行政院國家科學委員會專題研究計畫 成果報告

一維空間上馬可夫鏈的收斂門檻
研究成果報告(精簡版)

計 畫 類 別 ： 個別型
計 畫 編 號 ： NSC 98-2628-M-009-003-
執 行 期 間 ： 98 年 08 月 01 日至 99 年 07 月 31 日
執 行 單 位 ： 國立交通大學應用數學系（所）

計 畫 主 持 人 ： 陳冠宇

處 理 方 式 ： 本計畫可公開查詢

中 華 民 國 99 年 10 月 06 日

研究成果報告內容

Markov first studied the stochastic processes that came to be named after him in 1906. During the past century, there have been many scientists engaged in exploring the qualitative behavior of Markov chains at a systematical way. In the recent decades, due to the maturity of theory, the interdisciplinary communication among researchers at different scientific majors is blooming and the fields include computer science, statistic physics, bioinformatics, engineering and many others. This leads to several new aspects on the quantitative analysis of Markov chains and makes the study get involved in more subfields in mathematics such as number theory and coding, combinatorics, graph theory, algebra and geometry.

The classical theory of Markov chains focused on the qualitative analysis such as the rate of convergence to the limiting distribution. In the past two decades, as the interest in chains with large state spaces increased, a subject different from the past emerged. Some measurement on the distance to the stationarity is specified and the number of steps required to reach the stability, called the mixing time, is highly spotlighted. In the end, the modern theory of Markov chains falls on the study of mixing times and one goal is to understand how the mixing time grows as the size of the state space increases.

In the quantitative analysis of Markov chains, a remarkable phenomenon known as the cutoff phenomenon was introduced by Aldous and Diaconis in early 1980s to capture the fact that some Markov chains converge abruptly to their invariant probabilities. This brilliant idea reveals the observation that the distribution of the chain is a good approximation to the limiting distribution after the so called “cutoff time” but never fits well before. Such a phenomenon has a close relation to the mixing time and is sensitive to measuring mechanics. The cutoff phenomenon is closely related to the mixing time problem and the cutoff time is an important flag that points out the time to stop the simulation in Markov chain Monte Carlo method.

Many measurements on the distance between Markov chains and their stationarity are of interest, including the total variation, separation, entropy and the L^p-distance. According to diverse purposes, each subject has its own favor. The variation and separation are of particular interests in statistics and their analysis falls on the study of coupling time and strong stationary time, where the first is a classical probabilistic technique and the second is introduced and studied by Aldous and Diaconis in 1980s. The entropy is mostly considered in statistic physics and the logarithmic Sobolev inequality is useful in studying the entropy convergence, in particular the underlying space has a large dimension. Regarding the L^p-distance, the case $p=1$ is exactly twice of the total variation. For $p>1$, Diaconis and Saloff-Coste (1996) introduced a discrete version of the logarithmic Sobolev inequality to bound the L^p-mixing time using a related constant, the logarithmic Sobolev constant. There are still a lot of heuristic ideas on estimating the convergence, such as representation theory, conductance profile, comparison technique and many others.

Since Diaconis announced the observation of cutoff phenomena in 1981, there are many scholars engaged in exploring such a sharp phase transition in Markov processes. Up to now, many practical models are studied and the existence of cutoff is determined, including a detailed description on the cutoff time. But, however, there are very rare theoretical researches on the mixing time of Markov chains and let alone the cutoff phenomenon, except some special topics. In 2003, I started the Ph.D. program on conquering the mixing time under the supervision of Laurent Saloff-Coste and obtained a bunch of results which are composed in 2006 as a Ph.D. dissertation in [1]. The materials considered in the thesis are all about discrete mathematics, but the heuristics is applicable to very general setting. In the context of the L^p-distance, we consider Markov processes with almost no assumption and make up the results in [2]. There include many necessary and sufficient conditions on the L^p-cutoffs and have miscellaneous examples as an illustration if the relation is not equivalent. During the time of submission, a very positive report from the referee is replied. As the underlying Markov process is assumed reversible, the spectral decomposition is useful in expressing the L^2-distance but the mixing time and cutoff phenomenon are still puzzles and hard to determine. An application on the theory of Fourier transform is used to achieve an equivalent condition on the L^2-cutoff and a formula on the L^2-mixing time. Regardless of the heavy requirements to work out the theorem in [3], this is the first time that a cutoff is determined theoretically and the cutoff time is formulated.

Our goal of this project is two-folds. By restricting our attention on the 1-dimensional case, the birth-and-death chains, we plan to reduce the equivalent condition on the L^2-cutoff and find out an easy expression of the cutoff time if any. The first goal has been completed due to a reduction of a subsidiary condition, whereas there is indeed only one remained. For the second goal, we work on several examples and obtain some ideas on the equivalence of cutoff. But, this needs more time to simplify the expression up to a reasonable and workable extent.

While the sharp phase-transit phenomenon disappears, the mixing time has the same order as the relaxation time, which is the inverse of the spectral gap, for all $p>1$. This leads to the study of the spectral gap of 1-dimensional Markov processes. As inspired by Miclo's observation of a qualitative behavior of the first eigenfunctions in 2006, we create an iterative scheme on the computation of the spectral gap. What surprised is that such an algorithm generates a sequence tending to the spectral gap with exponential convergence rate. Moreover, an upper bound on the difference to the spectral gap during the iteration is easy to compute. Different from the heavy computation of the power method, such an idea makes it possible to compute the relaxation time numerically at a lower cost. All results mentioned above are based on a solid mathematical proof and the draft is in preparation.

This project has some immediate prospects. First, our method in computing the spectral gap is based on Miclo's work, which depends strongly on the geometric structure of birth-and-death chains. Since the graph representation of 1-dimensional Markov chain can be categorized as trees in graph theory, one should be able to extend Miclo's observation to a more general extent. (In fact, he has done some works.) This makes it possible to implement our method to random walks on trees.

The second aspect is the computation of the logarithmic Sobolev constant. Such a constant is useful in bounding the L^p-mixing time but, however, the exact value is available only for very few simple examples. It is very easy to modify the algorithm on the numerical computation of spectral gaps for birth-and-death chain so that a possible convergent sequence is generated for the logarithmic Sobolev constant. We have implemented the new idea on several non-trivial 1-dmensional cases and the outcome of the iterations points out a way to prove the algorithm mathematically. This leads to other research topics, such as the numerical computation of logarithmic Sobolev constants and the entropy cutoff of birth-and-death chains.

Reference

[1] Guan-Yu Chen. *The cut-off phenomenon for finite Markov chains.* PhD thesis, Cornell University, 2006.

[2] Guan-Yu Chen and Laurent Saloff-Coste. *The cutoff phenomenon for ergodic Markov processes.* Electronic Journal of Probability, 13 (2008), 26--78.

[3] Guan-Yu Chen and Laurent Saloff-Coste. *The L^2-cutoff for reversible markov processes*. J. Funct. Anal., 258:2246--2315, 2010.

[4] Guan-Yu Chen. *An iterative scheme on the spectral gap of birth-and-death chains.* In preparation.

無研發成果推廣資料

98 年度專題研究計畫研究成果彙整表

計畫主持人：陳冠宇	計畫編號：98-2628-M-009-003-
計畫名稱：一維空間上馬可夫鏈的收斂門檻	

成果項目			量化			單位	備註（質化說明：如數個計畫共同成果、成果列為該期刊之封面故事...等）
			實際已達成數（被接受或已發表）	預期總達成數(含實際已達成數)	本計畫實際貢獻百分比		
國內	論文著作	期刊論文	0	0	100%	篇	
		研究報告/技術報告	0	0	100%		
		研討會論文	0	0	100%		
		專書	0	0	100%		
	專利	申請中件數	0	0	100%	件	
		已獲得件數	0	0	100%		
	技術移轉	件數	0	0	100%	件	
		權利金	0	0	100%	千元	
	參與計畫人力（本國籍）	碩士生	0	0	100%	人次	
		博士生	0	0	100%		
		博士後研究員	0	0	100%		
		專任助理	0	0	100%		
國外	論文著作	期刊論文	0	1	100%	篇	
		研究報告/技術報告	0	0	100%		
		研討會論文	0	0	100%		
		專書	0	0	100%	章/本	
	專利	申請中件數	0	0	100%	件	
		已獲得件數	0	0	100%		
	技術移轉	件數	0	0	100%	件	
		權利金	0	0	100%	千元	
	參與計畫人力（外國籍）	碩士生	0	0	100%	人次	
		博士生	0	0	100%		
		博士後研究員	0	0	100%		
		專任助理	0	0	100%		

其他成果 (無法以量化表達之成果如辦理學術活動、獲得獎項、重要國際合作、研究成果國際影響力及其他協助產業技術發展之具體效益事項等，請以文字敘述填列。)	無

	成果項目	量化	名稱或內容性質簡述
科教處計畫加填項目	測驗工具(含質性與量性)	0	
	課程/模組	0	
	電腦及網路系統或工具	0	
	教材	0	
	舉辦之活動/競賽	0	
	研討會/工作坊	0	
	電子報、網站	0	
	計畫成果推廣之參與（閱聽）人數	0	

國科會補助專題研究計畫成果報告自評表

請就研究內容與原計畫相符程度、達成預期目標情況、研究成果之學術或應用價值（簡要敘述成果所代表之意義、價值、影響或進一步發展之可能性）、是否適合在學術期刊發表或申請專利、主要發現或其他有關價值等，作一綜合評估。

1. 請就研究內容與原計畫相符程度、達成預期目標情況作一綜合評估

   ■達成目標

   □未達成目標（請說明，以 100 字為限）

   　　□實驗失敗

   　　□因故實驗中斷

   　　□其他原因

   說明：

2. 研究成果在學術期刊發表或申請專利等情形：

   論文：□已發表 □未發表之文稿 ■撰寫中 □無

   專利：□已獲得 □申請中 ■無

   技轉：□已技轉 □洽談中 ■無

   其他：（以 100 字為限）

   本計畫所設定之目標大部分已經完成，研究成果也陸續在登錄中。然而，本人對於該主題更進一步的研究已有相當程度之瞭解，所以尚未將目前之論文初稿寄送至期刊發表。待本人確定後續之研究是否與現階段之成果有不可分割之完整性後，本人將盡快把目前之研究成果發表至學術期刊上。

3. 請依學術成就、技術創新、社會影響等方面，評估研究成果之學術或應用價值（簡要敘述成果所代表之意義、價值、影響或進一步發展之可能性）（以 500 字為限）

   馬可夫鏈的定性分析以及實務上的應用（尤其是統計物理學、資訊科學和分子生物學）在過去這一個世紀以來已經有相當成熟的發展。然而在實務的應用上，即便是很簡單的數學模型，定性分析所提供的幾個物理量依然是無法準確的估計出來。這對於模型之建立與模擬可能造成極大的誤差。本研究專題主要是針對某一特定模型之物理量，提供一個數學演算法來逼近目標值。並且針對該演算法，提供一個預測值與目標值之間的誤差上限。令人驚訝的是，該演算法的收斂速度很快，其誤差值是以指數函數的方式在遞減。這在實務上有很大的應用性與啟發性。