无处不在的样条函数：从逼近论、离散数学到概率统计学

许艳 著

SWJTUP 西南交通大学出版社

无处不在的样条函数: 从逼近论、离散数学到概率统计学

Ubiquitous Splines: From Approximation, Discrete Mathematics to Probability and Statistics

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内容提要

样条函数之父 Schoenberg 开启了样条函数理论研究的先河. 20 世纪 70 年代后，产生于逼近论的样条函数结合计算机科学技术，经过 40 多年的发展，已经成为沟通多个数学学科的桥梁. 本书以多元样条函数为主要工具，研究基础数学和概率统计学领域的交叉问题. 从样条函数理论的历史发展脉络来看，多元样条理论的发展可以带动与之相关的组合数学、离散几何学以及概率统计等数学分支的发展. 虽然这些交叉问题各自在相互不了解的情况下独立发展了几十年，但是数学的相关性与和谐性使得这些分支在最近的十几年内相互交融. 本书的主要目的是介绍样条这个具有生命力的数学工具以及这些方兴未艾的学科问题.

图书在版编目（CIP）数据

无处不在的样条函数：从逼近论、离散数学到概率统计学 / 许艳著. —成都：西南交通大学出版社，2020.4

ISBN 978-7-5643-7417-4

Ⅰ. ①无… Ⅱ. ①许… Ⅲ. ①样条函数 Ⅳ. ①O241.5

中国版本图书馆 CIP 数据核字（2020）第 065144 号

Wuchubuzai de Yangtiao Hanshu: Cong Bijinlun, Lisan Shuxue dao Gailü Tongjixue

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责任编辑	孟秀芝
封面设计	曹天擎
出版发行	西南交通大学出版社 （四川省成都市金牛区二环路北一段 111 号 西南交通大学创新大厦 21 楼）
发行部电话	028-87600564　028-87600533
邮政编码	610031
网址	http://www.xnjdcbs.com
印刷	四川煤田地质制图印刷厂
成品尺寸	170 mm × 230 mm
印张	9.75
字数	165 千
版次	2020 年 4 月第 1 版
印次	2020 年 4 月第 1 次
书号	ISBN 978-7-5643-7417-4
定价	48.00 元

序　言

B-样条函数是逼近论和数值分析中的重要工具，具有多个优美的性质，如局部支集性、非负性，对数凸性等，正因为B-样条函数具有如此多优美的性质，其在曲线曲面设计、方程数值求解、图像处理、小波等领域具有广泛的应用。与抽象的数学理论不同，B-样条函数是十分具体的，具体到可以写出它的显式表达公式，可以写出它的Fourier 变换的显式表达公式，可以写出它的导数的显式表达公式，并可快速计算出任意阶 B-样条函数在任意点的函数值。在传统数学教学中，人们更多从应用角度去看待 B-样条，但 B-样条函数却有着十分丰富的数学内涵。正如同它的桥形函数图像所显示的，B-样条函数也的确是连接多个不同数学领域的桥梁。人们可从离散几何、组合计数、概率、统计等多个不同角度对 B-样条进行理解和定义，并可将一个领域的结果，通过B-样条函数传递到另外一个领域，或者反之。这对这些领域的研究、发展都是十分有裨益的。正因为如此，本书主要针对B-样条的一些数学内涵及其在几个完全不同的领域中所扮演的角色进行介绍。许艳博士分别从几个不同角度进行选材，如多面体、Eulerian数以及概率统计等。这些选材十分新颖且具有前沿性，亦让我们感觉B-样条像一块奇异的宝石，在多个领域都散发着耀眼光芒。这可以帮助读者深入理解样条函数及其与多个不同领域的关联，并可以此为契机，帮助读者进入这些领域的研究前沿。

许志强

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前　言

1946 年 Schoenberg 对样条函数奠基性的工作[1], 开启了样条函数理论研究的先河. 20 世纪70 年代后, 产生于逼近论的样条函数结合计算机科学技术, 经过 40 多年的发展, 已经成为计算数学的重要工具. 样条函数具有理论深刻与应用广泛的双重意义. 它的应用范围包括数学、工程技术以及社会科学等领域. 例如, 样条函数在数学领域已应用于数值分析、曲线曲面的构造、微分方程的求解等, 在工程技术领域已用于信号分析、图像处理、计算机识别、地震勘探数据处理、边缘检测、音乐与语音合成、机械故障诊断等, 在社会科学领域已成功应用于计量经济学和统计等交叉学科. 随着样条理论的深入研究与发展, 人们发现样条函数与基础数学的一些领域, 如离散几何学、组合数学、渐近分析以及概率统计学等的关联也日趋紧密.

本书主要针对数值差商和与样条函数相关的基础数学及概率统计学领域中的交叉问题进行讨论. 本书的主要内容为：超收敛数值差商公式研究、离散几何中的样条函数方法、组合学中的样条函数方法、渐近分析中的双正交系统以及统计学中的样条函数方法。本书的具体内容如下：

数值差商一直是计算数学研究的核心课题, 与很多基础数学问题关联紧密. 例如，多元样条函数就有差商的定义方式, 因而多元差商理论的发展与多元样条函数理论的发展息息相关. 本书以一个数值差商公式猜想的证明开篇, 介绍充分光滑函数在节点距离很近的时候, 如何用该函数的 Hermite 插值多项式的差商来替代原函数的差商, 因而插值多项式可以转变为在另一组节点上的差商计算, 从而可以将这组节点间距取得足够大,

以便计算能够顺利进行.

第2章先介绍王兴华、王何宇和来明骏[2] 对充分光滑函数给出的数值差商公式余项的估计, 并且推导出了若干超收敛的数值差商公式及其余项的 Lagrange 表示. 但他们给出的这类超收敛公式余项的 Lagrange 表示定理仅仅限定在节点不超过4个的情况. 他们猜想这一结论对于任意正整数个节点成立. 我们证明了这一猜想, 得到了比较广泛的一类超收敛的数值差商公式余项的 Lagrange 表示定理. Brodskii[3], de Boor[4], Floater[5], 王兴华[6] [7] 等人关于数值差商公式余项的结果作为该定理的特例. 这一猜想的证明拓宽了数学家 Carl de Boor[4] 关于数值差商公式的适用范围, 也使得 Bridskii[3] 所得到的数值差商公式余项的估计成为本定理的特例.

第3章在离散几何问题的研究中, 引入样条函数方法. 将离散几何中的超立方体切面问题转化为与之等价的样条函数问题. 超立方体切面问题的研究最早可以追溯到 Laplace 和 Pólya 的研究工作. 他们分别利用概率方法给出了切面体积的积分表示和渐近形式. Pólya 所给出的体积公式在离散几何的相关问题的研究中具有十分重要的地位. 例如著名的 Good 猜想, 其证明就是由 Hensley 利用概率论的方法巧妙地估计了 Pólya 所给出的公式. 此外, Hensley 还给出了另一个关于切面最大值的猜想. 1989年, K. Ball[8]对 Pólya 所给出的体积积分公式进行估计, 证明了 Hensley 猜想. 2001年, Borwein[9]也曾给出类似于 Pólya 的积分公式. 但是上述关于超立方体切面的结果大多由概率方法得到. 在本书中, 我们提出了一种样条方法, 给出了 Laplace 和 Pólya 结果的样条证明, 考察了 B 样条函数及其导函数在 L^p 空间的渐近性并且给出了逼近阶, 从而使得 Laplace 和 Pólya 关于超立方体切面体积的渐近结果作为该定理的简单推论. 该定理不但可用于立方体切面的研究, 而且在计数组合学中亦发挥着重要的作用.

在本书的第4章提出了一种解决离散数学问题的新方法. 利用样条理论考虑了一系列的计数组合学问题, 为离散对象的研究提供了一种新的分析方法框架. 例如, 在组合数学中，组合计数问题、整数剖分函数以及组合序列对数凹性质都与样条函数理论相关, 甚至组合学中著名的Worpitzky恒等式可以看作样条函数理论中的 Marsden 恒等式特例。关于经典 Eulerian 数的一系列结果都可以作为 B样条函数的特例. 组合数的渐近分析一直是组合数学中引人入胜的问题. 一直以来，人们关注如何利用概率方法来解决这类问题. 我们发现, 一类组合渐近问题可以利用产生于逼近论的样条函数来优雅地解决. 不同于以往的概率方法, 样条方法能够更为精确地刻画组合数的逼近形式. L. Carlitz [10] 等人利用中心极限定理得到 Eulerian 数渐近公式的逼近阶为 $\frac{3}{4}$ 阶. 我们利用样条方法给出了更为精确的逼近阶.

组合序列的对数凹性是计数组合学研究的重要问题之一. 一般而言, 研究组合序列的对数凹性有以下几种方法：直接的组合方法、多项式实零点方法、解析法、混合体积法、代数方法等. 美国科学院院士 R. P. Stanley [11]和教授 F. Brenti[12] [13] 等人在这一领域做了大量翔实而深刻的研究. 在此, 我们给出一种研究组合序列对数凹性的新方法 —— 样条函数方法. 利用该方法, 我们证明了多种广义 Eulerian 数的对数凹性. 特别地, E. Steingrímsson 教授证明了 广义下降多项式 $D_d^n(t)$ 的系数 $D(d,n,k)$ 关于 k 具有单峰性. 利用样条方法, 我们得到了 $D(d,n,k)$ 关于 k 具有对数凹性这一更强结果.

将样条函数与混合体积联系起来, 给出了一类混合体积的样条解释. 利用这种解释可以得到一类具有对数凹性的组合序列, 从而部分回答了 Schmidt 和 Simion [14] 提出的关于混合体积的公开问题. 利用该结果, 给

出了细化 Eulerian 数、下降多项式的显式和递归表示.

第5章研究样条函数理论的初衷是将多项式逼近推广到分片多项式的插值. 这一理论的快速发展得益于样条函数在计算机辅助设计中对于构造自由曲线曲面的应用. 同时, 样条函数也应用于小波分析、稀疏数据表示以及图像处理等领域. 为了拓广到正交多项式以及正交样条函数, 样条函数之父 Schoenberg 构造了一类正交基底, 借以得到有限区间上的均匀样条函数. 这类正交基底被称为“Legendre 样条”.构造均匀样条 Legendre 多项式这样的简单例子并没有使得人们看到构造更多的正交样条或者有效的算法的可行性. 因而这一理论从 Schoenberg 之后并没有太多的进展. 但是鉴于正交多项式和特殊函数在数学中的重要性, 以及由它们所衍生出来的众多应用, 这部分着重讨论了各类正交多项式的渐近性质.

我们从一元均匀 B 样条与 Bernoulli 多项式的双正交关系谈起，衍生出众多正交多项式与特殊函数的双正交关系. 建立一套全新的研究多项式渐近性质的理论框架. 本章着重讨论了渐近于 Hermite 多项式和 Laguerre 多项式的函数列性质. 构造一类渐近于 Hermite 正交多项式的 Appell 多项式序列, 使得该序列与渐近于 Gauss 函数的函数类 ϕ的 n 阶导数之间构成了一组双正交系统. 利用这一结果, 可以得到多种正交多项式和组合多项式的渐近性质以及一些新的组合恒等式. 特别地, 由 N 阶 B 样条所生成的 Appell 多项式序列恰为 N 阶 Bernoulli 多项式. Bernoulli 多项式与 B 样条的导函数之间便构成了一组双正交系统, 且标准化之后的 Bernoulli 多项式随着 $N \to \infty$ 渐近到 Hermite 多项式. 由二项分布所生成的 Appell 序列为 Euler 多项式, 从而 Euler 多项式与二项分布的导函数之间构成了一组双正交系统, 且标准化之后的 Euler 多项式随着 $N \to \infty$ 渐近到 Hermite 多项式. 给出了 Appell 序列的生成函数满足尺度方程的

充要条件. 给出了渐近于 Hermite 多项式的函数列的判定定理. 应用该定理, 验证了广义 Buchholz 多项式、广义 Ultraspherical (Gegenbauer) 多项式和广义 Laguerre 多项式渐近于 Hermite 多项式的性质. 给出了渐近于 Laguerre 多项式的函数列的构造方法和判定定理. 利用 Laguerre 多项式给出了 Meixner-Pllaczek 多项式和 Meixner 多项式的渐近形式. 超几何正交多项式的 Askey 格式揭示了正交多项式之间的渐近关系. 应用上述方法验证了部分 Askey 格式成立.

第6章讨论了样条函数在概率统计学中的应用. 样条函数原本是计算数学家研究的课题, 但由于其具有独特的性质, 样条函数很快就引起了概率论和统计学家们的兴趣. 多元样条函数的概率解释始于 1956 年 Watson 的工作. 此后 S. Karlin, C. A. Micchelli 和 Y. Rinott 于 1986 年系统地给出了多元样条函数作为特殊的概率密度函数的解释,从而导出多元样条函数的递归公式, 并且得到了多元样条函数的对数凹性质.

本研究的重要性还在于提出了利用 Dirichlet 概率密度函数所定义的广义多元样条函数. 这也是此后由 M. Unser 等人所给出的分数阶样条函数的理论基础. 2010 年, Peter Massopust 和 Brightte Forester 在论文 *Multivariate Complex B-splines and Dirichlet Averages* 中系统地给出了多元复样条的概率解释. 中科院研究员许志强于 2009 年将上述概念推广至多元 F 样条, 给出了多元 F 截断幂、多元 F-箱样条的定义, 从而将多元多项式样条和多元 E 样条作为该定义的特例. 由此可以将包含多元复样条和分数阶样条在内的样条函数的定义统一起来. 从而给出了新的计算多面体上积分的工具. 瑞典数学家 Svante Janson 在论文 *Euler - Frobenius Numbers and Rounding*(2013) 中将我们关于多元样条函数与组合数学、离散几何学的研究成果运用概率论的方法进行重新推广和证明, 给出了

Euler–Frobenius 和广义 Eulerian 数的概率分布, 将我们得到的 Eulerian 数相关的理论成果用概率论的语言加以证明和重写.

近30 年来,样条函数估计方法业已发展成一支比较活跃的统计学新分支. 鉴于国内学者在该领域涉足不深, 现根据作者近年来在该方面的研究体会和积累的资料, 以回归分析和非参数分析为重点, 对该分支的主要内容和发展现状做一粗浅的介绍.介绍这一领域的历史发展脉络, 以期为以后有志于这一领域研究的学者起到抛砖引玉的作用.

从这些历史发展脉络我们能够看出, 多元样条理论的发展可以带动与之相关的组合数学、离散几何学以及概率统计等数学分支的发展. 虽然多个分支的问题各自在相互不了解的情况下独立发展了几十年, 但是数学的相关性与和谐性使得这些分支在最近的十几年内相互交融. 这也是我们写这本专著的目的，向读者介绍样条这个具有生命力的工具以及这些方兴未艾的学科.

Preface

Schoenberg's fundamental work on spline functions in 1946[1] is the corner stone in the history of the spline theory. Spline functions originally derived from the approximation theory. As the computer science and technologies developing, the spline theory has became an important tool in computational mathematics over 40 years after 1970s. It has both profound theoretical and applicable significance. Its applications include the fields such as mathematics, engineering, and even social sciences. Splines have been applied to numerical analysis, curve and surface construction, differential equation, etc. In the field of engineering, it has been used in signal analysis, image processing, computer recognition, seismic exploration data processing, edge detection, music and speech synthesis, mechanical fault diagnosis and other fields. In the social sciences, spline theory has been successfully applied to econometrics and statistics in the 1990s. With the deepening development of the spline theory, people found that the splines are closely related to some areas in fundamental mathematics, such as discrete geometry, combinatorial mathematics, asymptotic analysis and probabilistic statistics.

The book focuses on the divided difference and the problems related to the splines theory in the fundamental mathematics, probability theory and statistics. The main contents are as follow: the several divided difference formulas with super-convergence are investigated; the spline methods in discrete geometry are proposed, the splines in combinatorics, biorthogonal systems and the statistics.

Divided difference is the important topic in computational mathematics, which is closely related to many basic problems. Such as, the multivariate splines have a definition of divided differences. Therefore, the development of multivariate difference theory is quite related to the development of the multivariate spline theory. The book begins with a proof of the conjecture of the divided difference. If the nodes of the sufficient smoothness functions are very close, it is very difficult to calculate the divided differences of the functions. So the Hermite interpolation polynomials of the function can calculate the divided differences on another set of nodes. The distances of this set of nodes can be made large enough such that the computation of the divided differences can be carried out smoothly.

In chapter 2, Xinghua Wang, Heyu Wang and MingJun Lai estimated the remainders of the numerical divided difference formula for sufficient smooth function and derived the Lagrange expression of several divided difference formulas with super-convergence. But the conditions of formulas are only limited for 4 knots. The conjecture about several divided difference formulas with super-convergence for any positive integers are proposed by them. We proved the conjecture and derived a type of more general super convergent remainders for Lagrange interpolation which contains Brodskii[3], de Boor [4], Floater [5], Xinghua Wang's[6] [7] recent derivative expansions as special cases. It also extended the range of the divided differences given by mathematician Carl de Boor and made the Bridskii's formula as a special case of the theorem.

Spline methods in discrete geometry are proposed in chapter 3. The volumes of portions of hypercubes determined by hyperplanes play important roles in discrete geometry and other branches of Mathematics. It seems that Laplace and Pólya investigated this problem in the context of a question in probability. They gave the integral expression and asymptotic formula for the volume of a central slab of a hypercube. Pólya's formula and its close relatives are striking important in solving the problems arising in cube slicing. For example, Good conjecture was solved by Hensley with the help of probabilistic methods and Pólya's formula. Hensley also gave another conjecture about the upper bound for the volume of the slice. Ball used probabilistic methods, ending it up making ingenious estimates on integrals corresponding to the integral formula for the volume treated by Pólya. In this dissertation, we observed that the volume of the slice can be transformed to an equivalent problem in spline theory. Having related it directly to B-splines [15], we can take advantage of many powerful spline techniques to derive various results of these objects. the asymptotic properties of B-splines and their derivatives are investigated and the convergence orders are also derived. The results given by Laplace and Pólya are reproved with brevity and elegance by using spline notation. The asymptotic properties of B-splines are not only play a part in cube slicing but also striking important in combinatorial enumeration.

In chapter 4, a novel method for discrete mathematics is studied. The related problems in enumeration combinatorics were solved by multivariate splines which constructed the frames of fundamental theory of spline methods in discrete problems. For instance, problems in combinatorial enumerations, integer partition function, log-concavity for some combinatorial sequences are studied. The famous Worpitzky identical equation in combinatorics can be considered as the special case of the Marsden identical equation in splines. There are series results of the classical Eulerian numbers which are derived from the B-spline. The asymptotic analysis is the attractive topic in combinatorics. People always concern about how to use the probabilistic methods to solve such problems. But we find that a class of the combinatorial asymptotic problems can be solved elegantly by using spline functions derived from approximation theory. Different from probability methods, the spline methods describe the approximation rate of combination number more accurately. L. Carlitz [10] et al. obtained the asymptotic formula of Eulerian numbers with the approximation order of $\frac{3}{4}$ by using the central limit theorem. But a more accurate approximation order is gotten by the spline theory.

The log-concavity of combinatorial sequences is one of the important problems in enumeration combinatorics. In general, there are several methods to study the log-concavity of combination sequences: polynomial real root method, the analytic method, the mixed volume method, and the algebraic method, etc. Combinatorial mathematician R. P. Stanley[11], F. Brenti[12] [13] and others have done a lot of profound research in this field. We present a new spline method to study the log-concavity of the combinatorial sequences. The log-concavity of various generalized Eulerian numbers is proved by this method. In particular, E. Steingrímsson proved that the coefficients of the generalized descent polynomial $D_d^n(t)$, denoted by $D(d,n,k)$ are unimodal on k. We got the stronger results that $D(d,n,k)$ on k are log-concavity by the spline theory.

Spline explanations for some mixed volumes are derived by exploring the relations between mixed volumes and splines. Constructing log-concave sequences by using the explanation, a partial answer to the open problems which was proposed by Schmidt and Simion [14]. The explicit and recursive representations of refined Eulerian Numbers and decreasing polynomials are given.

The initial motivation for the development of spline functions in chapter 5 was to extend the vast knowledge on polynomial approximation and interpolation to spline functions. These extensions then developed rapidly because of their applicability in computer aided design of free-form curves and surfaces, as well as in wavelets and frames for sparse data representation and image processing. In an attempt to extend orthogonal polynomials to orthogonal splines, Schoenberg constructed an orthogonal basis for a class of uniform spline functions on a finite interval, in which the orthogonal basis functions were referred to as the "Legendre splines". The construction and results of this simple case of a uniform spline analogue of Legendre polynomials do not show promise of the availability of efficient algorithms or a general theory for orthogonal splines, and there has been no progress since then. Since orthogonal polynomials and special functions form an important discipline with many applications, this chapter aims to make another attempt to extend the vast knowledge of the asymptotic properties of the orthogonal polynomials and special functions to spline functions.

The biorthogonal relations between the orthogonal polynomials and special functions are derived from the biorthogonal property of uniformed B-splines and Bernoulli polynomial. A new theoretical framework is established to study the asymptotic properties of the polynomials. In this chapter, we focus on the properties of the functions asymptotic to Hermite polynomials and Laguerre polynomials. Hermite polynomials can be considered as a biorthogonal relation between the derivatives of the Gaussian and the Hermite polynomials. We extend the biorthogonal relation between Hermite polynomials and the derivatives of the Gaussian to a family of functions ϕ that approximate the Gaussian function and to construct a family of Appell sequences of "biorthogonal polynomials" that approximate to Hermite polynomials. The Appell polynomials and the distributional derivatives of ϕ form a biorthognal system. In particular, the Appell polynomials generated by the uniform B-spline of order N are the classical Bernoulli polynomials of order N and the Appell polynomials generated by the binomial distributions of order N are the classical Euler polynomials of order N. After suitably normalized, they converge to Hermite polynomials as $N \to \infty$. A necessary and sufficient condition for two Appell polynomial sequences whose generating functions satisfy the α-scaling equation is derived. as corollaries of the theorem for polynomial sequences that approximate to Hermite polynomials, the asymptotic properties of generalized Buchholz polynomials, Ultraspherical (Gegenbauer) polynomials and Laguerre polynomials are verified. Similarly, the asymptotic formulas for Meixner-Pllaczek polynomials and Meixner polynomials are derived from the theorem for polynomial sequences that approximate to generalized Laguerre polynomials. The Askey scheme of the hypergeometric orthogonal polynomials has verified.

In the last chapter of the book, we discuss the applications of the spline functions in probability and statistics. The splines are the topics originally from computational mathematics, but due to their unique properties, It becomes attractive to the people from probability theory and statistics. The probabilistic interpretation of multivariate spline functions started from the work of Watson in 1956. C. A. Micchelli and Y.Rinott systematically generalized the interpretation as a special probability density function to derived the recurrence formula and the logconcavity of the multivariate spline in 1986.

The importance of this paper also lies in the fact that a generalized multivariate spline function defined by the Dirichlet probability density