Different methods for Noise Analysis including Fokker-Plank, Dynamical programming, and Multi-scale Time Analysis.

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Abstract:

Extended Kramers Model based on Fokker-Plank Stochastic Differential Equation for velocity of Chemical reactions and can be applied to noise models, such as Brownian noise caused by the thermal agitation of the molecules of the fluid along with different single molecule experiments, such as optical tweezers, scanned tip microscopies, and single molecule fluorescence methods, as well as radio and sound noise that can be modeled by Dynamical Programming along with multi scale time analysis for Electromagnetic compatibility and electromagnetic interference.

Keywords: Fokker-Plank Stochastic Differential Equation, Brownian noise, Dynamic Programming.

The commcmorat1on of 100 years since introduction of Fokker-Planck Stochastic Differential Equation coincides with the commemoration of 250 years of history of Rutgers University,

I. Introduction with statement of chemical equations, discussion of Boltzmann type kinetic equations, Kramers approach with remaining problems and modem approaches.

The mathematical structure of the models of Boltzmann type kinetic equations for reacting gas mixtures for particles undergoing inelastic interactions with reactions of bimolecular and dissociation-recombination type is very complicated, because of the collisional operators that usually in the full Boltzmann equations, are expressed by 5-fold integrals.

Consequently direct numerical applications of these models present several computational difficulties.

The search for the simpler solution had its long way till the introduction of the equation for the Brownian motion by Albert Einstein.

With the application of Transition State Theory to Arrhenius equation,

$$\mathbf{R = C}\, e^{-\frac{E_b}{kT}} \qquad \textbf{(1)}$$

where R is the rate of chemical reaction, Eb the activation energy barrier , k is the Boltzmann constant, T is the temperature, and C is a constant transforms C to

$$\mathbf{C = kT/h}\ , \qquad \textbf{(2)}$$

where h is Plank's constant, this however, does not consider the state of equilibrium of the reactants.

In the theory of the velocity of chemical reactions the problem of study by Kramers was based on empirical knowledge that the reactants are in the state of equilibrium. His introduction of diffusion equation is given in the following form of Fokker-Plank equation,

$$m\frac{\partial^2 x}{\partial t^2} = -(\partial U(x))/\partial x - \gamma m\, \partial x/\partial t + F(t), \qquad (3)$$

where m is reduced mass in the potential of mean force U, and F is a noise of a random fluctuating force, originating from the thermal motion, γ is a viscosity or memory friction.
It was based on the assumptions about a particle that moves in an external field of force and additionally is subject to the irregular forces of a surrounding medium in temperature equilibrium . which he called Brownian motion(or an integral over the Brownian noise.

$$W(t) = \int_0^t \left(\frac{dW(t)}{d\tau}\right) d\tau, \text{ where W(t) is a Wiener process. (4)}$$

The conditions are such that the particle is thought of as caught in a potential hole but may escape in the course of time by passing over a potential barrier. The problem is to calculate the probability of escape in its dependency on temperature and viscosity of the medium.

The study had the following problems, pointed out in his original paper:

1. The study for the sake of simplicity was only a one-dimensional model.

2. However, as long as no perfect temperature equilibrium is attained, the equation of M a x w ell velocity distribution holds only approximately. This is even the case when the external force is zero.

According to his description, the B r o w n i a n forces of the medium illustrate the mechanism which strives to bring about temperature equilibrium. The value of the viscosity coefficient γ (which may depend on T even in the manner of an exponential function) is a measure for the intensity with which the molecules in the different states react with the surrounding medium.

3. The model illustrates also the ambiguity involved in the conception ,,transition state".

4. Quantum mechanical ,,tunnel-effects" for which there is no room in our model, could also play a part.

5. both Kramers and Grote-Hynes improvement give a well-defined rate constant, and therefore cannot account for dispersed kinetics or dynamic disorder. Such a clear separation of time scale is no longer true for proteins, which are sluggish systems as demonstrated by the fluctuation observed at the slow and broad range of time scales

Further investigations in the subject led to the development of new theoretical approaches, such as State Transition Theory, which includes multidimensional approach.

2. Dynamical programming was introduced by Richard Bellman in the mid 50-ties during the Proceedings of the National Academy of Sciences. It can be thought of as very natural in light of the existence of the dynamic time warping algorithm that is applied to computing the global distance between time series.{1.Bellman R. Equipment replacement policy J Soc Ind Appl Math,3(3),133-136, 2. Bellman R. Dynamic programming and Lagrange multipliers, PNAS 42, 767-769, 3. Bellman R. Dynamic programming Princeton UP 4.Sanford M. Roberts Editor Dynamic Programming in Chemical Engineering and Process Control AP)

This method was of special interest for me as one of the problems that I solved working with the late Professor Lawrence Shepp was in the field of dynamic programming. He was a member of National Academy of Science, and worked on many applied problems in Bell Laboratories.

The overview can be found in[l. R.W.H. Sargent Optimal control Journal of Computational and Applied Mathematics 124 (2000) 361-371 www.elsevier.nl/locate/cam2. Alsmeyer, F., Marquardt, W., Olf, G., 2002. A new method for phase equilibrium measurements in reacting mixtures. Fluid Phase Equilibria203, 31-51. 3. Jonathan *How.16.323 Principles of Optimal Control.* Spring 2008. Massachusetts Institute of Technology: MIT OpenCourseWare, https://ocw.mit.edu.License: Creative Commons BY-NC-SA.]

Why this method was abandoned, and it is very difficult to find in the recent literature? Dynamic Programming is based on the **Principle of Optimality:** Suppose the optimal solution for a problem passes through some intermediate point (x_1,t_1) , then the optimal solution to the same problem starting at (x_1,t_1) must be the continuation of the same path. The explanation to the Principle is in that we are looking for solution in finding optimal decision procedure only through controlled dynamics, and we obtain the evolution of the system, when the system obeys controllability assumptions or conditions. Hence the conditions would require **sets to be compact and bounded**, and the solution would exist within the domain that we are working with. Usually we are looking for the solution that would satisfy “as a consequence of the requirement for the thermal equilibrium assumption that is dependent on how large is the viscosity or memory friction with the probability of equilibrium becoming larger.” (Reaction rate theory· fifty years after Kramers Peter Hanggi et al) that has a lot of difficulties of checking during the reaction. As some researchers could not rely on imaginary assumptions for iterations that was considered as kind of contradiction with the Principle of Optimality, the tendency of using dynamic programming left place for other methods.

subject to x'= a(x,u,t), x(t0)= fixed, t_f= fixed f The iteration algorithm would be for vector **x**

X' (t) = f (x(t), a) (t >0); **$x(0)=x_0$**, (5)

$\vec{x}_{k+1} = \vec{x}_k + a_k p_k$ (6)

for some scalar a_k and direction $\mathbf{p_k}$**.** The direction canbe found from e.g. Taylor series expansion or other iterative methods.

Other methods for unconstrained problems can include:
1. Polynomial approximation
2. Golden section ("Optimal Control of Hydrosystems" Larry Mays)
involves deleting variables range or elimination of intervals in
one-dimensional case and is related to Fibonacci numbers
3. Bisection(S Giove"A bisection algorithm for fuzzy quadratic optimal control""www.unive.it/media/allegato/DIP/Economia/mmef-ex .. ./Giove_2_1_2007.pdf)

Dynamic programming considers the problems of minimizing Shortest Paths, e.g. classic navigation problems, Routing through a street maze, and road maps as time/state, discrete/continuousproblems.

$$\mathbf{min\ J = h(x(t_f)) + \int_{t_0}^{t_f} g(x(t), u(t), t))\ dt} \qquad \mathbf{(7)}$$

that allows other constrains also.

The solution starts from
1)mapping spatial/temporal grid over
space/time and
2) Evaluation of final costs of possible final states $\mathbf{x_i(t_f)}$,then
3) Going back up 1 step in time and consider all possible ways of completing the problem and so on.
4) Approximate integral cost at state $\mathbf{x^j}$ **at time** $\mathbf{t_k}$, and apply control $\mathbf{u^{ij}_k}$ to move to state x at time $\mathbf{t_{k+1} = t_k + \Delta t}$.

$$\int_{t_k}^{t_{k+1}} \mathbf{g(x(t), u(t), t))\, dt} \quad \approx \quad \mathbf{g(\, x_k^i\, ,\, u_k^{ij}\, ,\, t_k\,)\, \Delta t} \qquad \mathbf{(8)}$$

Solution for control inputs directly from system model

$$\mathbf{x_{k+1}^j \approx x_k^i + a(\, x_k^i\, ,\, u_k^{ij}\, ,\, t_k\,)\, \Delta t \Longrightarrow a(\, x_k^i\, ,\, u_k^{ij}\, ,\, t_k\,) = (x_{k+1}^j - x_k^i\,)/\, \Delta t} \qquad \mathbf{(9)}$$

That can be solved to find $\mathbf{u_k^{ij}}$.
In case of linear system model and a quadratic cost function

$$\mathbf{x'(t) = A(t)x(t) + B(t)u(t)} \qquad \mathbf{(10)}$$

$$\mathbf{J} = \frac{1}{2}\, x(t_f\,)^T\, \mathbf{H}\, x(t_f) + \frac{1}{2} \int_{t_0}^{t_f} (x(t\,)^T R_{xx}(t)\, x(t\,) + (u(t\,)^T R_{uu}(t) u(t\,) dt \qquad \mathbf{(11)}$$

For initiaI **conditions H,** $\mathbf{R_{xx}(t) \geq 0}$ **and** $\mathbf{R_{uu}(t) > O}$**, then**

$$\mathbf{H(x,u,\breve{J}x,\, t) = 2\, [x(t)^T\, Rxx(t)x(t) + u(t)^T\, Ruu(t)u(t)] + \breve{J}x(x(t),t)[A(t)x(t) + B(t)u(t)]} \quad \mathbf{(12)}$$

And the problem is to minimize H subject

$$\frac{\partial H}{\partial u} = \mathbf{u(t)^T Ruu(t) + \breve{J}x\, (x(t),t)B(t) = O,\ where\ } \frac{\partial^2 H}{\partial u^2} = \mathbf{R_{uu}(t) > o} \qquad \mathbf{(13)}$$

$$\mathbf{Which\ gives\ the\ optimal\ control\ law\ } \breve{u}(t) = -R_{uu}^{-1}(t) B(t)^T\, \breve{J}x\, (x(t),t)^T \qquad \mathbf{(14)}$$

3.**The method of time scale**

The first to use time scale for particles was Smoluchowski Smuluchovski devised that after a time span $\tau = 1/\xi$
the particle loses the memory of the initial velocity. It is called the Smuluchovski time scale and the average velocity is zero or constant. From Langevin equation

$$\langle \overrightarrow{v(t)} * \overrightarrow{v(t)} \rangle_{\vec{v}_0} = \mathbf{v_o^2\, exp\, (-2\xi t) + \frac{C_{\vec{v}_0}}{2\xi}\, (1 - exp\, (-2\xi t))\, ,} \qquad \mathbf{(15)\ ,\ where}$$

$$\frac{d\vec{v}}{dt} = -\xi\, v + \vec{F} \qquad \mathbf{(16)}$$

And the friction constant $\xi = 6\pi\eta a/m$, where η is the viscosity of the solvent and a is the radius of the particle

$$\vec{0} = -\xi\vec{v} - \frac{1}{m}\vec{\nabla}\, \Phi + \vec{F}\mathbf{,\ where\ } \Phi(\vec{r}) \mathbf{\ is\ the\ external\ potential.} \qquad \mathbf{(17)}$$

For derivation of Smuluchovski time scale the initial velocity may be taken equal to $\sqrt{3kT/m}$.

The distance the particle travel divided by its diameter then would be equal to

$\frac{\sqrt{3kT/m}}{a\xi} = \frac{\sqrt{3kT/m}}{6\pi\eta a^2} = \mathbf{10^{-5}}$ for normal colloidal particles. (Theory of Polymer Dynamics W.J. Briels http://cbp.tnw.utwente.nl/PolymeerDictaat/index.html)

The student of Kramers Van Kampen exploited Fokker-Planck equation for approximation of solutions of master equation.

At the end to the discussion of the second approach of time scale or master equation, it Is worth to list additional encountered problems as an introduction to the newly developed methods such as
l)optical tweezers,
2)scanned tip
microscopes, and
3)single molecule fluorescence, as well as
4)radio and sound noise and new challenges facing them.
Dispersed kinetics and dynamic disorder has been the subject of intensive theoretical investigations. The first approach assumes the fluctuating rate constant is phenomenologically dependent on a time-varying control parameter, such as the activation barrier height, or the area of the bottleneck. Although this approach is conceptually straight forward, the control parameters are usually not experimentally accessible. As a result, their dynamics is often assumed empirically on ad hoc basis.

One of examples is Brownian motion governed by Langevin dynamics.

The second one assumes a kinetic scheme involving multiple discrete conformational states with different rate constants. However, there is often no sufficient information about the kinetic parameters or the connection topology among the multiple states

The possible approaches to the solution of the above problems

The quantum state tomography QST could be considered as an attempt to solve most of the above problems. Its aim is to statistically reconstruct an unknown state from the outcomes of repeated measurements performed on identical copies of the state. Among the proposed estimation methods we mention,

1. variations of maximum likelihood and least squares estimator,
2. linear inversion ,
3. Bayesian inference,
4. estimation with incomplete measurements,
5. continuous variables tomography.

However, composite systems such as trapped ions, due to the

exponential increase in dimension in order to identify and estimate the state with a reduced number of measurements demand special approaches.

All of the above discussion apply to different single molecule experiments, such as optical tweezers, scanned tip microscopes, and single molecule fluorescence methods, as well as radio and sound noise in as much as all these seemingly exact methods have effects of l) dispersion, 2)some kind of memory friction that in its turn affects possible state of equilibrium

4. Resolution.

In the late 50-es, Richard Feynman predicted with his famous expression that "there' s plenty of room at the bottom" that in the future people would be able "arrange the atoms one by one the way they want them" and he implied "that high resolution microscopes would allow a direct look at single molecules in biological samples". The topic of resolution is very important in view of the recent Article by Xiao-Li Meng A trio of inference problems that could win you a Nobel Prize in statistics (if you help fund it), which focuses on Multi-resolution inference, Resolution via filtration and decomposition, and other topics of resolution.

After 50 years in light of the above discussion about memory friction, the Smoluchowski time scale, velocity memory loss, and the iterative methods for equilibrium, the new research is at the bottom of the challenging problems that present "the fields of nanotechnology and single molecule (SM) microscopy developed after the Feynman's prediction. In the 80's so called scanning probe and near-field microscopes were developed that use sharp, nanoscale tips to image, probe and manipulate individual atoms or molecules .... An SM microscope needs to efficiently reject background, such as autofluorescence as well as elastic Rayleigh and inelastic Raman scattering of the medium surrounding the target molecule, by optically isolating the desired Stokes-(red-)shifted fluorescence signal. A common way to decrease background.

Excitation volume usually is combined with conventional optics. "In epifluo-rescence microscopy the illumination and detection volumes are constrained by focusing light to illuminate an area several μ m in diameter and using the same optics to detect fluorescence with an area detector." The use of fluorescence resonance energy transfer (FRET) that is energy transfer between two light-sensitive molecules for measurement of distances between molecules in structural biology to the development of concepts of multidimensional conformational landscape and dynamics of biopolymers "SM version of FRET is able to quantitatively dissect the temporal sequence of events in folding transitions, including the adoption of rare and transient intermediates that may exist under either equilibrium or non-equilibrium conditions." (Walter et al. Page 9)
"Local heating can influence enzymatic activity and change the local viscosity of the medium, whereas steep thermal gradients may produce convention currents that can adversely affect the measurements. Local heating in the vicinity of the optical trap can be calculated and several techniques have been developed to measure the temperature directly." (Keir C. Neuman and Attila Nagy Single-molecule force spectroscopy: optical tweezers, magnetic tweezers and atomic force microscopy Nat Methods. June/08 5(6): 491-505. doi :10.1038/nmeth. 1218.)

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