Euro Gold Medal 2013 Laureate Lecture

Panos M. Pardalos

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  http://nnov.hse.ru/en/latna/

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Summary (Partial) of my Research

- On the passage from local to global in optimization
- Optimization with very large and massive datasets
- Critical element selection problems in networks
- Research in Biomedicine
  - epilepsy research
  - network models of a human brain
  - data mining and optimization
- Research in energy systems

On the passage from local to global in optimization

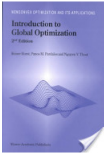
- Concave minimization
- General linear complimentarity problem
- Complexity issues
  - complexity of Kuhn-Tucker Conditions
  - complexity of local minimization
  - phase transition problems
- Global optimization approaches to discrete optimization problems
  - maximum clique problem
  - nonlinear assignment problems
  - Steiner tree problem
  - satisfiability problem
- Hierarchical optimization
- Optimality conditions in non-convex optimization
- Applications in medicine, science and engineering

From local to global in optimization

Panos M. Pardalos,
On the passage from local to global in optimization, in Mathematical Programming: State of the Art (Edited by J.R. Birge and K.G. Murty), The University of Michigan 1994, pp. 220-247

Panos M. Pardalos and Ben J. Rosen,
Constrained global optimization: algorithms and applications, Springer-Verlag New York, 1987

Reiner Horst and Panos M. Pardalos and Nguyen Van Thoai,
Introduction to global optimization, Kluwer Academic Pub, 1995, 2-nd edition 2000,
A Chinese translation of the book has been published by Tsinghua University Press in 2003.



Journal of Global Optimization

- R. Horst and P.M. Pardalos,
  Handbook of Global Optimization, Kluwer Academic Publishers, 1995
- P.M. Pardalos and E. Romeijn,
  Handbook of Global Optimization Volume 2: Heuristic Approaches, Kluwer Academic Publishers, 2002

Journal of Global Optimization, Springer

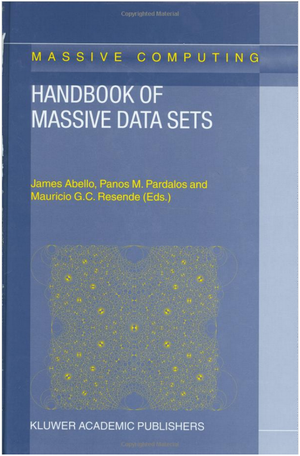
Editor-in-Chief, 1993-2013

What is Big Data?

- The **proliferation of massive datasets** brings with it a series of special computational challenges.
- This **data avalanche** arises in a wide range of scientific and commercial applications.
- With rapid advances in computer and information technologies, many of these challenges are beginning to be addressed.

Handbook of Massive Data Sets

J. Abello and P.M. Pardalos and and M. Resende, ***Handbook of Massive Data Sets***, Kluwer Academic Publishers, 2002



Optimization on Very Large Graphs

- The graphs we have to deal with in some applications are very massive. Examples are the WWW graph and the **call graph**.
- The various gigantic graphs that have lately attracted notice share some properties:
  - They tend to be **sparse**: The graphs have relatively few edges, considering their vast numbers of vertices.
  - They tend to be **clustered**. In the World Wide Web, two pages that are linked to the same page have an elevated probability of including links to one another.

Optimization on Very Large Graphs (cont.)

- They tend to have a **small diameter.** The diameter of a graph is the longest shortest path across it.
- Graphs with the three properties of **sparseness**, **clustering** and **small diameter** have been termed **”small-world” graphs.**

The Call Graph

- In the **call graph**, the vertices are telephone numbers, and two vertices are connected by an edge if a call was made from one number to another.
- A **call graph** was constructed with data from AT&T telephone billing records. Based on one 20-day period it had 290 million vertices and 4 billion edges.
- The analyzed one-day **call graph** had 53,767,087 vertices and over 170 millions of edges

The Call Graph (cont.)

- This graph appeared to have 3,667,448 connected components, most of them tiny.
- A **giant connected component** with 44,989,297 vertices (more than 80 percent of the total) was computed.
- The distribution of the degrees of the vertices follows the **power-law distribution**.

References

J. Abello and P.M. Pardalos and M. Resende,
On maximum clique problems in very large graphs, External Memory Algorithms, 1999, pp. 119-130

V. Boginski and S. Butenko and P. M. Pardalos,
Modeling and optimization in massive graphs, Novel Approaches to Hard Discrete Optimization, 2003, pp. 17-39

Market Graph

- Each stock corresponds to a **vertex** in the network.
- Link between two stocks (vertices) is represented by a weighted edge, where the weight reflects **degree of similarity** between stocks.
- Market network is a **complete weighted graph**.
- Mining market data: filter the information in complete weighted graph in order to extract the **most valuable information**.
- Remark: Common measure of similarity is **correlation** calculated from time series of observations.

References

- V. Boginski and S. Butenko and P.M. Pardalos,
  On structural properties of the market graph, in Innovations in financial and economic networks, Edward Elgar Publishers, 2003
- V. Boginski and S. Butenko and P. M. Pardalos,
  Statistical analysis of financial networks, Computational Statistics and Data Analysis, 2005, pp. 431443
- V. Boginski and S. Butenko and P. M. Pardalos,
  Mining market data: A network approach, Computers & Operations Research, 2006, pp. 3171-3184
- A. Vizgunov and B. Goldengorin and V. Kalyagin and A. Koldanov and P. Koldanov and P.M. Pardalos,
  Network approach for the Russian stock market, Computational Management Science, 2013
- A. Koldanov and P. Koldanov and V. Kalyagin and P.M. Pardalos,
  Statistical procedures for the market graph construction, Computational Statistics & Data Analysis, 2013
- G. Bautin and V. Kalyagin and A. Koldanov and P. Koldanov and P.M. Pardalos,
  Simple measure of similarity for the market graph construction, Computational Management Science, 2013, pp. 105-124

Market Graph Analysis Tools

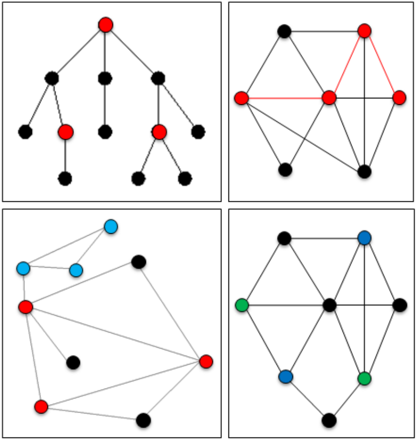
- Minimum Spanning Tree.
- Planar Maximally Filtered Graph.
- Maximum cliques and clique partitions.
- Maximum independent sets.

Analysis of the Russian Stock Market

- The market network constructed using **correlation** as a measure of similarity between stocks.
- We considered **11 shifted periods of 500-day each** from September 1, 2007 to September 16, 2011
- Results are surprising:
  - Russian stock market is dominated by a few **highly correlated** stokes with the biggest value.
  - The nodes of the maximum clique for the threshold are 9 most valuable stocks.
  - The stocks in the clique account for 89% of the total value of the market.
  - The most valuable stocks have the strongest connections between their return.

Critical Elements Detection

Given a graph $G(V, E)$ and an integer k, find a set of at most k **elements**, whose deletion minimizes the **connectivity** of the residual network.



Elements?

- Nodes (arcs)
- Paths
- Cliques
- Node subsets

Connectivity?

- Max flow
- Number of pairwise connections
- Number of components

Critical Elements Detection

The problem is proven to be NP-hard in the general case for different elements:

- Nodes (Arcs)
- Paths
- Cliques

A. Arulsevan and C. W. Commander and L. Elefteriadou and P. M. Pardalos, ***Detecting Critical Nodes in Sparse Graphs***, Computers and Operations Research, 2009, pp. 2193-2200

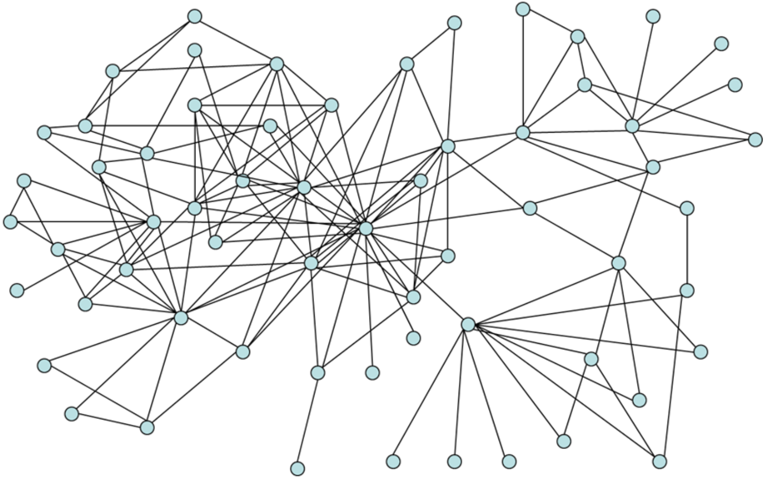
T. N. Dinh and Y. Xuan and M. T. Thai and P. M. Pardalos, ***On New Approaches of Assessing Network Vulnerability: Hardness and Approximation***, IEEE ACM Transactions on Networking, 2012, pp. 609-619

J. Walteros and P. M. Pardalos, ***A Decomposition Approach for Solving Critical Clique Detection Problems***, Experimental Algorithms, Springer, 2012, pp. 393-404

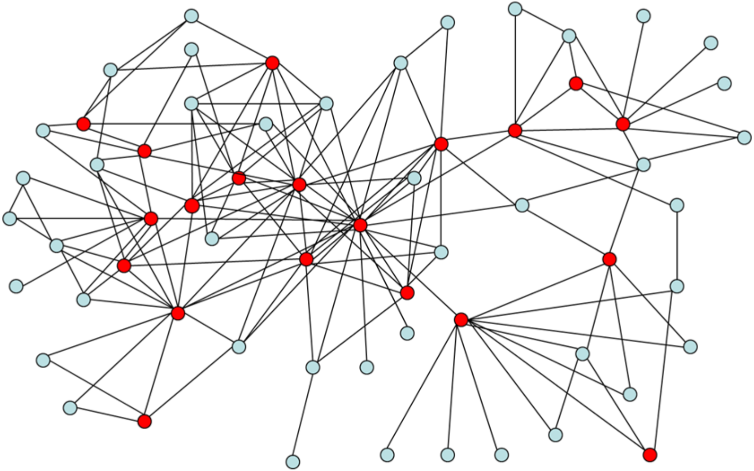
Applications

- Evacuation planning
- Fragmentation of terrorist organizations
- Epidemic contagion analysis and immunization planning
- Social network analysis (Prestige and dominance)
- Transportation (Cross-dock and hub-and-spoke networks)
- Marketing and customer services design
- Biomaterials and drugs design

Critical Nodes Detection Problem



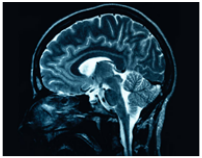
Critical Nodes Detection Problem

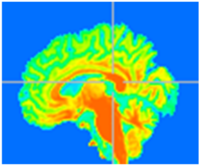


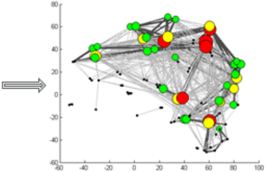
Human Brain Networks

Human Brain Networks

- Network modeling approach to study **complex systems**
- Statistically dependent **neural activity patterns** in distinct brain regions
- **Functional interactions** through neural impulses and information exchange
- Brain networks: nodes represent **brain regions**; connections represent **functional interactions**







F. Skidmore and D. Korenkevych and Y. Liu and G. He and E. Bullmore and P. M. Pardalos,
Connectivity brain networks based on wavelet correlation analysis in Parkinson fMRI data, Neuroscience Letters, 2011, pp. 47-51

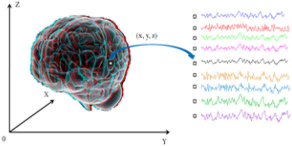
Human Brain Networks (cont.)

Parkinsons Brain

- Small world properties of brain networks
- Noise reduction with wavelet analysis
- Anatomical brain partition
- Connectivity networks based on wavelet correlations

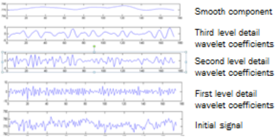
MRI session

Brain activity recorded as time series



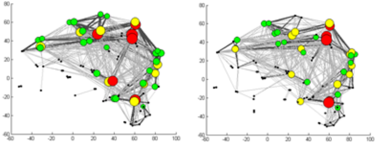
Wavelet transform

Components in time-frequency domain



Correlation analysis

Weighted brain networks



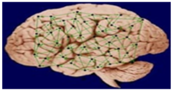
Healthy individual

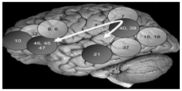
PD patient

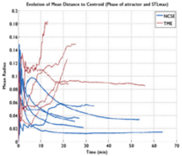
Epilepsy

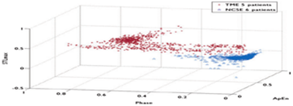
Brain state transition study and epilepsy research

- Nonlinear dynamic modeling
- Patients classification of epilepsy
- Pattern discovery and machine learning
- Epileptic seizure prediction
- Network modeling and optimization
- Epileptic brain state transition study
- Seizure monitoring / warning system









Selected references

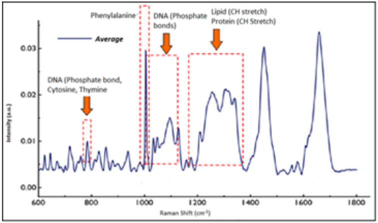
- J. Zhang and P. Xanthopoulos and C. Liu and S. Bearden and B. M Uthman and P. M. Pardalos,
  Real-time differentiation of nonconvulsive status epilepticus from other encephalopathies using quantitative EEG analysis: A pilot study, Epilepsia, 2010, pp. 243-250
- L. Iasemidis and D. Shiau and J. Sackellares and P.M. Pardalos,
  Quadratic binary programming and dynamic system approach to determine the predictability of epileptic seizures, Journal of Combinatorial Optimization, 2001, pp. 9-26
- L. Iasemidis and J. Sackellares and D. Shiau and W. Chaovalitwongse and P. Carney and J. Principe and M. Yang and V. Yatsenko and S. Roper and P.M. Pardalos,
  Seizure Warning Algorithm Based on Optimization and Nonlinear Dynamics, Mathematical Programming, 2004, pp. 365385

The William Pierskalla best paper award for research excellence in health care management science, INFORMS.

Data Mining Applications: Raman Spectroscopy

Raman spectra data analysis

- Data mining for nano toxicity quantification (collaboration with P.E.R.C.)
- Pick de-convolution of Raman spectrograms
- Feature Selection/dimensionality reduction techniques for classification of various cell lines and cell deaths



Selected references

- G. Pyrgiotakis and E. Kundakcioglu and K. Finton and P. M. Pardalos and K. Powers and B. Moudgil, ***Cell death discrimination with Raman spectroscopy and support vector machines***, Annals of biomedical engineering, Springer, 2009, pp. 1464-1473
- M. Fenn and P. Xanthopoulos and G. Pyrgiotakis and S. Grobmyer and P.M. Pardalos and L. Hench, ***Raman spectroscopy for Clinical Oncology***, Advances in Optical Technologies, Hindawi Publishing Corporation, 2011
- M. Fenn and V. Pappu and P. Georgeiv and P.M. Pardalos, ***Raman spectroscopy utilizing Fisher-based feature selection combined with Support Vector Machines for the characterization of breast cell lines***, Journal of Raman Spectroscopy, 2013

Patents

- **Multi-dimensional multi-parameter time series processing for seizure warning and prediction** (with Sackellares James Chris, Iasemidis Leonidas D., Shiau Deng-Shan, Dance Linda, and Chaovalitwongse Wanpracha) Patent 7,263,467 (Issued on August 28, 2007).
- **Optimization of Multi-dimensional Time Series Processing for seizure warning and prediction** (with Sackellares James Chris, Iasemidis Leonidas D., Shiau Deng-Shan, Yatsenko Vitaliy, and Chaovalitwongse Wanpracha) Patent 7,373,199 (Issued on May 13, 2008).
- **Optimization of spatio-temporal pattern processing for seizure warning and prediction** (with Sackellares James Chris, Iasemidis Leonidas D., Shiau Deng-Shan, and Chaovalitwongse Wanpracha) Patent 7,461,045 (Issued on December 2, 2008).
- **Sensor registration by global optimization procedures** (with Mauricio Guilherme de Carvalho Resende and Michael Jacob Hirsch) Patent 7,653,513 (Issued January 26, 2010).
- **Sensor registration by global optimization procedures** (with Mauricio Guilherme de Carvalho Resende and Michael Jacob Hirsch) Patent 7,974,816 (Issued July 5, 2011).

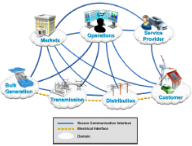
Dynamics of global energy systems

- Changes in oil and gas production and trade flows (shale gas and oil, new fields in USA / Canada, oil production in Iraq, changes in global economy and geopolitical balance)
- Renewable energy (solar, wind, biofuels etc.)
- Focus on energy efficiency / sustainable energy systems (climate changes)
- CO_2 emission remain at record high
- Issues with Fossil Fuel Subsidies
- Over 1 billion people have no access to electricity
- Energy/Water/Environmental issues
- Advances in Technology/Modeling/Optimization

Dynamics of global energy systems

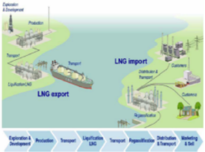
Smart Grid must predict and intelligently respond to the behavior and actions of power users

- Electricity demand is growing worldwide
- Making the grid more flexible
- Security concerns
- Network expansion problems



Energy Systems are Interdependent

- Increased use of natural gas for electricity generation
- Liquified Natural Gas terminals
- Natural gas transportation and distribution systems
- Long-term planning horizon for expansion planning



Hydro-Thermal Scheduling

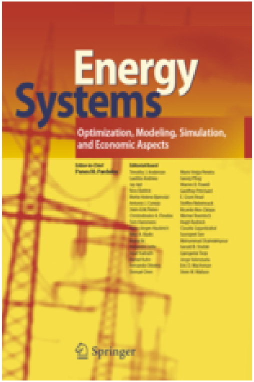
- Uncertainties in weather, demand, and prices
- Scenario reduction
- CO_2 emissions constraints

Our Recent Research

- Smart Grid
- Islanding
- Reliability Analysis
- Stochastic Unit Commitment Problem
- Expansion Planning
- Hydro-Thermal Scheduling

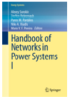
Energy Systems Journal, Springer

Editor-in-Chief

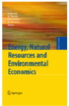


Published Books

- A. Sorokin, S. Rebennack, P. M. Pardalos, N. Illiadis, M. V. F. Pereira (eds.), ***Handbook of Networks in Power Systems***, Springer, 2012

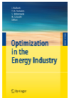


- E. Bjorndal, M. Bjorndal, P. M. Pardalos, M. Ronnqvist (eds.), ***Energy, Natural Resources and Environmental Economics***, Springer, 2010



- S. Rebennack, P. M. Pardalos, M. V. F. Pereira, N. Illiadis (eds.), ***Handbook of Power Systems***, Springer, 2010

- J. Kallrath, P. M. Pardalos, S. Rebennack, and M. Scheidt (eds.), ***Optimization in the Energy Industry***, Springer, 2009



Selected references

- N. Fan and H. Xu and F. Pan and P. M. Pardalos, ***Economic Analysis of the N -k Power Grid Contingency Selection and Evaluation by Graph Algorithms and Interdiction Methods***, Energy Systems, 2011, pp. 313324
- S. Rebennack and J. Kallrath and P. M. Pardalos, ***Energy Portfolio Optimization for Electric Utilities: Case Study for Germany***, Natural Resources and Environmental Economics, 2010, pp. 221-246
- Q. Zheng and P. M. Pardalos, ***Stochastic and Risk Management Models and Solution Algorithm for Natural Gas Transmission Network Expansion and LNG Terminal Location Planning***, Journal of Optimization Theory and Applications, 2010, pp. 337-357
- Q. Zheng and S. Rebennack and N. Iliadis and P. M. Pardalos, ***Optimization Models in the Natural Gas Industry***, in Handbook of Power Systems I, 2010, pp. 121-148

Concluding remarks

ΧΡΥΣΟΝ ΓΑΡ ΟΙ ΔΙΖΗΜΕΝΟΙ ΓΗΝ ΠΟΛΛΗΝ ΟΡΥΣΣΟΥΣΙ ΚΑΙ ΕΥΡΙΣΚΟΥΣΙΝ ΟΛΙΓΟΝ

"Seekers after gold dig up much earth and find little"

"The lord whose oracle is at Delphi neither speaks nor conceals, but gives signs"

- Heraclitus

I shall be telling this with a sigh
Somewhere ages and ages hence:
Two roads diverged in a wood, and I,
I took the one less traveled by,
And that has made all the difference.

- Robert Frost