Markov process with discrete states and continuous or discrete time. The conditions which guarantees the physical interpretations also implies that the approximations are stable.

Solna, February 7, 1962

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C Kinberg

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APPENDIX

Iterative calculation of the stationary solution :

The stationary solutions of (2.1.4) and (3.1.3) are given by

$$(A.1) \quad Qf = 0$$

where f is a vector and Q a matrix.

Write this as

$$(A.2) \quad f = (hQ + I)f$$

Due to the properties of the Q matrix the eigenvalues of

$$(A.3) \quad hQ + I$$

has all its eigenvalues within the unit circle if

$$h \leq \frac{k^2}{2A}$$

The sequence of vectors f^r obtained by

$$(A.4) \quad f^r = (hQ + I)f^r$$

will then converge to the solution of (A.2) and (A.4) can thus be used for an iterative determination of the solution.

Writing (A.4) in components we get

$$(A.5) \quad f_i^r = A_i' f_{i-1}^r + B_i' f_i^r + C_i' f_{i+1}^r$$

where

$$A'_i = ha_i = A_i$$

$$B'_i = hb_i + 1 = B_i$$

$$C'_i = hc_i = C_i$$

The iterative solution of the stationary solution is thus equivalent to the solution of the difference approximation to the partial differential equation as shown in section 3.