Ernesto Estrada

Institute of Applied Mathematics (IUMA),
Universidad de Zaragoza, Pedro Cerbuna 12, E-50009 Zaragoza, Spain;
ARAID Foundation, Government of Aragón, 50018 Zaragoza, Spain,
ernesto.estrada.roger@gmail.com,
http://www.estradalab.org

CAREER PROFILE (Education and Employment)

Employment

2019 -	Senior Researcher, ARAID Foundation, Institute of Applied Mathematics (IUMA), University of Zaragoza, Spain
2008 – 2018	Full Professor and Chair, Complexity Sciences, University of Strathclyde
2003 – 2008	"Ramón y Cajal" Researcher in Complex Systems, University of Santiago de Compostela, Spain
2002 – 2003	Research Scientist of Computational Chemistry, Safety & Environmental Assurance Centre (SEAC), Unilever, Colworth, UK
2001 – 2002	Research Associate, Department of Organic Chemistry, University of Santiago de Compostela, Spain
1999 – 2000	Postdoctoral Researcher, Lisa Meitner-Minerva Institute for Computational Quantum Chemistry, Hebrew University of Jerusalem, Israel
1997	Postdoctoral Researcher, Department of Physical Chemistry, University of Valencia, Spain
1993 – 1998	Assistant Researcher, Department of Computer-Aided Drug Design Center for Bioactive Chemicals, Central University of Las Villas, Cuba

Education

1997	PhD in Chemistry, Central University of Las Villas, Cuba
1990	MSc (Hons) in Chemistry, Central University of Las Villas, Cuba

AWARDS

- **2018** Elected Honorary Member of the *Italian Society of Chaos and Complexity*
- **2018** Pregl Colloquium Speaker, National Institute of Chemistry, Slovenia
- **2014** Elected Member of the *Academia Europaea*
- Awarded 1964 *Chair of Mathematics* at University of Strathclyde
- *Royal Society Wolfson Research Merit Award* for '*scientists of outstanding achievement and potential to the UK*', given by the Royal Society of London
- **2012** Plenary Speaker at the *2012 SIAM Annual Meeting*, Minneapolis, USA
- **2007** Award '*Outstanding Scientist'*, International Academy of Mathematical Chemistry, Croatia
- **2005** Elected Full Member of the '*International Academy of Mathematical Chemistry*', Croatia
- **1998** *National Prize of the Cuban Academy of Science*, Section of Natural Science, La Habana, Cuba

MEASURES OF STEEM

- Elected as:
  - Member of the Scientific Committee of the *23rd Conference of the International Linear Algebra Society*, Galway, Ireland, 2020
  - Member of the *Academia Europaea*, 2014
  - Full-Member of '*International Academy of Mathematical Chemistry*', 2005
  - Member of the Society's Newton International Fellowships Committee: Physical Sciences, 2017-2019
  - Plenary speaker at the 2012 SIAM Annual Meeting, Indianapolis, USA
- Editorial roles
  - Editor-in-Chief: Journal of Complex Networks (Oxford University Press), 2013-present
  - Associate Editor: SIAM Journal of Applied Mathematics, 2016-present
  - Section Editor: Encyclopedia of Complexity and Systems Science (Springer-Nature), 2016-
  - Member of the Editorial Board of: *MATCH Communications in Mathematical and in Computer Chemistry*, 2005-present; *Entropy*, 2015-present; *Journal of Chemical Information and Computer Science*, 2001-2003
- Expert for:
  - Israel Science Foundation for Revision of Research Grants

- Projects of the European Commission
- Governmental Experts, MAPRA Network, Animal and Plant Health, European Food Safety Authority
- Vienna Science and Technology Fund (WWTF), 2016.

- Reviewer for Grant Applications of the EPRSC, Vienna Science and Technology Fund WWTF, Romanian National Council for Research and Development, and the Netherlands Organisation for Scientific Research (NWO) for Veni Grants in the Innovational Research Incentives Scheme
- Over 55 invited talks, and plenary and keynote addresses at international conferences and a further 60+ invited talks at institutions and societies.

INNOVATION & COMMERCIALIZATION ACTIVITY

- Industrial collaborations with
  - *Weir Oil and Gas.* Developed complex network models of fractures in rocks of petrophysical interest. These models were implemented by the business to facilitate exploration processes.
  - *Isochron Ltd*. Developed business forecasting using network techniques that were implemented by the company for regular use.
  - *I2 Ltd*. Developed visual intelligence and investigative analysis software.
  - *Market Sentinel* on online conversation monitoring and analytics, and semantic search.
- Patents:
  1. Procedure for the preparation of 1-(5-bromofur-2-yl)-2-bromo-2-nitroethene and its microcide action, N. Castañedo, R. Goizueta, J. Pérez, J. González, E. Silveira, M. Cuesta, A. Martínez, E. Lugo, **E. Estrada**, A. C. Carta, O. Navia and M. S. Delgado. Cuban Patent 4894 (1994). European Patent Application 95500056.7. Publication number: 0 678 516 A1. Canadian Patent Application 2,147,594. Japan Patent Application 222002. U. S. Patent, application number 60008011
     - The product Furvina from this patent is an efficient antimicrobial with broad-spectrum activity against Gram-positive and Gram-negative bacteria, yeasts and filamentous fungi. It is currently in medical use in Cuba marketed as Dermofural ointment for treatment of human skin and nail infections and as Furvinol for veterinary use.
  2. Substituted Hydroxyacetophenon Derivatives. J. Quincoces, **E. Estrada**, K. Peseke, International Patent WO/2006/003010; International Application Number: PCT/EP2005/007307
     - This product has been licenced to Riemser Arzneimittel Ag, Germany, for its exploitation as an anticancer compound, which is active against 60 cancerous cellular lines.

Programme Committee (PC) Membership

2019
- COMPLENET'19. 10th International Conference on Complex Networks, March 18-21, Tarragona, Spain.
- (Programme Chair) COMPLEXIS 2019 - 4th International Conference on Complexity, Future Information Systems and Risk, May 2-4, Heraklion, Greece.

2018
- Complex Networks 2018. 7th International Conference on Complex Networks and Their Applications, Nov 11-13, Cambridge, UK.
- Summer Solstice Conference on Discrete Models of Copmplex Systems, June 25-27, Gdansk, Poland.
- (Honor Advisory Committee) Mol2Net 2017. International Conference Series on Interdisciplinary Sciences, Bilbao, Spain.

2017
- First Latin American Conference on Complex Networks, 25th-29th September, Puebla, Mexico.
- Complex Networks 2017. 6th International Conference on Complex Networks and Their Applications, Nov 29- Dec. 1, Lyon, France.
- Contagion'17. Modeling of Disease Contagion Processes, 6th Edition, Sept. 21th, Amsterdam, The Netherlands.
- (Honor Advisory Committee) Mol2Net 2017. International Conference Series on Interdisciplinary Sciences, Nov. 15-30, Bilbao, Spain.

2016
- 5th International Workshop on Complex Networks and Their Applications, Nov. 30-Dec 2, Milan, Italy.

2015
- NetSci 2015, International School and Conference on Network Sciences, June 1-5, Zaragoza, Spain.
- NetSci-X 2015, International School and Conference on Network Sciences, January 14-16, Rio de Janeiro, Brazil.

2014
- 10th International Conference on Signal-Image Technology & Internet-Based Systems, November 23-27, Marrakech, Morocco.
- IWBBIO 2014. International Work-Conference on Bioinformatics and Biomedical Engineering, April 7-9, Granada, Spain

2013

- 9th International Conference on Signal-Image Technology & Internet-Based Systems, Kyoto, Japan, December 2-5,
- IWBBIO 2013. International Work-Conference on Bioinformatics and Biomedical Engineering, Granada, Spain, March 18-23.

2012

- ACM-SAC BIO 2012. Conference Track on Bioinformatics and Computational Systems Biology. Riva del Garda, Italy, March.

Research Grants

2015-2017 **£42,600.00** Grant: "MultiplexCities. A holistic view of data analytics for cities", Newton Fund and the British Council, UK.
£10,000.00 Bridging the Gap Grant from the Institute of Future Cities for initiating research on data analytics of future cities, UK.

2015 – 2019 **£72,000.00** Grant: Engineering and Physical Sciences Research Council (EPSRC), UK. "Study of geometrical and topological properties of networks"

2014 – 2018 **£75,000.00:** Wolfson Research Merit Award, Royal Society of London, UK for "Physico-mathematical modelling of communication patterns in complex networks"

2014 – 2018 **£72,000.00** Grant: Engineering and Physical Sciences Research Council (EPSRC), UK. "Study of new matrix functions for networks"

2013 – 2017 **£72,000.00** Grant: Engineering and Physical Sciences Research Council (EPSRC), UK and the Weir Group "Modelling Complex Networks of Fractures in Rocks of Petrophysical Interest"

2012 **£5,000.00** Grant: Scottish Funding Council for developing a joint research project with the company Isochron on business forecasting using network techniques

2010 – 2012 **£181,000.00** Grant: Engineering and Physical Sciences Research Council and the Research Councils UK Digital Economy Programme, on the project MOLTEN: Mathematics Of Large Technological Evolving Networks

2009 **£9,143.00** Grant: "Bridging the Gap" from the Engineering and Physical Sciences Research Council (EPRSC), U.K. on the project "Water Supply Networks"

2008 – 2011 **£25,000.00** Grant: "New Professors Fund" from the University of Strathclyde, Glasgow, U.K. for the development of interdisciplinary researches in complex networks

2004 **11,000.00 Euros**: Unilever UK Central Resources Limited Grant: "Development of structural alerts for chromosome aberrations and other genetic toxicological endpoints for organic compounds. Use of the TOPS-MODE approach"

2002 – 2005 **$60,000.00**: FONDECYT, Chile. Grant to Motivate the International Cooperation: "QSPR models to predict physico-chemical properties of herbicides from quantum-chemical descriptors"

2001 – 2003 **$10,648.40**: FAPESP (Fundação de Auxílio Pesquisa Estado de São Paulo) Brasil: "Synthesis of prenylated compounds with antibacterial and antimicrobial activities"

2000 – 2002 **49,042.00 Euros**: Ministry of Science and Technology, Spain: "Synthesis and studies of new coumarins, furocoumarins and tetracyclic derivatives of coumarins with pharmacological interest"

2001 **45,436.51 Euros:** Regional Government of Galicia, Spain: "System for Molecular Design"

Principal Invited Lectures

2018 Invited speaker at the Pregl Colloquium, Chemistry Institute, Ljubljana, Slovenia, 21th June.
2018 Keynote speaker and teacher at the conference and school Spatial Networks. Theory and Applications, Bristol, UK, Sep 11-14.
2018 Invited speaker and teacher at the conference and school Complex Networks with application on Climate, Neuroscience, Power Grid, Epidemiology, Sao Paulo, Brazil, 27th September-1st October.
2018 Invited speaker at Graph Theory and Physics, London, UK, May 30.

2018 Invited plenary speaker at The 8th International Conference on Network Analysis (NET 2018), Moscow, Russia, May 17-20.
2018 Invited lecturer at School on "Nonlinear Time Series Analysis and Complex Networks in the Big Data Era", ICTP-SAIFR (Sao Paulo, Brazil), February 19 – March 2, 2018.
2018 Keynote speaker at 4th Winter School "Social Networks, Paris 22-26 January 2018.
2018 Invited lecturer at 4th Winter School "Social Networks, Paris 22-26 January 2018.
2018 Keynote speaker at the 3rd International Conference on Complexity, Future Information Systems and Risk, March 20 - 21, 2018, Funchal, Madeira – Portugal.
2018 Pregl Colloquium Speaker, National Institute of Chemistry, Slovenia
2017 Keynote speaker at the Short Course and Symposium on Spatial Networks, Oxford University, 11th-14th September.
2017 Invited lecturer at the Short Course and Symposium on Spatial Networks, Oxford University, 11th-14th September.
2017 Invited speaker at 12th SICC International Tutorial Workshop "Topics in Nonlinear Dynamics, Control of Complex Networks of Nonlinear Circuits and Systems", 7-8 September, Catania, Sicily, Italy
2017 Invited seminar at the Mediterranean School of Complex Networks, 3-8 Sept 2017, Salina, Sicily, Italy
2017 Invited speaker at the First Latin American Conference on Complex Networks, 25th-29th September, Puebla, Mexico
2017 Invited lecturer at the First Latin American Conference on Complex Networks, 25th-29th September, Puebla, Mexico.
2017 Invited speaker at the ECS Security Symposium on Collective Dynamics, 11th May, Bristol, UK.
2017 Invited lecturer at the Condensed Matter Section of the German Physical Society, 19-24 March, Dresden, Germany
2016 Invited lecturer at the Winter School on Data Analytics, December 17-19, 2016, Nizhny Novgorod, Russia.
2016 Invited lecturer at The 5th International Workshop on Complex Networks and their Applications, 30th Nov.-2nd Dec., Milan, Italy.
2016 Invited lecturer at the IV Workshop and School on Dynamics, Transport and Control in Complex Networks, São Carlos, Brazil, September 28th-October 2nd.
2016 Invited speaker at the 2016 International Conference on Mathematical Chemistry, Tianjin, China, July 4-8.
2016 Invited speaker at the International Symposium "Frontiers in Network Science", June 26-28, Hamburg, Germany.
2016 Invited speaker at the 2016 Summer Solstice - 8th International Conference on Discrete Models of Complex Systems, Aveiro, Portugal, June 20-22.
2016 Invited lecturer at school **"**Complex Networks", Bertinoro, Italy, 11-16 July.
2016 Invited lecturer at school **"**Complex Networks: Theory, Methods & Applications", Lake Como, Italy, 18-22 May.
2016 Keynote Speaker at the 1st IMA Conference on Theoretical and Computational Discrete Mathematics, University of Derby, 22nd-23th March.
2016 Keynote speaker at the 7th Workshop on Complex Networks (CompleNet 2016), Dijon, France, March 23-25.
2015 Invited lecturer at the ICTP-SAIFR School on Complex Networks and Applications to Neurosciences, Sao Paulo, Brazil, September 28th-October 16th
2015 Invited speaker at the SIAM Conference on Applied Linear Algebra (LA15), Atlanta, USA, October 26-30.
2015 Plenary speaker at GAMM Workshop on Applied Numerical Linear Algebra, Magdeburg, Germany, July 9-10.
2015 Invited lecturer at the International School on Complex Networks, NetSci 2015, Zaragoza, Spain, June 1-5
2015 Invited Speaker at NetSci 2015 Satellite Conference on Multilayer Networks, in Zaragoza, Spain, June 1-5
2015 Plenary Speaker at NetSci 2015 Satellite Conference on Networks in Education, in Zaragoza, Spain, June 1-5
2015 Plenary Speaker at NetSci-X 2015 in Rio de Janeiro, January 14-16
2014 Plenary Speaker at the European Conference on Complex Systems, Lucca, Italy
2013 Invited Speaker at The 36th German Conference on Pattern Recognition (GCPR 2014), Münster, Germany
2013 "How to navigate in a complex world", Invited "Science Talks" at the Faculty of Science, Kennesaw State University, Atlanta, USA
2013 Invited Speaker at the IQC workshop on quantum computation and complex networks, Institute of Quantum Computing and Perimeter Institute for Theoretical Physics, Waterloo, Canada, May 24-26.
2012 Plenary Speaker at 4th International Interdisciplinary Chaos Symposium on Chaos & Complex Systems, Turkey
2012 "Complex networks: A tour'd horizon", Plenary Speaker at 2012 SIAM Annual Meeting, Minneapolis, USA
2012 Invited speaker at the conference "Applications of Graph Spectra in Computer Sciences", CRM Barcelona, Spain
2012 "Communicability in complex networks: Quantum vs. classical approaches" invited talk at the meeting "Function Prediction in Complex Networks", Kavli Royal Society International Scientific Centre
2011 Plenary Speaker at *The 1st International Symposium on Innovative Mathematical Modelling*, Tokyo, Japan
2010 Plenary Speaker at *Joint IAPR International Workshops on Structural and Syntactic Pattern Recognition (SSPR 2010) and Statistical Techniques in Pattern Recognition (SPR 2010)*, Cesme, Turkey
2010 "A Graph Theoretic Approach to Atomic Displacements in Fullerenes". Keynote Speaker Lecture, *Computers in Scientific Discovery*, University of Sheffield, Sheffield
2009 "Communicability and the evolution of communities in networks", Invited Lecture, *The Unexpected Link: Using Network Science to Tackle Social Problems*, Budapest, Hungary
2009 "Spectra of Complex Networks: Centrality Measures and Applications", Invited Lecture, *Applications of Physics in Financial Analysis, 7th International Conference*, Tokyo, Japan
2008 "Golden Spectral Graphs and Networks", Invited Lecture, *Spectral Graph Theory in Rio*, Rio de Janeiro, Brazil
2005 "Subgraph centrality, bipartivity and spectral scaling in complex networks.", Invited Talk, Conference on Complex Networks: Evolution and Statistical Properties, Salou, Spain
2004 "A universal topological property of complex networks.", Invited Talk, Nordic Workshop on Networks. NORDITA, Niels Bohr Institute, Copenhagen, Denmark

2001 "Characterization of protein folding degree in lattice and real proteins." Lecture, The Sixteenth International Course & Conference on the Interfaces among Mathematics, Chemistry & Computer Sciences, Dubrovnik, Croatia

2001 "Wiener number in the context of generalized topological indices", Lecture, The Harry Wiener International Memorial Conference on the Role of Topology in Chemistry, University of Georgia, Athens, Georgia, USA

2000 "Extending the molecular connectivity indices. From bond connectivity to long-range connectivity indices.", Lecture, Symposium for the 25th Anniversary of the Connectivity Indices. 220th National Meeting of the American Chemical Society, Washington DC, USA

Invited Seminars and Colloquia

2018 ""d-path Laplacians and long-range interactions in network dynamics", Institute for Physics & Astronomy University of Potsdam, Germany, October.

2018 "Natural geometric embedding of networks", Colloquium at the Department of Mathematics, University Carlos III, Madrid, Spain, October.

2018 "d-path Laplacians and long-range interactions in dynamics on graphs", Department of Mathematics, University of Santiago de Compostela, Spain, July

2018 "Machine learning on complex networks in hyperspherical space", IFICS, University of Balearic Islands, Palma de Mallorca, Spain, 27th June.

2018 "Communicability geometry in networks", Department of Mathematics, Queen Mary University of London, London, UK.

2018 "Communicability in networks", Department of Mathematics and Computer Sciences, University Rovira i Virgili, Tarragona, Spain.

2017 "Long-range interactions and dynamics on networks"; Colloquium at the Department of Mathematics, Politecnico di Torino, Turin, Italy.

2017 "Matrix functions in mathematical chemistry", Institut des Sciences Moléculaires de Marseille, Aix-Marseille Université, France.

2017 **"**k-path Laplacians and generalised diffusion on networks"; Department of Statistics, University College London, UK

2017 **"**Anomalous diffusion on networks"; Department of Mathematics and Statistics, Herriot-Watts University, UK.

2016 "The geometry of complex networks", Department of Mathematics & Statistics, University of Limerick, Ireland.

2016 "Complex networks. A Tour d'Horizon", National Oceanography Institute, Southampton, UK.

2016 "The geometry of communication in networks", Max-Planck Institute for Dynamics and Self-organization (MPIDS) in Göttingen, Germany.

2015 "Communicability geometry and the spatial efficiency of networks", Seminar the Group of Complex Systems and the Doctoral Programme in Complex Systems, Polytechnic University of Madrid, Madrid, Spain, 13th November 2015.

2015 "Random rectangular graphs. Theory and applications", Seminar at the Department of Mathematics, Bristol University, U.K., 19th June, 2015

2015 "Communicability angles and the spatial efficiency of networks", Seminar at the Department of Mathematics, Oxford University, U.K., 18th June, 2015

2014 "Communicability in complex networks. Theory and Applications", Seminar at the Department of Actuarial Mathematics, Herriot-Watts University, Edinburgh, U.K., February 2014

2013 "Path Laplacian Matrices. Theory & Application", Seminar, GERAD, University of Montreal, Canada, November

2013 "Communicability and Information Diffusion on Complex Networks", Colloquium at the Department of Mathematics, Dartmouth College, Hanover, USA, November 2013

2013 "Communicability and Information Diffusion on Complex Networks", Seminar at the Laboratory for the Modeling of Biological and Socio-Technical Systems, Northeastern University, Boston, USA, November 2013

2013 "How Peer Pressure Shapes Consensus in Social Groups", Talk presented at the Computational Social Science Workshop organised by Georgia Institute of Technology and Emory University, November 2013

2013 "Golden spectral graphs", Seminar at the Department of Mathematics and Computer Sciences, Emory University, Atlanta, USA, October 2013

2013 "Communicability in Social Networks", Political Sciences Colloquium, Emory University, Atlanta, USA, October.

2013 "How not to get lost when navigating through a city, the Internet or the brain?" Seminar at the Network Research Group, Swansea University, Wales, UK, 25th June 2013

2012 "Communicability in complex networks" invited talk at the Inaugural Session of the SIAM Students Chapter, University of Edinburgh

2012 "An Invitation to Complex Networks" invited talk at the Inaugural Session of the SIAM Students Chapter, University of Manchester

2012 "Networks on Hyperspheres", Colloquium at Centre of Mathematical Researches, CIMAT, Guanajuato, Mexico, **2012** "Communicability in complex networks", Colloquium at Centre of Mathematical Researches, CIMAT, Mexico, 2012

2011 "Communicability in complex networks", seminar at the Department of Mathematical Engineering, Universite Catholique de Louvain, Louvain-la-Neuve, 2nd December 2011

2011 "Path Laplacian matrices. Theory and Applications", seminar at the Applied Analysis group, Department of Mathematics and Statistics, University of Strathclyde, Glasgow, 24th November 2011

2011 "Communicability and subgraph centrality in complex networks", seminar at Department of Physics, University of Catania, Sicily, Italy, 22nd November 2011

2011 "Communicability in complex networks", seminar at Bristol Centre for Complexity Sciences, Dept. of Engineering

Mathematics & School of Biological Sciences, 9th November 2011

2011 "Decoding Matrix Structure by Matrix Functions", Colloquium at the Department of Mathematics and Computer Science, Emory University, Atlanta, USA, April 2011

2011 "Approaching Network Structure by Spectral Methods", Mathematical Biology Seminar at the case Western Reserve University, Cleveland, Ohio, USA, April 2011

2011 "Communicability in Complex Networks", Seminar at Statistical and Applied Mathematical Sciences Institute, SAMSI, North Carolina, USA, April 2011

2011 "Complex Networks: Interdisciplinary Research" invited talk at the Inaugural Session of the SIAM Students Chapter, University of Strathclyde, Glasgow

2011 "Predicting toxicity from molecular structure. A topological tale", Invited Talk at the NC3Rs/Mathematics in Medicine Study Group workshop on Mathematical Modelling and Toxicology.

2010 "An excursion through the world of complex networks guided by matrix theory", Seminar at the Computational Mathematics and Applications Group, Rutherford Appleton Laboratory, Oxford, UK, 21st January 2010

2010 "Introduction to Complex Networks I. Network Science Tutorial for non-specialists." Workshop Complex Networks across the Natural and Technological Sciences. Institute for Advanced Studies. Glasgow. 19th-23th January, 2009

2009 "Introduction to Complex Networks II. Modern Concepts, Algorithms and Applications. Network Science Tutorial for non-specialists." Workshop Complex Networks across the Natural and Technological Sciences. Institute for Advanced Studies. Glasgow. 19th-23th January, 2009

2009 "Joining the Dots", Public Lecture at the Workshop: Complex Networks across the Natural and Technological Sciences. Institute for Advanced Studies. Glasgow. 19th-23th January, 2009

2009 "Introduction to Network Theory", PhD Workshop in Modelling Skills. Institute for Advanced Studies. Glasgow. 5th-6th November 2009

2009 "Golden Spectral Graphs and Networks". Lecture at the Workshop Complex Networks across the Natural and Technological Sciences. Institute for Advanced Studies. Glasgow. 19th-23th January, 2009

2009 "Information Mobility in Complex Networks". Workshop Applications of Complex Networks, Institute for Advanced Studies, Glasgow, 25th-29th May, 2009

2009 "Modelling Complex Networks through Matrix Functions". Centre for Interdisciplinary Computational and Dynamical Analysis (CICADA), university of Manchester. 11 - 14 January 2009

2009 "Communicability and Community Structure in Complex Network". BBSRC MATSYB network I2M: Immunology, Imaging and Modelling. School of Mathematics, University of Leeds. 2nd April, 2009

2009 "Centrality and Communicability in Complex Networks". Department of Computing Sciences and Mathematics, University of Stirling. 14th April 2009

2008 "Complex Networks: from Nature and Society to Technology", Lecture, Workshop *Complexity in the Brain*, University of Strathclyde, Glasgow

2008 "Centrality and Communities in Complex Socio-Economic Networks", Lecture, Tokyo Institute of Technology

2008 "Protein Origami: How to Quantify the Degree of Folding of Protein Chains", Lecture, Department of Applied Physics, University of Tokyo

2008 "Detecting communities in Complex Networks", Lecture, Institute of Industrial Sciences, University of Tokyo, Japan

2008 "Complex networks: From the cell to ecosystems", Lecture, Faculty of Sciences, University of Oporto, Portugal

2008 "Complex networks and Biology in the XXI century", Lecture, Institute for Marine Sciences, CSIC, Vigo, Spain

2008 "Mathematical Characterization of Local and Global Properties in Complex Networks", Lecture, Department of Informatics, University of Tokyo (May 19, 2008)

2008 "Topological characterization of complex biological networks", Seminar, Center for Mathematics Applied to the Life Sciences, University of Strathclyde and University of Glasgow, U.K. (February 20, 2008)

2008 "Protein Origami: The Degree of Folding of Proteins", Seminar, Bioinformatics Research Centre, University of Glasgow, U.K. (February 19, 2008)

2008 "Topological characterization of complex biological networks", Seminar, Translational Medicine Research Collaboration, The Sir James Black Centre, University of Dundee, U.K. (February 15, 2008)

2007 "A Novel Topological Approach to Molecular Design in Organic Chemistry", Lecture, Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences, Sofia, Bulgaria

2007 "From Small Molecules to "Small-Worlds", Lecture, Faculty of Experimental Sciences, University of Almería, Spain

2006 "The parts in the whole. The role of mathematics in the study of complex systems.", Lecture, VIII National Conference of Spanish Deans and Directors of Mathematics, 2006, Polytechnic University of Valencia, Valencia, Spain

2006 "How the Parts are Organized in the Whole? An Excursion to Complex Systems", Lecture, Second Meeting of The International Academy of Mathematical Chemistry (IAMC) Dubrovnik, Croatia

2005 "Structural characterization of complex networks", Lecture, VII Seminar of Discrete Mathematics, University Carlos III, Madrid, Spain

2004 "Characterization of the Degree of Folding of Proteins", Lecture, Faculty of Chemistry, University of Concepción, Chile

2003 "Quantitative Structure-Property and Structure-Activity Relationships. A Personal View", Lecture, Faculty of Chemistry, University of Concepcion, Chile

2002 "From 2D Drug Design to 3D Characterization of the Degree of Folding of Proteins", Lecture, Department of Chemistry, University of Campinas, Brazil.

2002 "An Introduction to Bioinformatics for Mathematicians". Invited Seminar, Institute of Mathematics, University of Santiago de Compostela, Spain (December 14, 2001)

1997 "Spectral Moments of the Edge adjacency Matrix. Applications to Molecular Design.", Seminar at the Group of Combinatorics, Graph Theory and Applications, Polytechnic University of Barcelona, Spain (April 10, 1997)

Principal Contributed Papers and Poster Presentation

1 "Two-walks degree assortativity in graphs and networks", A. Allen-Perkins, J. M. Pastor, E. Estrada, Poster, LANET 2017, 1st Latin American Conference on Complex Networks, Puebla, Mexico, 25-29 September, 2017. **Awarded Best Poster**.

2 "Communicability geometry in multiplexes", E. Estrada, Oral presentation, LANET 2017, 1st Latin American Conference on Complex Networks, Puebla, Mexico, 25-29 September, 2017.

3 "Mathematical analysis of k-path Laplacian operators on networks", E. Estrada, E. Hameed, N. Hatano, M. Langer, Oral presentation, LANET 2017, 1st Latin American Conference on Complex Networks, Puebla, Mexico, 25-29 September, 2017.

4 "Long walks and holes in networks", G. Silver, E. Estrada, Oral presentation, LANET 2017, 1st Latin American Conference on Complex Networks, Puebla, Mexico, 25-29 September, 2017.

5 "Centrality measures in simplicial complexes", E. Estrada. G. Ross, Oral presentation, LANET 2017, 1st Latin American Conference on Complex Networks, Puebla, Mexico, 25-29 September, 2017.

6 "Phase transition in the communicability clustering structure of graphs and networks", E. Estrada, N. S. Alalwal, Oral presentation, LANET 2017, 1st Latin American Conference on Complex Networks, Puebla, Mexico, 25-29 September, 2017.

7 "Random rectangular networks", E. Estrada, M. Sheerin, Poster, LANET 2017, 1st Latin American Conference on Complex Networks, Puebla, Mexico, 25-29 September, 2017.

8 "From Networks to Hypernetworks", Oral communication, NETSCI 09, International Workshop and Conference on Complex Networks and their Applications, Venice, Italy (June 29-July 3, 2009). Work together with Naomichi Hatano

9 "Matrix Functions for the Analysis of Complex Networks". Minisymposium Function of Matrices. SIAM Conference on Applied Linear Algebra. Monterey, CA. 26-29 October, 2009

10 "Proteins as Complex Networks", Lecture, IAMC, International Academy of Mathematical Chemistry, Dubrovnik, Croatia (June 10-14, 2009)

11 "Spectral Measures for Molecular Networks", Lecture, MCC 2009, International Conference Math/Chem/Comp, Dubrovnik, Croatia (June 4-9, 2009)

12 "Complex Networks and OMICS", Lecture, Symposium on Complex Networks: Biology, Ecology, Society; University of Santiago de Compostela, Spain (June 22, 2007)

13 "Complex Networks", Lecture, Second Meeting of the International Academy of Mathematical Chemistry; Dubrovnik, Croatia (June 8, 2006)

14 "Utility of Cyclodextrins for the Improvement of the Solubility of Sertaconazol", Poster, V Congress of the Spanish Society of Industrial Pharmacy, Valencia, Spain (February 6, 2001)

15 "New Tetracyclic Frameworks with Potential Antitumor Interest", Poster, XVIth International Symposium on Medicinal Chemistry, Bologna, Italy (November 22, 2000)

16 "In Silico Studies for the Screening and Design of Pharmacologically Active Compounds", Poster, XVIth International Symposium on Medicinal Chemistry, Bologna, Italy (November 22, 2000)

17 "New N,N-Disubstituted Piperazines as Serotonine and Dopamine Ligands", Poster, XVIth International Symposium on Medicinal Chemistry, Bologna, Italy (November 22, 2000)

18 "Toss-Mode in Predicting Biological, Toxicological and ADME Parameters of Organic Compounds", Lecture, The 15th Dubrovnik International Course & Conference Math/Chem/Comp 2000, Dubrovnik, Croatia (June 24, 2000)

19 "Design, Synthesis and in Vitro Determination of the Antimicrobian Activity of New Gamma-Nitrocyclohexanones", Poster, IV Iberoamerican Meeting of Pharmaceutical and Food Sciences, La Habana, Cuba (June 30, 2000)

20 "Use of the TOPS-MODE Approach for the Classification of Capsaicin Analogues with Analgesic Activity and for Structure-Property Relationships (QSPR) Studies", Poster, IV Iberoamerican Meeting of Pharmaceutical and Food Sciences, La Habana, Cuba (June 30, 2000)

21 "Predicting Chemical Reactivity (Log K) and Octanol/Water Partition Coefficient (Lipophilicty, Log P) of Furylethylene Compounds from Graph-Theoretical Molecular Descriptors", Poster, 16th Conference of Chemistry, University of Oriente, Santiago de Cuba, Cuba, (December 10, 1999)

22 "Use of a Novel Theoretical Approach to Calculate the Fragment Contribution of a Molecule to the Biological Activity", Poster, 16th Conference of Chemistry, University of Oriente, Santiago de Cuba, Cuba, (December 10, 1999)

23 "Use of Local Spectral Moments in Drug Design", Poster, 16th Conference of Chemistry, University of Oriente, Santiago de Cuba, Cuba, (December 10, 1999)

24 "Designing Antifungal and Antibacterial Compounds by a Substructural Graph-Theoreical Approach", Poster, 16th Conference of Chemistry, University of Oriente, Santiago de Cuba, Cuba, (December 10, 1999)

25 "Piecewise Linear Regression-Discriminant Analysis (PLR-DA) in QSAR Studies", Poster, III International Congress of the Cuban Chemical Society, University of Oriente, Santiago de Cuba (December 4, 1998)

26 "Designing Biologically Active Compounds from a Novel Substructural Graph-Theoretical Approach", Poster, III International Congress of the Cuban Chemical Society, University of Oriente, Santiago de Cuba (December 4, 1998)

27 "On the Nature of Topographic Indices Based on Electronic Properties of Molecules", Poster, 7th International Conference on Mathematical Chemistry and 3rd Girona Seminar on Molecular Similarity, Girona, Spain (May 31, 1997)

28 "Generalizations of Wiener Number and other Distance-Based Graph Theoretical Invariants", Poster, 7th International Conference on Mathematical Chemistry and 3rd Girona Seminar on Molecular Similarity, Girona, Spain (May 31, 1997)

29 "Spectral Moments of Bond Matrix. A Novel Substructural Approach to QSPR and QSAR Studies", Poster, 7th International Conference on Mathematical Chemistry and 3rd Girona Seminar on Molecular Similarity, Spain, May 1997

30 "Theoretical Studies for the Rational Functionalization of 2-Bromo-(3-Fur-2-yl)-3-oxo-Propyonamide", Poster, First Workshop on Molecular Modeling and Applications, La Habana, Cuba (March 28, 1997)

31 "Comparative Study of Antibiotic Activity of Gamma-Lactamic Compounds with the Use of Topological and Topographic Descriptors", Poster, 1st Workshop on Molecular Modeling & Applications, La Habana, Cuba , March 28, 1997

32 "Simulation of Antibiotics Penetration into Cerebrospinal Fluids in Bacterial Meningitis", Lecture, First International Workshop on Antibiotics, La Habana, Cuba (November 4, 1993)
33 "Quantitative Structure-Activity Relationships (QSAR) Study of the Action Mechanism of Antibacterial Furylethylenes Derivatives", Poster, First International Workshop on Antibiotics, La Habana, Cuba (November 4, 1993)
34 "Advances in the Registration of 1-(5-Bromofur-2-yl)-2-Bromo-2-Nitroethene in Veterinary Medicine", XIII Conference of Chemistry, University of Oriente, Santiago de Cuba, Cuba (January 25, 1990)
35 "Quantitative Determination of Polyatomic Anions in NaCl Matrices by using IR Spectroscopy", Oral presentation, XI Conference of Chemistry and II Congress of the Cuban Chemical Society, University of Oriente, Santiago de Cuba, Cuba (January 25, 1985).

Short Term Visiting Positions

2013	Visiting Professor at the Department of Mathematics and Computer Sciences and Fellow of the Institute for Quantitative Theory and Methods (QuanTM), *Emory University*, Atlanta, USA
2013 – 2014	Visiting Professor at the Centre of Mathematical Research, Guanajuato, Mexico
2012 – 2013	Visiting Professor at the Centre of Mathematical Research, Guanajuato, Mexico
2011	Visiting Research Fellow of the Statistical and Applied Mathematical Sciences (SAMSI), USA
2008	Visiting Research Fellow of the Institute of Industrial Science, The University of Tokyo, Japan Visiting research fellow of the Royal Society of Edinburgh International Exchange Programme and Edinburgh Mathematical Society for visiting the Department of Mathematics, University of Strathclyde, Scotland

PhD – Supervised Thesis (Inc. First Employment Post PhD)

2003 **Enrique Molina-Pérez** (Ph. D., Chemistry, University of Camagüey, Cuba). (Associate Professor at the University of Camagüey, Cuba).
2006 **Santiago Vilar**, (Ph. D., Pharmacy, University of Santiago de Compostela, Spain, 2006), (post-doc at Columbia University, USA).
2012 **Franck Kalala-Mutombo**, Ph. D. Mathematics, at the Department of Mathematics & Statistics, University of Strathclyde, 2012; (Lecturer at the Mombashi University, R. D. Congo).
2015 **Eusebio Vargas-Estrada**, Ph. D. Mathematics, Department of Mathematics & Statistics, University of Strathclyde, 2015, (Research Assistant to Prof Brandes at the University of Konstanz, Germany).
2018 **Matthew Sheerin**, Ph. D. Mathematics, Department of Mathematics & Statistics, University of Strathclyde, (Software Engineer position at Metaswitch Networks in Edinburgh).

In progess:

- **Grant Silver**, Ph. D. Student at the Department of Mathematics & Statistics, University of Strathclyde. Viva in 2018.
- **Ehsan Mejeed Hameed**, Ph. D. Student, Department of Mathematics & Statistics, University of Strathclyde. Viva in 2018.
- **Alhanouf Alhomaidhi**, Ph. D. Student, Department of Mathematics and Statistics, University of Strathclyde. Viva in 2019.
- **Grant Ross**, Ph. D. Student, Department of Mathematics and Statistics, University of Strathclyde. Viva in 2019.
- **Najlaa Alalwal,** Ph. D. Student, Department of Mathematics and Statistics, University of Strathclyde. Viva in 2019.

DESCRIPTION OF THREE KEY ACHIEVEMENTS

1. Network communicability theory

One of the main paradigms of network theory is that information flows between two nodes of a network through the shortest path connecting them. However, there is neither mathematical nor empirical evidence that information travels this way in real-world networks. In addition, the fact that senders of information typically have a complete lack of knowledge about the global structure of a network makes this hypothesis invalid. Furthermore, sending information on networks based on local topology produces paradoxical results. That is, while passing information to the most connected neighbours of a node almost surely guarantees that it travels through the shortest path, it also produces that information get lost due to the high transitivity in which the hubs of the network are involved in. In 2008, I introduced the communicability concept [CT31], which is based on the assumption that information flows through a network in a diffusion-like process which uses all the available routes connecting pairs of nodes in the graph, in counterposition to the idea that information flows only through the shortest-paths of the network. We have generalised this concept [CT24], interpreted it physically [CT17], and expanded it in several contexts (see papers in the corresponding section of my CV). The self-communicability index, known as the subgraph centrality [CT39] and the sum of all subgraph centralities of a graph, known as the Estrada index of the graph, has also found many applications across the fields. In total, my papers in this area have received 2,032 citations according to Scopus and 3,057 according to Google Scholar, with average citations per paper of 58.0 and 87.3, respectively.

In recent years there has been an increasing number of works by many groups around the world, supporting this concept with experimental evidence. For instance, the all-routes communicability outperforms the shortest-path communication in detecting changes in the contralesional hemisphere following strokes in humans, in the detection of symptoms of multiple sclerosis, in the study of variants of epilepsy, in the prediction of abnormal brain states, in the early detection of Alzheimer's disease, in the prediction of functional protein complexes, in the analysis of genetic diseases, in the optimization of wireless networks, in the evolution of granular materials, in the classification of grass pollen and vegetation patterns, and in the identification of the transcription factor critically involved with self-renewal of undifferentiated embryonic stem cells, to mention just a few of the most recent findings (see Fig. 1).

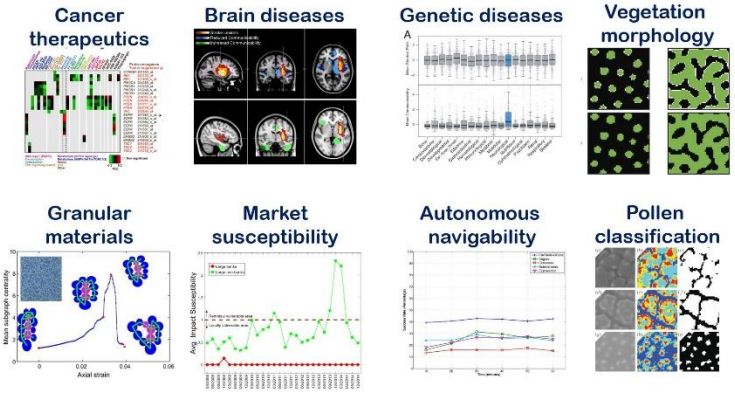

Figure 1. Some applications of the communicability function.

More recently, I have proved that the communicability function induces a Euclidean geometry for networks [CT16, CT11, CT5]. This hyperspherical embedding of networks has already found applications in detecting critical edges in network dynamics [CT6], for studying network spatial efficiency [CT6] and for clustering analysis of networks [CT1]. All in all, the topic is still under development but it already has great acceptance by the scientific community who has applied it in many fields and contribute to its theoretical development.

2. Mathematical tools for data analytics on networked systems

The progress of a scientific field, such as networked data analysis, depends significantly on the availability of theoretical and computational tools of high quality that allow the practitioners of the field to perform effectively their tasks. As an applied mathematician I am interested in: (i) developing new mathematical tools for characterising network (structural and dynamical) properties; (ii) improving the existing ones where they are not appropriate for certain tasks; (iii) finding the structural or physical meaning of those tools used in the field for which such interpretation does not exist (see Fig. 2). In this area I have developed new measures that quantify the global and local bipartivity of networks [NS21, NS46], balance in signed networks [NS24], walk entropies [CT9, NS25], degree heterogeneity [NS32], node-edge connectivity (ABC index) [NS58, NS38], network clumpiness [NS37], simplex centralities in simplicial complexes [NS4], among others (see CV). I have extended other existing approaches, such as the definition of the *d*-path Laplacian operators for networks which generalise the graph Laplacian to include long-range interactions [NS12, NS29], defined the random rectangular graphs which generalise the random geometric graphs [NS23], have generalised existing topological indices to characterise molecular graphs to allow its optimisation for describing quantitatively molecular properties [NS47]. I have also provided a structural interpretation of the clustering coefficients (local and global) of networks [NS19], of the graph energy [NS19], clarified the topological meaning of the information centrality [NS34], and provided the combinatorial interpretation of the assortativity coefficient used for detecting communities in networks [NS30]. I have advanced a theory that explain destructive quantum interference in molecules [Bc1], which in collaboration with Nobel prize winner Roald Hoffmann has been extended to explain this important phenomenon for the development of molecular electronic devices. These works have received 2,652 (Scopus) or 3,685 (Google Scholar) citations, with 44.9 and 62.4 citations per paper, respectively.

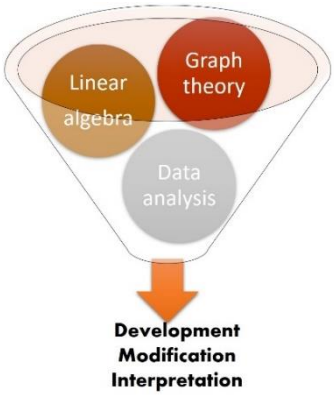

Figure 2. Using applied mathematics to develop, modify and interpret network tools.

I have also advanced some applications of these new mathematical methods in different areas. For instance, I have contributed to the applications of *d*-path Laplacian operators for generalising diffusion on graphs and proving the existence of superdiffusive behaviour under certain conditions [NS1, NS12]. Also in the application of these operators for generalising the Kuramoto model for synchronization in networks [NS5], as well as for generalising epidemic models on plants [NS3]. Random rectangular graphs have been applied by my group to the representation of agricultural plots/fields [NS18], fractures in rocks for oil and gas exploration [NS10] and for studying the spatial effects on synchronization [NS22]. I have also contributed to the study of the influence of indirect peers pressure on the diffusion of innovations [NS26], management of landscape connectivity [NS36], food web robustness [NS41], efficiency of airline transportation companies in Europe [NS21] as well as to molecular studies (several papers in CV). All these works are characterised by a phenomenological approach in which theory and data-driven processes go hand to hand to develop the mathematical tools that best describe the processes under study.

Some of these mathematical methods have been implemented in computational tools available for the analysis of networks by subject-specific users who have used them in a plethora of applications. Some examples are: the analysis of evolution of granular materials, analysis of the stability of fullerenes, detection of brain anticommunities, heterogeneity of rat amygdala, analysis of stock markets dynamics, prediction of financial crisis, prediction of drug safety, epidemic spreading as well as to oil and gas exploration.

3. Chem- and bio-informatics analysis of networked systems

Molecules are the smallest of all complex systems when compared at geometric scales. However, when represented as networks of interactions they are composed of a few hundreds to a few thousand nodes (see Fig. 3). I have contributed to the development of mathematical methods for data analysis of these systems at the three different size scales: molecular, macromolecular and intermolecular. In total my papers in this area have attracted 2,465 citations according to Scopus (2,982 according to Google Scholar) with average citations per paper of 45.6 and 55.2, respectively. For instance, I have developed cheminformatic methods and tools for the representation of the topological, geometric and electronic structure of small organic molecules, which are the basis of most human and veterinary medicines, food additives and plant pesticides. The *Topological Sub-Structural Molecular Design* (TOPS-MODE) approach (see CB40) was developed for the purpose of cheminformatic analysis of drug-like molecules, and it has been widely used in the literature for predicting physico-chemical, biological, pharmacological, toxicological and environmental impact of organic molecules. I have contributed to studies applying this method to the binding of substrates to P-glycoprotein [CB2], chromosome aberrations of organic compounds [CB13], antiproliferative activity of natural products from Brazilian propolis [CB14], drug binding to serum albumin [CB15], design of anti-HIV [CB19], anticancer [CB47], anticonvulsant [CB45], and sedative/hypnotic compounds [CB52], prediction of skin sensitization [CB31, CB22], and neurotoxicity of organic molecules [CB37], among others. Notice that I am coauthor of two international patents, one of a compound with antibacterial and antifungal activities, currently in clinical use, and another with anticancer activity.

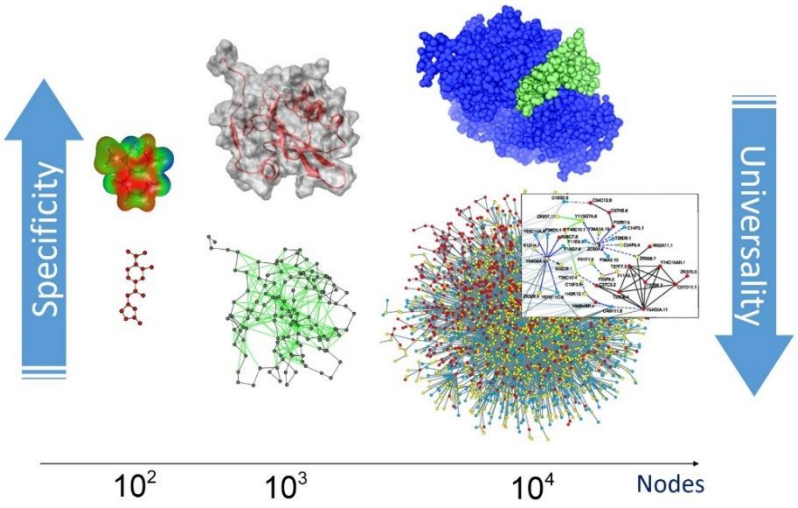

Figure 3. Scales of the molecular universe.

At a larger size scale we find biomacromolecules like DNA, RNA and proteins. In this case, particularly for proteins, we can represent a network consisting of amino acid residues as nodes and both covalent and nonbonding interactions as edges. In this area of structural bioinformatics I have contributed with a method to characterise the degree of folding of protein chains [CB33, CB20], to the analysis of protein packing [CB10], to the identification of holes (potential binding sites) in proteins [CT25], as well as the application of these methods to the analysis of the stability of protein-ligand complexes [CB16, CB28], to the functional analysis of azurins and pseudoazurins [CB17], and the development of a method to quantify the contribution of amino acids to the degree of folding of a protein [CB21].

Finally, at the larger size scale we find giant arrangements of interacting macromolecules, such as protein-protein interaction networks. In this case I have used the measures of sub-graph centrality and bipartivity for the identification of essential proteins in the PPI of yeast [CT37, CT38] as well as to the prediction of hormesis using real-world data [CB18]. The paper [CT38] was the first indicating the usability of network theory to make biological predictions on real-world data. It appeared in the cover of the journal *Proteomics* and I was interviewed for the podcast of the journal.

Publications

SENIOR-AUTHOR PUBLICATIONS (including Scopus (Google Scholar) citation counts, *for senior author)

ORCID ID: orcid.org/0000-0002-3066-7418
SCOPUS ID: 7005488279

	Google Scholar[1]	Scopus
Number of citations:	11,617	8,012
h-index:	58	50

Books

2015 *A First Course in Network Theory*.
E. Estrada, P. Knight
Oxford University Press. **[Cited (34) times]**.

2011 *The Structure of Complex Networks. Theory and Applications*.
E. Estrada
Oxford University Press. **[Cited (405) times]**.

2010 *Network Science: Complexity in Nature & Technology*.
Edited by E. Estrada, M. Fox, D. J. Higham, G.-L. Oppo
Springer. **[Cited (60) times]**.

Papers

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2) Topological melting in networks of granular materials
Alawal, N., Arenas, A., Estrada, E.*
Journal of Mathematical Chemistry, **2018**, in press.

3) Gaussianization of the spectra of graphs and networks. Theory and applications
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4) Second-order consensus protocols based on transformed d-path Laplacians.
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Pereda, M., Estrada, E.*
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7) Communicability captures traffic flow in cities.
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8) Back to the origins. Using matrix functions of Hückel Hamiltonian for quantum interference.
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9) Path-Laplacian operators and superdiffusive processes on graphs. II. Two-dimensional lattice.
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12) Synchronization in networks of Rössler oscillators with long-range interactions.
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Estrada, E.* Gambuzza, L. V., Frasca, M.
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15) Quantum interference, graphs, walks, and polynomials.
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16) The electron density function of the Hückel (tight-binding) model.
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17) Spatial "artistic" networks. From deconstructing integer-functions to visual arts.
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18) Integer Digit-Functions. An Example of Math-Art Integration.
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20) Random Neighborhood Graphs as Models of Fracture Networks on Rocks: Structural and Dynamical Analysis.
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Estrada, E.*, Ali Alhomaidhi, A., Al-Thukair, F.
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24) Accounting for the role of long walks on networks via a new matrix function.
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Estrada, E., Benzi, M.*
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Estrada, E.*, Hatano, N.
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