London Mathematical Society
Lecture Note Series 484

Discrete Quantum Walks on Graphs and Digraphs

Chris Godsil and Hanmeng Zhan

LONDON
MATHEMATICAL
SOCIETY
EST. 1865

CAMBRIDGE

Discrete Quantum Walks on Graphs and Digraphs

Discrete quantum walks are quantum analogues of classical random walks. They are an important tool in quantum computing and a number of algorithms can be viewed as discrete quantum walks, in particular Grover's search algorithm. These walks are constructed on an underlying graph, and so there is a relation between properties of walks and properties of the graph. This book studies the mathematical problems that arise from this connection, and the different classes of walks that arise. Written at a level suitable for graduate students in mathematics, the only prerequisites are linear algebra and basic graph theory; no prior knowledge of physics is required. The text serves as an introduction to this important and rapidly developing area for mathematicians and as a detailed reference for computer scientists and physicists working on quantum information theory.

CHRIS GODSIL is Distinguished Professor Emeritus at the University of Waterloo. He has written three books: *Algebraic Combinatorics* (1993), *Algebraic Graph Theory* (2004, co-authored with Gordon Royle) and *The Erdos-Ko-Rado Theorem: Algebraic Approaches* (2015, co-authored with Karen Meagher).

HANMENG ZHAN is a postdoctoral fellow at Simon Fraser University. For her thesis on discrete quantum walks via algebraic graph theory, she received two awards from the University of Waterloo: the University Finalist for the Governor General's Gold Medal and the Inaugural Mathematics Doctoral Prize.

LONDON MATHEMATICAL SOCIETY LECTURE NOTE SERIES

Managing Editor: Professor Endre Süli, Mathematical Institute, University of Oxford, Woodstock Road, Oxford OX2 6GG, United Kingdom

The titles below are available from booksellers, or from Cambridge University Press at www.cambridge.org/mathematics

374 Geometric analysis of hyperbolic differential equations: An introduction, S. ALINHAC
375 Triangulated categories, T. HOLM, P. JØRGENSEN & R. ROUQUIER (eds)
376 Permutation patterns, S. LINTON, N. RUŠKUC & V. VATTER (eds)
377 An introduction to Galois cohomology and its applications, G. BERHUY
378 Probability and mathematical genetics, N. H. BINGHAM & C. M. GOLDIE (eds)
379 Finite and algorithmic model theory, J. ESPARZA, C. MICHAUX & C. STEINHORN (eds)
380 Real and complex singularities, M. MANOEL, M.C. ROMERO FUSTER & C.T.C WALL (eds)
381 Symmetries and integrability of difference equations, D. LEVI, P. OLVER, Z. THOMOVA & P. WINTERNITZ (eds)
382 Forcing with random variables and proof complexity, J. KRAJÍČEK
383 Motivic integration and its interactions with model theory and non-Archimedean geometry I, R. CLUCKERS, J. NICAISE & J. SEBAG (eds)
384 Motivic integration and its interactions with model theory and non-Archimedean geometry II, R. CLUCKERS, J. NICAISE & J. SEBAG (eds)
385 Entropy of hidden Markov processes and connections to dynamical systems, B. MARCUS, K. PETERSEN & T. WEISSMAN (eds)
386 Independence-friendly logic, A.L. MANN, G. SANDU & M. SEVENSTER
387 Groups St Andrews 2009 in Bath I, C.M. CAMPBELL *et al* (eds)
388 Groups St Andrews 2009 in Bath II, C.M. CAMPBELL *et al* (eds)
389 Random fields on the sphere, D. MARINUCCI & G. PECCATI
390 Localization in periodic potentials, D.E. PELINOVSKY
391 Fusion systems in algebra and topology, M. ASCHBACHER, R. KESSAR & B. OLIVER
392 Surveys in combinatorics 2011, R. CHAPMAN (ed)
393 Non-abelian fundamental groups and Iwasawa theory, J. COATES *et al* (eds)
394 Variational problems in differential geometry, R. BIELAWSKI, K. HOUSTON & M. SPEIGHT (eds)
395 How groups grow, A. MANN
396 Arithmetic differential operators over the *p*-adic integers, C.C. RALPH & S.R. SIMANCA
397 Hyperbolic geometry and applications in quantum chaos and cosmology, J. BOLTE & F. STEINER (eds)
398 Mathematical models in contact mechanics, M. SOFONEA & A. MATEI
399 Circuit double cover of graphs, C.-Q. ZHANG
400 Dense sphere packings: a blueprint for formal proofs, T. HALES
401 A double Hall algebra approach to affine quantum Schur–Weyl theory, B. DENG, J. DU & Q. FU
402 Mathematical aspects of fluid mechanics, J.C. ROBINSON, J.L. RODRIGO & W. SADOWSKI (eds)
403 Foundations of computational mathematics, Budapest 2011, F. CUCKER, T. KRICK, A. PINKUS & A. SZANTO (eds)
404 Operator methods for boundary value problems, S. HASSI, H.S.V. DE SNOO & F.H. SZAFRANIEC (eds)
405 Torsors, étale homotopy and applications to rational points, A.N. SKOROBOGATOV (ed)
406 Appalachian set theory, J. CUMMINGS & E. SCHIMMERLING (eds)
407 The maximal subgroups of the low-dimensional finite classical groups, J.N. BRAY, D.F. HOLT & C.M. RONEY-DOUGAL
408 Complexity science: the Warwick master's course, R. BALL, V. KOLOKOLTSOV & R.S. MACKAY (eds)
409 Surveys in combinatorics 2013, S.R. BLACKBURN, S. GERKE & M. WILDON (eds)
410 Representation theory and harmonic analysis of wreath products of finite groups, T. CECCHERINI-SILBERSTEIN, F. SCARABOTTI & F. TOLLI

411 Moduli spaces, L. BRAMBILA-PAZ, O. GARCÍA-PRADA, P. NEWSTEAD & R.P. THOMAS (eds)
412 Automorphisms and equivalence relations in topological dynamics, D.B. ELLIS & R. ELLIS
413 Optimal transportation, Y. OLLIVIER, H. PAJOT & C. VILLANI (eds)
414 Automorphic forms and Galois representations I, F. DIAMOND, P.L. KASSAEI & M. KIM (eds)
415 Automorphic forms and Galois representations II, F. DIAMOND, P.L. KASSAEI & M. KIM (eds)
416 Reversibility in dynamics and group theory, A.G. O'FARRELL & I. SHORT
417 Recent advances in algebraic geometry, C.D. HACON, M. MUSTAŢĂ & M. POPA (eds)
418 The Bloch–Kato conjecture for the Riemann zeta function, J. COATES, A. RAGHURAM, A. SAIKIA & R. SUJATHA (eds)
419 The Cauchy problem for non-Lipschitz semi-linear parabolic partial differential equations, J.C. MEYER & D.J. NEEDHAM
420 Arithmetic and geometry, L. DIEULEFAIT *et al* (eds)
421 O-minimality and Diophantine geometry, G.O. JONES & A.J. WILKIE (eds)
422 Groups St Andrews 2013, C.M. CAMPBELL *et al* (eds)
423 Inequalities for graph eigenvalues, Z. STANIĆ
424 Surveys in combinatorics 2015, A. CZUMAJ *et al* (eds)
425 Geometry, topology and dynamics in negative curvature, C.S. ARAVINDA, F.T. FARRELL & J.-F. LAFONT (eds)
426 Lectures on the theory of water waves, T. BRIDGES, M. GROVES & D. NICHOLLS (eds)
427 Recent advances in Hodge theory, M. KERR & G. PEARLSTEIN (eds)
428 Geometry in a Fréchet context, C.T.J. DODSON, G. GALANIS & E. VASSILIOU
429 Sheaves and functions modulo *p*, L. TAELMAN
430 Recent progress in the theory of the Euler and Navier–Stokes equations, J.C. ROBINSON, J.L. RODRIGO, W. SADOWSKI & A. VIDAL-LÓPEZ (eds)
431 Harmonic and subharmonic function theory on the real hyperbolic ball, M. STOLL
432 Topics in graph automorphisms and reconstruction (2nd Edition), J. LAURI & R. SCAPELLATO
433 Regular and irregular holonomic D-modules, M. KASHIWARA & P. SCHAPIRA
434 Analytic semigroups and semilinear initial boundary value problems (2nd Edition), K. TAIRA
435 Graded rings and graded Grothendieck groups, R. HAZRAT
436 Groups, graphs and random walks, T. CECCHERINI-SILBERSTEIN, M. SALVATORI & E. SAVA-HUSS (eds)
437 Dynamics and analytic number theory, D. BADZIAHIN, A. GORODNIK & N. PEYERIMHOFF (eds)
438 Random walks and heat kernels on graphs, M.T. BARLOW
439 Evolution equations, K. AMMARI & S. GERBI (eds)
440 Surveys in combinatorics 2017, A. CLAESSON *et al* (eds)
441 Polynomials and the mod 2 Steenrod algebra I, G. WALKER & R.M.W. WOOD
442 Polynomials and the mod 2 Steenrod algebra II, G. WALKER & R.M.W. WOOD
443 Asymptotic analysis in general relativity, T. DAUDÉ, D. HÄFNER & J.-P. NICOLAS (eds)
444 Geometric and cohomological group theory, P.H. KROPHOLLER, I.J. LEARY, C. MARTÍNEZ-PÉREZ & B.E.A. NUCINKIS (eds)
445 Introduction to hidden semi-Markov models, J. VAN DER HOEK & R.J. ELLIOTT
446 Advances in two-dimensional homotopy and combinatorial group theory, W. METZLER & S. ROSEBROCK (eds)
447 New directions in locally compact groups, P.-E. CAPRACE & N. MONOD (eds)
448 Synthetic differential topology, M.C. BUNGE, F. GAGO & A.M. SAN LUIS
449 Permutation groups and cartesian decompositions, C.E. PRAEGER & C. SCHNEIDER
450 Partial differential equations arising from physics and geometry, M. BEN AYED *et al* (eds)
451 Topological methods in group theory, N. BROADDUS, M. DAVIS, J.-F. LAFONT & I. ORTIZ (eds)
452 Partial differential equations in fluid mechanics, C.L. FEFFERMAN, J.C. ROBINSON & J.L. RODRIGO (eds)

453 Stochastic stability of differential equations in abstract spaces, K. LIU
454 Beyond hyperbolicity, M. HAGEN, R. WEBB & H. WILTON (eds)
455 Groups St Andrews 2017 in Birmingham, C.M. CAMPBELL *et al* (eds)
456 Surveys in combinatorics 2019, A. LO, R. MYCROFT, G. PERARNAU & A. TREGLOWN (eds)
457 Shimura varieties, T. HAINES & M. HARRIS (eds)
458 Integrable systems and algebraic geometry I, R. DONAGI & T. SHASKA (eds)
459 Integrable systems and algebraic geometry II, R. DONAGI & T. SHASKA (eds)
460 Wigner-type theorems for Hilbert Grassmannians, M. PANKOV
461 Analysis and geometry on graphs and manifolds, M. KELLER, D. LENZ & R.K. WOJCIECHOWSKI
462 Zeta and *L*-functions of varieties and motives, B. KAHN
463 Differential geometry in the large, O. DEARRICOTT *et al* (eds)
464 Lectures on orthogonal polynomials and special functions, H.S. COHL & M.E.H. ISMAIL (eds)
465 Constrained Willmore surfaces, Á.C. QUINTINO
466 Invariance of modules under automorphisms of their envelopes and covers, A.K. SRIVASTAVA, A. TUGANBAEV & P.A.GUIL ASENSIO
467 The genesis of the Langlands program, J. MUELLER & F. SHAHIDI
468 (Co)end calculus, F. LOREGIAN
469 Computational cryptography, J.W. BOS & M. STAM (eds)
470 Surveys in combinatorics 2021, K.K. DABROWSKI *et al* (eds)
471 Matrix analysis and entrywise positivity preservers, A. KHARE
472 Facets of algebraic geometry I, P. ALUFFI *et al* (eds)
473 Facets of algebraic geometry II, P. ALUFFI *et al* (eds)
474 Equivariant topology and derived algebra, S. BALCHIN, D. BARNES, M. KĘDZIOREK & M. SZYMIK (eds)
475 Effective results and methods for Diophantine equations over finitely generated domains, J.-H. EVERTSE & K. GYŐRY
476 An indefinite excursion in operator theory, A. GHEONDEA
477 Elliptic regularity theory by approximation methods, E.A. PIMENTEL
478 Recent developments in algebraic geometry, H. ABBAN, G. BROWN, A. KASPRZYK & S. MORI (eds)
479 Bounded cohomology and simplicial volume, C. CAMPAGNOLO, F. FOURNIER-FACIO, N. HEUER & M. MORASCHINI (eds)
480 Stacks Project Expository Collection (SPEC), P. BELMANS, W. HO & A.J. DE JONG (eds)
481 Surveys in combinatorics 2022, A. NIXON & S. PRENDIVILLE (eds)
482 The logical approach to automatic sequences, J. SHALLIT
483 Rectifiability: a survey, P. MATTILA
484 Discrete Quantum Walks on Graphs and Digraphs, C. GODSIL & H. ZHAN

London Mathematical Society Lecture Note Series: 484

Discrete Quantum Walks on Graphs and Digraphs

C. GODSIL
University of Waterloo

H. ZHAN
Simon Fraser University

CAMBRIDGE
UNIVERSITY PRESS

CAMBRIDGE UNIVERSITY PRESS

Shaftesbury Road, Cambridge CB2 8EA, United Kingdom

One Liberty Plaza, 20th Floor, New York, NY 10006, USA

477 Williamstown Road, Port Melbourne, VIC 3207, Australia

314–321, 3rd Floor, Plot 3, Splendor Forum, Jasola District Centre, New Delhi – 110025, India

103 Penang Road, #05–06/07, Visioncrest Commercial, Singapore 238467

Cambridge University Press is part of Cambridge University Press & Assessment, a department of the University of Cambridge.

We share the University's mission to contribute to society through the pursuit of education, learning and research at the highest international levels of excellence.

www.cambridge.org
Information on this title: www.cambridge.org/9781009261685
DOI: 10.1017/9781009261692

First published 2023

Printed in the United Kingdom by TJ Books Limited, Padstow Cornwall

A catalogue record for this publication is available from the British Library.

ISBN 978-1-009-26168-5 Paperback

Contents

Preface

A discrete quantum walk is determined by a unitary matrix U, the *transition matrix* of the walk. If the initial state of the system is given by a vector z, then the state of the system at time k is $U^k z$. The problem is to choose U and z so that we can do something useful, and indeed we can – Grover showed how an implementation of this setup could be used to enable quantum computers to search a database faster than any known classical algorithm.

The framework we have just described is impossibly general; a quantum computer can conveniently implement only a small subset of the set of unitary matrices. There is also a mathematical difficulty, in that it may be impossible to derive useful predictions of the behaviour of the walk without imposing some structure on U.

As we have described it, the transition matrix U is an operator on the complex inner product space $\mathbb{C}^d$. However, for the reasons just given, much of the work on discrete quantum walks considers the case where U is an operator on the space of complex functions on the arcs (ordered pairs of adjacent vertices) of a graph X. Physically meaningful questions must be expressed in terms of the absolute values of the entries of the powers U^k. Thus, we might ask if, for a given initial state z, there is an integer k such that the absolute values of the entries of U^k are close to being equal.

The goal of our work on this topic has been to attempt to relate the properties of the walk to the properties of the underlying graph, and this book is both an introduction to the topic and a report on our progress.

We start our treatment with the most famous topic, Grover's search algorithm. We offer two approaches, but in both cases we find that the transition matrix arises as a product $U = RC$, where R and C are unitary matrices with simple structure and are defined in terms of an underlying graph. In fact, R and C are both involutions, and the algebra they generate is a matrix representation of the dihedral group. We make use of this fact to determine the spectral decomposition of U in terms of the underlying graph. (If the graph is k-regular on n vertices, U is of order $nk \times nk$, so we have reduced the scale of the problem.) We then apply the resulting theory to the study of properties of our walks, and determine useful parameters. Of course, each time we identify a parameter of a walk, we have introduced a possibly new graph parameter, and many interesting questions raise their heads.

In the second part of the book we relax our assumptions that R and C are involutions. We find that, to properly specify the resulting walks, we must specify a linear ordering on the arcs leaving a vertex. As any graph theorist is aware, embeddings of graphs in an orientable surface are specified by cyclic orderings of the arcs leaving a vertex. Hence we offer a detailed treatment of graph embeddings and graph covers. Following this, we consider walks based on shunts and walks on the line. We close the book with a treatment of what we call vertex-face walks, which are explicitly derived from embeddings of graphs in orientable surfaces.

We note that this book is based on the Ph.D. thesis of the second author (https://uwspace.uwaterloo.ca/handle/10012/13952). The intended audience is mathematicians, particularly those who might be interested in new graph theory problems arising from the study of discrete quantum walks. The book by Portugal [58] provides a complementary view. We do not think any knowledge of physics is required to profit from this work; the required background is linear algebra (spectral decomposition) and some field theory. We have tried to keep things self-contained, but Godsil and Royle [35] may prove a useful backup.

Cambridge University Press has a website devoted to this book at https://www.cambridge.org/gb/academic/subjects/mathematics/discrete-mathematics-information-theory-and-coding/discrete-quantum-walks-graphs-and-digraphs?

1

Grover Search

1.1 States

Any quantum system has a state space, which is a complex inner product space. For us, this will usually be finite dimensional, just $\mathbb{C}^d$ for some d. The actual states are the 1-dimensional subspaces of this vector space. We could specify a subspace U of the complex inner product space V by giving an orthonormal basis $u_1, \dots, u_k$, but it is often more convenient to define U in terms of the orthogonal projection P onto U – this is the idempotent Hermitian matrix with image equal to U. In fact, if v^* denotes the conjugate transpose of the vector (or matrix) v, then

$$P = \sum_i u_i u_i^*,$$

but, despite appearances, P is independent of the choice of orthonormal basis for U.

Operations on the state space correspond to unitary matrices. If U is unitary and the state of our system is given by a unit vector z, then the vector Uz defines the new state. If we choose to work with projections, our initial state is given by zz^*, and the state after we apply U is Uzz^*U^*.

The outcome of a measurement of a quantum system modelled by $\mathbb{C}^d$ can be taken to be an element of $\{1, \dots, d\}$. However, the result is actually a random variable: there are probabilities $p_1, \dots, p_d$ summing to 1, such that we observe outcome i with probability p_i. Thus, we have a probability density defined on the set $\{1, \dots, d\}$. This means we can view the outcome of a measurement as a probability density. This probability density will depend on the initial state of our system, the operations we apply to the system, and the choice of measurement.

Mathematically, a measurement is represented by a sequence $M_1, \dots, M_e$ of positive semidefinite matrices such that $\sum_i M_i = I$. The simplest case is when $e = d$ and $M_i = e_i e_i^T$ (here e_i denotes the characteristic vector of i, and ^{T} denotes the transpose). We describe this as 'measurement relative to the standard basis.' If the state of the system is zz^*, then the probability that we observe the ith outcome is

$$\mathrm{tr}(M_i zz^*) = z^* M_i z,$$

which is equal to the inner product $\langle M_i, zz^* \rangle$; if we are measuring relative to the standard basis, the probability is

$$z^* e_i e_i^T z = |\langle z, e_i \rangle|^2.$$

Thus, it is the square of the absolute value of the ith entry of z.

1.2 Discrete Walks

For our purposes, a *discrete quantum walk* is specified by a unitary matrix U. We call it the *transition matrix* of the walk. If U is $d \times d$, we view it as acting on a quantum system with state space $\mathbb{C}^d$. The system evolves under repeated applications of U; thus, if the initial state of the system is represented by the unit vector z, then after m steps, the state of the system would be $U^m z$. If we measure the system after k steps relative to the standard basis, the outcome will be e_j with probability

$$|\langle e_j, U^m z \rangle|^2.$$

Our view of a discrete quantum walk is more general than taken by physicists. We find the generality useful, but there are two problems. The first is mathematical: at this level of generality, we may lack the mathematical tools needed to determine interesting properties of parameters of the walk. The second is physical: some unitary matrices decribe operations that are not easily implemented in practice; thus, we will see that U is usually defined as a product of simple unitary matrices, often sparse.

One common feature of nearly all discrete walks in this book will be that the state space is the set of complex functions on the arcs of a graph. Here an *arc* of a graph is an ordered pair of adjacent vertices. Thus, if X is an undirected graph with m edges, then it has $2m$ arcs, and the associated state space will have dimension $2m$.

1.3 Grover Search

We present one of the most important applications of quantum walks, Grover's search algorithm. Basically we have a system with state space $\mathbb{C}^d$ and two unitary operators R and S. The operators have a special form; they are *reflections*. We explain what this means.