复杂网络研究中的优化问题
---- Optimization Problems in Complex Network Research

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复杂网络的提出

- 复杂网络是一种具有**非简单拓扑结构特征**的网络，这些特征既不在简单的格点网络中出现，也不在随机网络中出现，但却在现实世界的网络中出现。（维基百科 Wikipedia）

- 开创性工作：
  - 小世界网络模型 （Watts & Strogatz, ***Nature***, 1998）
  - 无尺度网络模型 （Barabasi & Albert, ***Science***, 1999）

A.-L.Barabasi 最近在NATURE PHYSICS,（Vol.8 January 2012，IF: 18.4) 上发表了一篇题为 "网络论的兴起 （The network takeover）"的文章。

文章的主要论点如下：

1. 复杂性理论在几十年的研究中没有得到有效的进展。
2. 从以爆炸速度增加的数据财富中得益最多的领域是网络理论，它本质性地重塑了我们对复杂性的研究。
3. 各具体复杂网络的节点的属性和之间的连接有很大差别，但大部分却由一系列基本的规则支配着，确定和限制着它们的行为。
4. 网络科学远比物理学大，而物理学深深卷入其中。要像前辈物理学家在上个世纪开创了量子力学一样，投入网络理论的研究，直到它的完成。

The network takeover

Albert-László Barabási

Reductionism, as a paradigm, is expired, and complexity, as a field, is tired. Data-based mathematical models of complex systems are offering a fresh perspective, rapidly developing into a new discipline: network science.

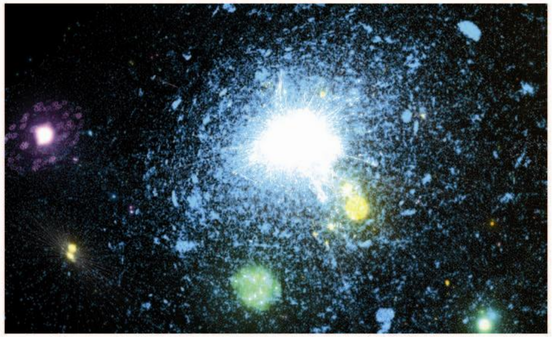
Reports of the death of reductionism are greatly exaggerated. It is so ingrained in our thinking that if one day some magical force should make us all forget it, we would promptly have to reinvent it. The real worry is not with reductionism, which, as a paradigm and tool, is rather useful. It is necessary, but no longer sufficient. But, weighing up better ideas, it became a burden.

"You never want a serious crisis to go to waste," Ralph Emmanuel, at that time Obama's chief of staff, famously proclaimed in November 2008, at the height of the financial meltdown. Indeed, forced by an imminent need to go beyond reductionism, a new network-based paradigm is emerging that is taking science by storm. It relies on datasets that are inherently incomplete and noisy. It builds on a set of sharp tools, developed during the past decade, that seem to be just as useful in search engines as in cell biology. It is making a real impact from science to industry. Along the way it points to a new way to handle a century-old problem: complexity.

A better understanding of the pieces cannot solve the difficulties that many research fields currently face, from cell biology to software design. There is no 'cancer gene'. A typical cancer patient has mutations in a few dozen of about 300 genes, an elusive combinatorial problem whose complexity is increasingly a worry to the medical community. No single regulation can legislate away the economic malady that is slowly eating at our wealth. It is the web of diverging financial and political interests that makes policy so difficult to implement. Consciousness cannot be reduced to a single neuron. It is an emergent property that engages billions of synapses. In fact, the more we know about the workings of individual genes, banks or neurons, the less we understand the system as a whole. Consequently, an increasing number of the big questions of contemporary science are rooted in the same problem: we hit the limits of reductionism. No need to mount a defence of it. Instead, we need to tackle the real question in front of us: complexity.

The complexity argument is by no means new. It has re-emerged repeatedly during the past decades. The fact that it is still fresh underlines the lack of progress achieved so far. It also stays with us for good reason: complexity research is a thorny undertaking. First, its goals are easily confusing to the outsider. What does it aim to address — the origins of social order, biological complexity or economic interconnectedness? Second, decades of research on complexity were driven by big, sweeping theoretical ideas, inspired by toy models and differential equations that ultimately failed to deliver. Think synergetics and its slave modes; think chaos theory, ultimately telling us more about unpredictability than how to predict nonlinear systems; think self-organized criticality, a sweeping collection of scaling ideas squeezed into a sand pile; think fractals, hailed once as the source of all answers to the problems of pattern formation. We learned a lot, but achieved little: our tools failed to keep up with the shifting challenges that complex systems pose. Third, there is a looming methodological question: what should a theory of complexity deliver? A new Maxwellian formula, condensing into a set of elegant equations every ill that science faces today? Or a new uncertainty principle, encoding what we can and what we can't do in complex systems? Finally, who owns the science of complexity? Physics? Engineering? Biology, mathematics, computer science? All of the above? Anyone?

These questions have resisted answers for decades. Yet something has changed in the past few years. The driving force behind this change can be condensed into a single word: data. Fuelled by cheap sensors and high-throughput technologies,



Network universe. A visualization of the first large-scale network explicitly mapped out to explore the large-scale structure of real networks. The map was generated in 1999 and represents a small portion of the World Wide Web[1]; this map has led to the discovery of scale-free networks. Nodes are web documents; links correspond to URLs. Visualization by Mauro Martino, Alec Pawling and Chaoming Song.

美国*INFORMS*前主席 *Richard Larson* 推荐在“***Operations Research***”上（vol.56, no.5, September-October, 2008）发表了一篇题为“**抓住‘网络科学’的要害问题：运筹学家的视野和机遇**”的论文

论文的主要论点为：

1. **概要地介绍网络理论的起源、方法论以及重要的成果。**

2. **对传统以图理论为基础进行的网络研究同工程师、决策者需要的网络理论的比较。**

3. **建议以运筹方法对复杂网络的重要属性和公开问题进行**‘optimization-based reverse engineering’研究

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Catching the “Network Science” Bug: Insight and Opportunity for the Operations Researcher

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Recent efforts to develop a universal view of complex networks have created both excitement and confusion about the way in which knowledge of network structure can be used to understand, control, or design system behavior. This paper offers perspective on the emerging field of “network science” in three ways. First, it briefly summarizes the origins, methodological approaches, and most celebrated contributions within this increasingly popular field. Second, it contrasts the predominant perspective in the network science literature (that abstracts away domain-specific function and instead focuses on graph theoretic measures of system structure and dynamics) with that of engineers and practitioners of decision science (who emphasize the importance of network performance, constraints, and tradeoffs). Third, it proposes *optimization-based reverse engineering* to address some important open questions within network science from an operations research perspective. We advocate for increased, yet cautious, participation in this field by operations researchers.

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1. Introduction

Recent attention on the large-scale structure of many vital network systems has led to the proliferation of new theories that attempt to explain, predict, and control network behavior and evolution. The ubiquity of the network paradigm across many important and practical applications—including the Internet and communication systems, manufacturing systems and supply chains, national infrastructures, military systems, global markets, and social organizations—has created significant interest in whether there exist universal properties of networks that may be discovered and then applied in order to understand and manage them. To empower operations researchers looking to capitalize on these research trends, this article provides a review and commentary about the potential benefits and pitfalls of recent approaches to “complex networks.”

As documented in a 2006 National Research Council (NRC) report, a new research field called “network science” is focused on an interdisciplinary view of complex network systems. The NRC Report describes progress in this field and summarizes efforts to establish network science as an academic discipline. The scientific literature over the last several years (as measured by the

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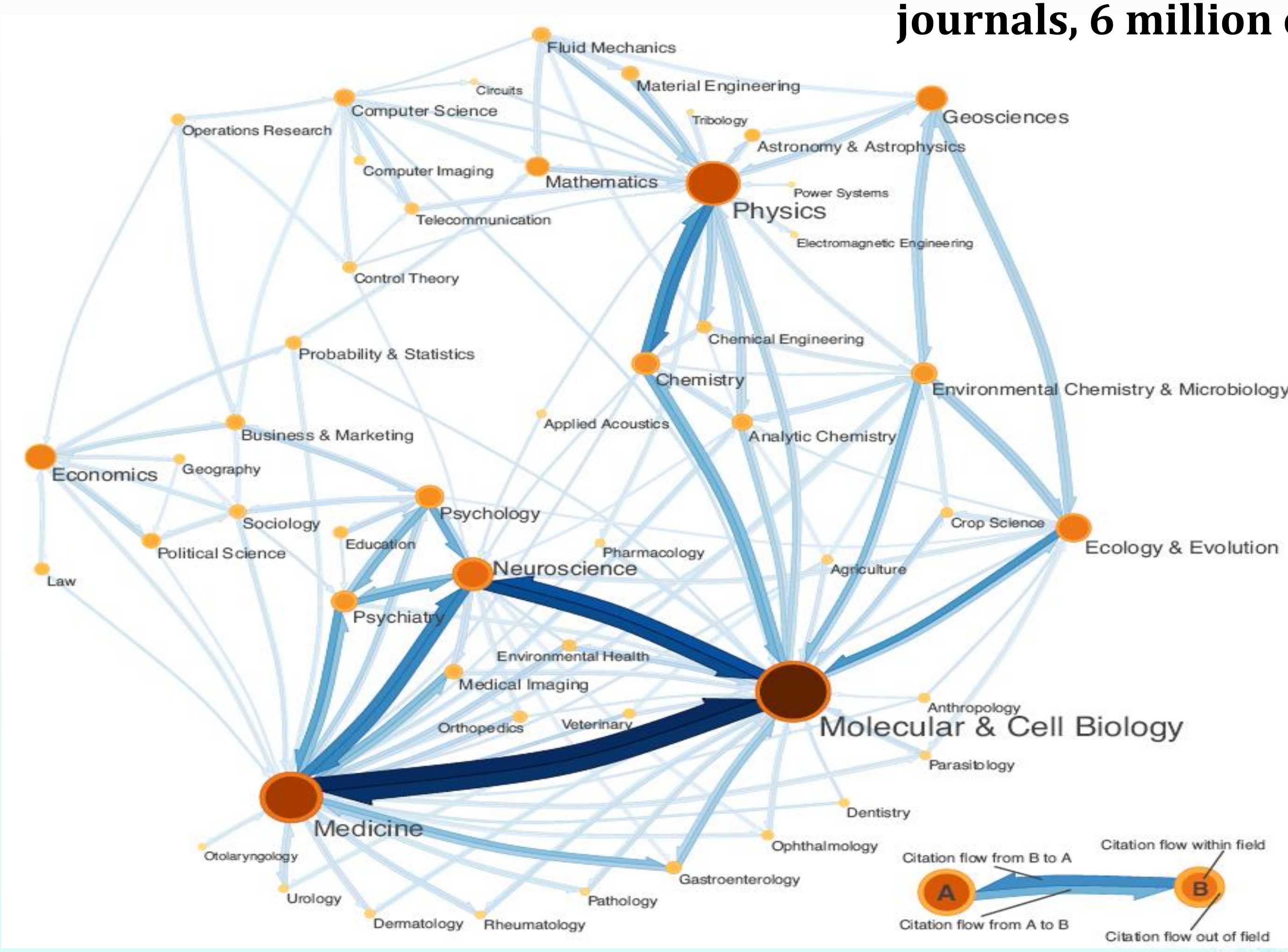
复杂网络的基本特征（续）

- Small World （小世界性质）
- Power Law /Scale free （幂律分布/无尺度网络）
- Clustering （聚合性）
- **Community Structure 社团结构**

“社团中的点相互连接紧密，而这些点同社团外的点连接较为松散。”

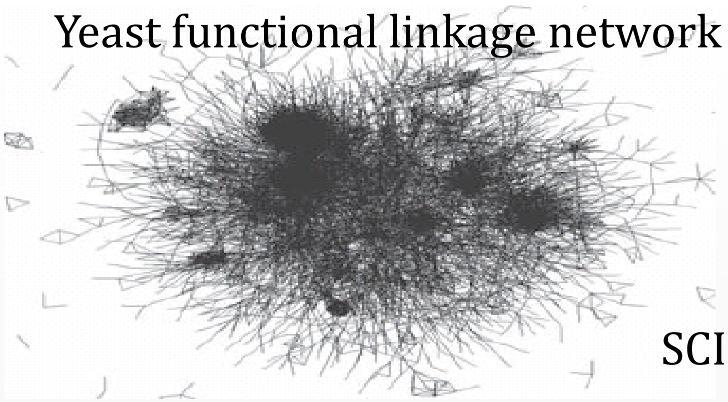
Martin Rosvall, Carl T. Bergstrom, PNAS, vol. 105, no.4. 1118-1123, 2007

Citation network of natural science papers： 6128 journals, 6 million citations，

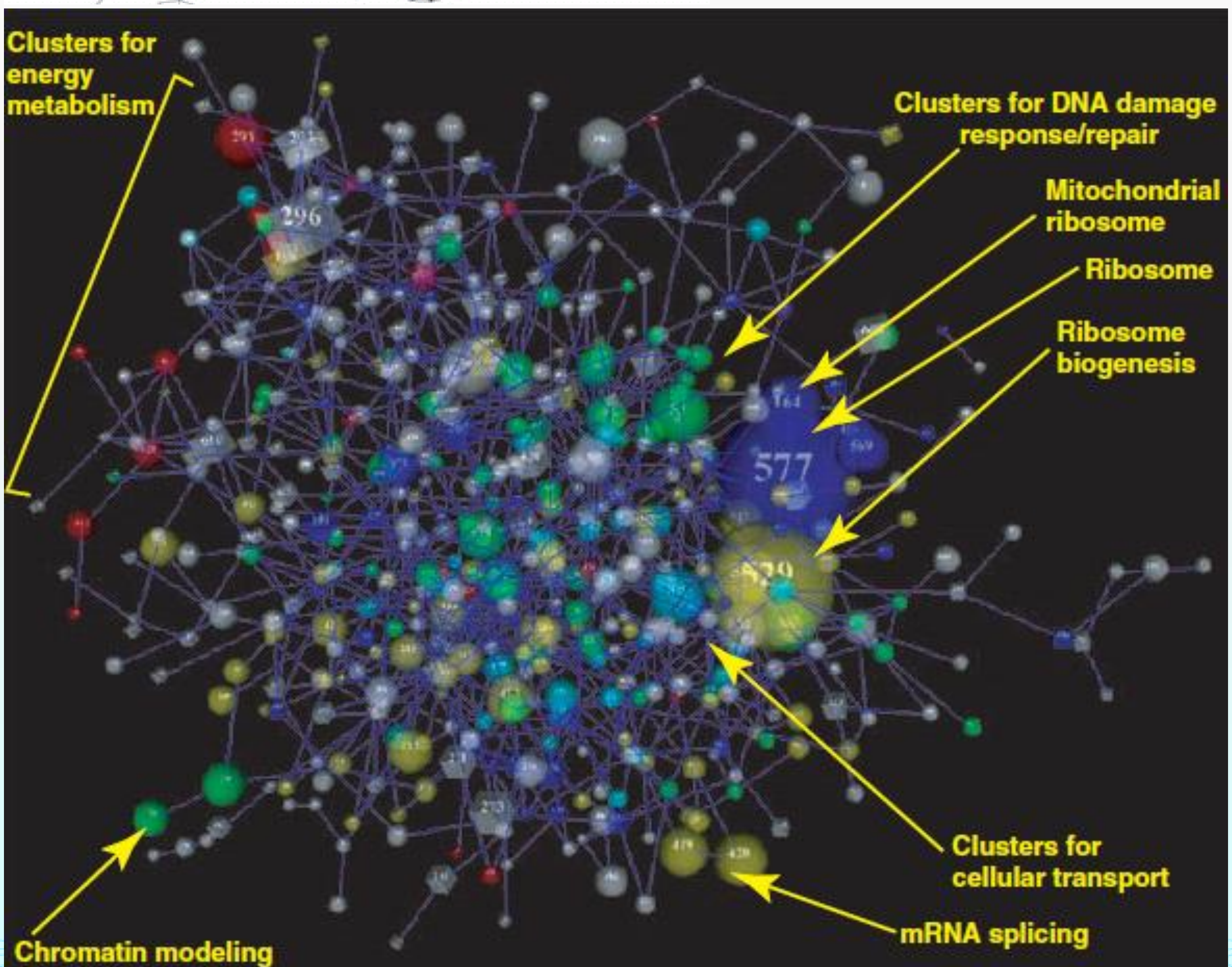


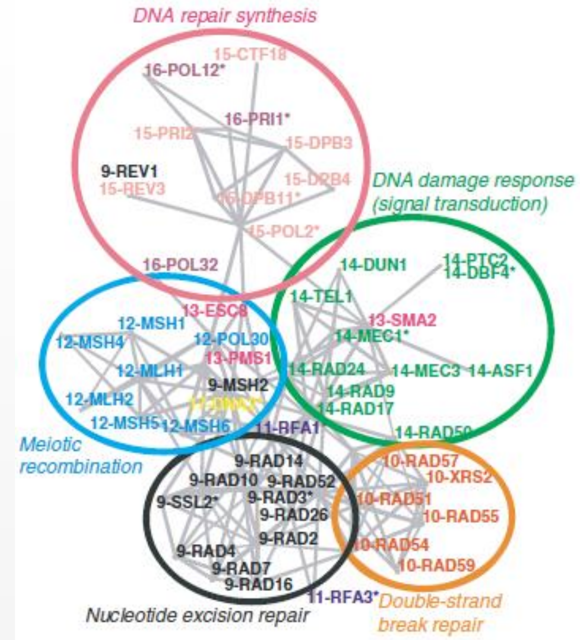
88 个模块，3024 条模块之间的连接。描述了各个学科之间的合作、交叉关系。

Yeast functional linkage network 酵母功能模块



SCIENCE Vol 306(26) 2004





DNA damage module

564 个模块，相互之间有 950 个密切的连接。

网络社团结构的其它经典例子

这些例子常常是作为社团结构算法设计时的测试问题（**benchmark problems**）

- ***Football team network***

  (S. White, P. Smyth, *SIAM* conference, 2004)

- ***Karate (空手道) club network***

  (W. W. Zachary, J. ***Anthropol. Res***. 33, 452 1977)

- ***Journal index network***

  (M. Rosvall and C. T. Bergstrom, ***Proc. Natl. Acad. Sci. U.S.A***. 104, 7327 2007)

以下发表物说明问题的重要性

- Girvan, M, Newman, M., ***Proc. Natl. Acad. Sci***, 2002
- Ravasz, E, Somera, A, Mongru, D, Oltvai, Z, Barabasi, A., ***Science***, 2002
- Radicchi, F, Castellano, C, Cecconi, F., ***Proc. Natl. Acad. Sci***, 2004
- Guimera, R, Mossa, S, Turtschi, A., ***Proc. Natl. Acad. Sci***, 2005
- Guimera, R, Amaral, L., ***Nature***, 2005
- Newman, M., ***Proc. Natl. Acad. Sci***, 2006
- Rosvall, M, Bergstrom, C., ***Proc. Natl. Acad. Sci***, 2007
- Fortunato, S, Barthelemy, M., ***Proc. Natl. Acad. Sci***, 2007
- Weinan, E, Li, T, Vanden-Eijnden, E., ***Proc. Natl. Acad. Sci***, 2008
- Rosvall, M, Bergstrom, C., ***Proc. Natl. Acad. Sci***, 2008
- Peter J. Mucha, *et al.*, ***Science*** 2010
- Yong-Yeol Ahn, James P. Bagrow & Sune Lehmann， ***Nature***, 2010

我们就下面几步来说明**社团结构问题**研究同运筹学的关系

- 社团结构的**定义**
- 试从图论来看社团结构问题
- 网络学家/物理学家的解

1. 模块优度方法
2. 模块优度方法存在的缺陷

- 运筹学对方法缺陷的探测（optimization-based reverse engineering）研究

1. 对存在问题的分析
2. 社团结构问题的完整运筹学模型

问题的定性定义

- 给定网络或者图$N = (V, E)$, 将其划分为K个子网络或者子图 $N_1=(V_1,E_1)$, ..., $N_K=(V_K,E_K)$, 这里 K 不是预先给定的，每个子网络满足：

- **The nodes in a sub-network are densely linked but are sparsely linked with that in other sub-networks**

"社团中的点相互连接紧密，而这些点同社团外的点连接较为松散。"

F. Radicchi et. al. *Proc. Natl. Acad. Sci. USA (PNAS)*, Vol.101, No.9, *2658-2663*, 2004

问题的数学定义

数学定义之一为, 对任意点 集合*Vs*中的点 *v*，

$$L(\{v\}, Vs) > L(\{v\}, V\backslash Vs),$$

此处 $L(Vi, Vj)$ 是集合 *Vi* 和 *Vj* 之间的边数. 这一定义称为社团结构的**强定义**（**strong definition**）.

F. Radicchi *et. al.* , *Proc. Natl. Acad. Sci. USA (PNAS)*, **Vol.101, No.9, *2658-2663*, 2004**

问题的数学定义 (续)

数学定义之二为,

$$L(Vs, Vs) > L(Vs, V\backslash Vs)$$

这一定义称为社团结构的**弱定义 (weak definition)**.

F. Radicchi *et. al.* , *Proc. Natl. Acad. Sci. USA (PNAS)*, Vol.101, No.9, *2658-2663,* 2004

问题的数学定义（续）

数学定义之三为,

$$L(Vs, Vs) > L(Vs, Vj),\ \ any\ \ j \neq s$$

这一定义称为社团结构的**最弱定义 (most weak definition)**.

Hu, Y., *at al*., Comparative definition of community and corresponding identifying algorithm

***Physical Review E*，** 78(2) 026121, 2008

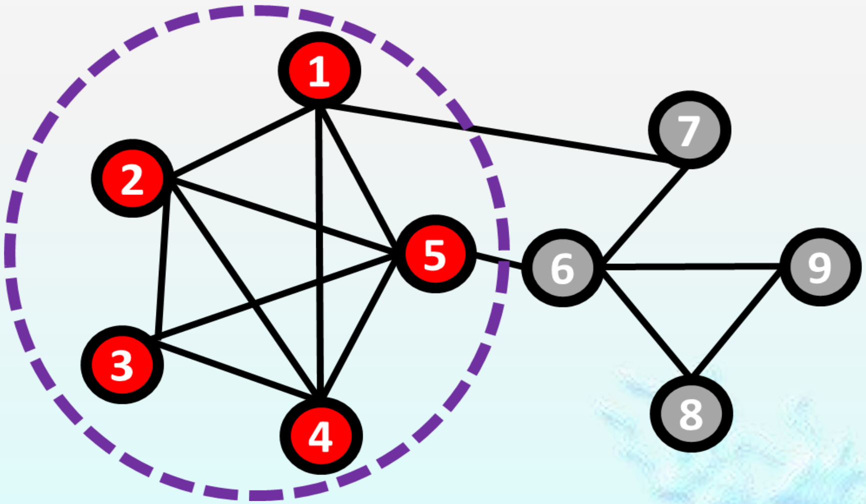
从图论角度的思考

有哪些图论中的经典问题同“社团结构问题”有关

1. 图的最大团问题---最大独立集问题

   是一个NP完全问题。

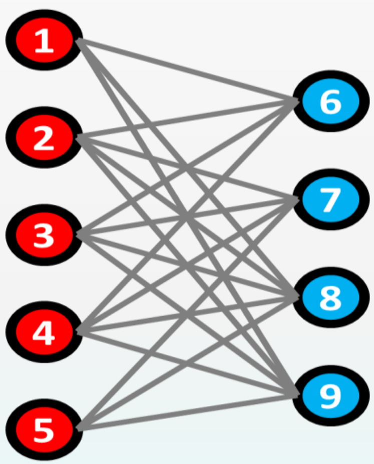
找到一个社团，其它的点就不管了，这是“Local Method”的一类方法的思路。

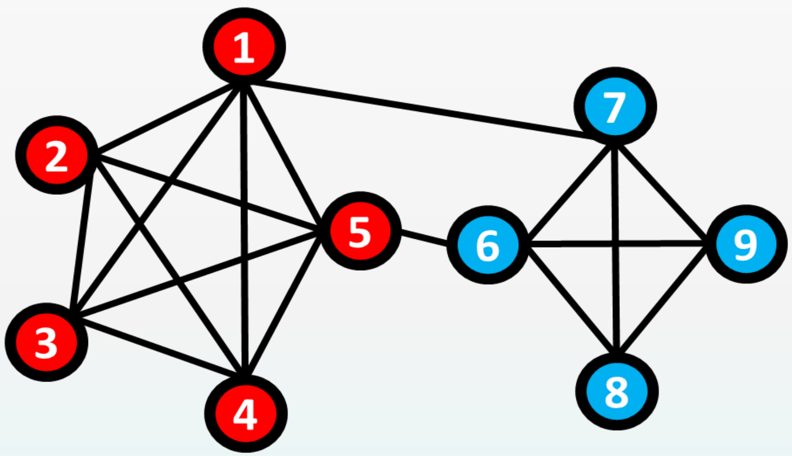


从图论角度的思考（续）

2. 二分图问题

考虑一个二分图和它的补图



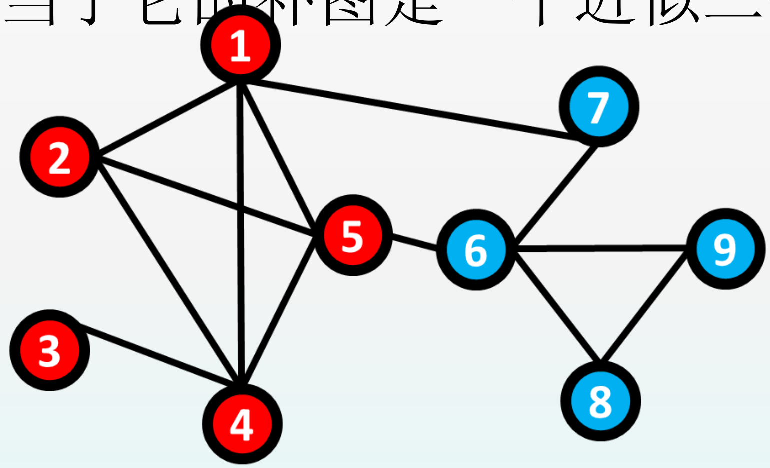


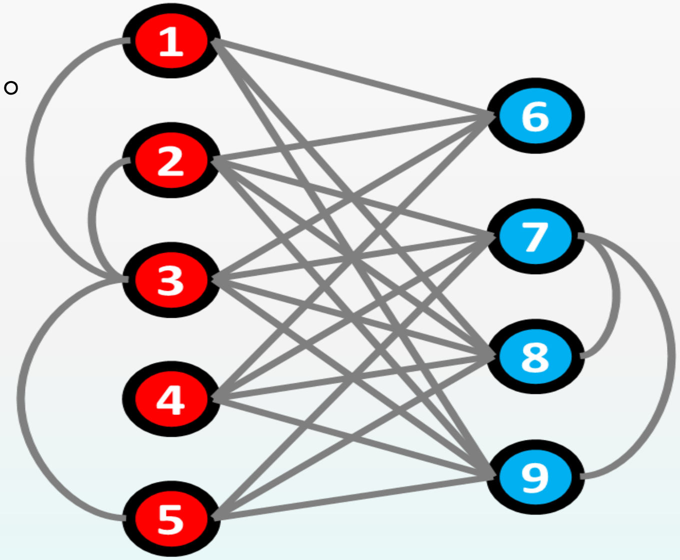
一个图是否有由两个完全子图组成的一个Community Structure，当且仅当它的补图是一个完全二分图。有线性复杂性的算法找出这个结构。

从图论角度的思考（续）

一个图有两个接近完全子图的社团组成的 Community Structure

相当于它的补图是一个近似二分图。





我们对所要研究Community Structure的网络的补图，即右图，来看图论中已有的算法。

从图论角度的思考（续）

对一个误差为k条边的近似二分图，基于Reed *et al.* 和 Hűffner的工作，Guo *et al.* 提出了去除k条边后找出二分图的算法，计算复杂性（parameterized complexity）为

$$O(2^k k|E|^2)$$

这样我们得到了社团数为二、但社团不必为完全子图的结构。

Reed B, *et al*, Finding odd cycle transversals, *Operations Research Letters*, 2004

Hüffner F., Algorithm engineering for optimal graph bipartization, *Proceedings of the 4th WEA*, Springer-Verlag , 2005

Guo J., *et al*, Improved fixed parameter algorithms for two feedback set problems, *Proceedings of the 9th WADS*, Springer-Verlag , 2005

从图论角度的思考（续）

- 实际网络的社团数大大超多“2”
- 即使是将一个网络分成两个社团的问题，当社团离完全图的缺边数为⅛时（已经是非常稠密的社团了），此时的计算复杂度变成，

$$O(2^{|E|/8}k|E|^2)$$

- 这一例子不一定精确，这是用来说明社团问题的复杂性。
- 二分图的例子是寻找社团结构的“**Global Methods**”的思路。

网络学家/物理学家的解

- 一个通常的做法是对每个划分给出一个度量，较合理的划分有较高的度量。优化该度量以得到最优或次优的社团结构。

- 第一个、也是目前最有效的度量是 “*modularity*”，译成“模块优度”.

- 由 **Newman and Girvan** (***Physical Review E***, **2004**, 到我写这个报告时，被引用次数 **3349**)。是物理学家的“启发式算法”的典范。

Modularity Q --- 模块优度 Q

- **Newman and Girvan (*Physical Review E*, 2004) 定量地定义一个社团分划的优度 *Q*为**

$$Q(N_1,\ldots,N_K)=\sum_{s=1}^{K}\left[\frac{L(V_s,V_s)}{L(V,V)}-\left(\frac{L(V_s,V)}{L(V,V)}\right)^2\right]=\sum_{s=1}^{K}Q_s$$

- **此处 *N₁, ..., Nₖ* 为 *N* 的一个划分，求和号下的项的意义为，在 *Nₛ* 中的边和总边数的比率，减去在保持每块的度数不变、边的连接方式为随机的等价网络中 *Nₛ* 的边和总边数的期望比率。**

- **或更加详细地说明:**

$$Q(N_1,\ldots,N_K)=\sum_{s=1}^{K}\left[\frac{L(V_s,V_s)}{L(V,V)}-\left(\frac{L(V_s,V)}{L(V,V)}\right)^2\right]=\sum_{s=1}^{K}Q_s$$

- $\frac{L(V_s,V_s)}{L(V,V)}$ 是第 **s** 个社团中的边数和总边数的比率.
- $\frac{L(V_s,V)}{L(V,V)}$ 分子是 ***Vs*** 的度 **ds**, 全式含义为在网络中随机地连一条边，有一个顶点落在 ***Vs*** 中的概率。
- $\left(\frac{L(V_s,V)}{L(V,V)}\right)^2$ 是随机地连接一条边时，两个顶点都落在 ***Vs*** 中的概率。

Optimization of Q

使模块度Q达到最大值的社团分划是一个最优的社团结构。这是一个两步极大化问题：

$$\max_{K} \max_{V_1 \cup \bullet\bullet\bullet \cup V_K} \sum_{s=1}^{K} Q_s$$

光是里层的问题就是一个难解问题。

Optimization of Q（续）

- *Q*的最优化是一个*NP-hard*问题, 通常用启发式算法（*heuristic algorithms*）来解，包括模拟退火、遗传算法等等。
  (Newman, *PNAS*, 2006; Guimera, *Nature*, 2005).

- 除了*Q*-方法以外，还有许多别的方法。但*Q*-方法是使用最多、最有效的方法。

- 比较这些方法的优劣使用实证研究，即把方法用到在本报告开始时提到的许多有已知社团结构的网络例子上，看它们的识别精度。

Q-optimization 存在的问题

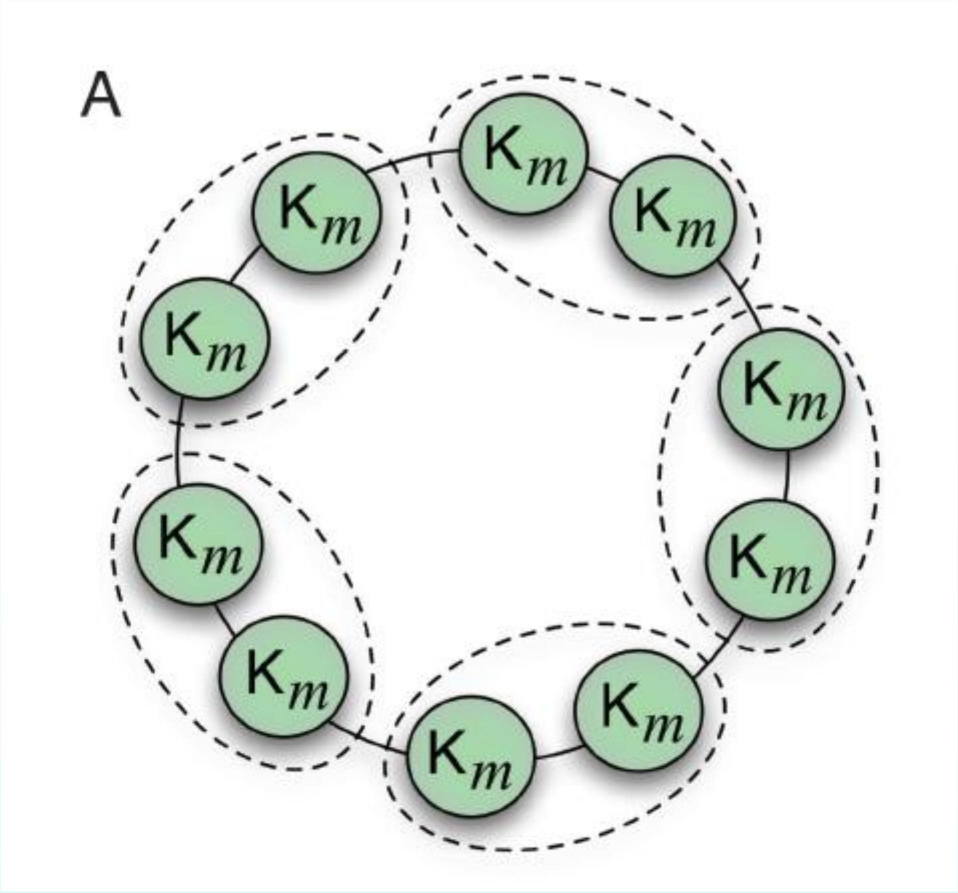
- 总的来讲，Q 方法是非常有效的，但有它的局限性。
- **Resolution limit** 精度局限

  错失精细的社团结构
- **Misidentification** 错分

  得到的社团结构不符合社团的定义
- **Definition-blind** 盲分

  得到的社团结构的定义随遇而安

Q 不能找出精细的结构



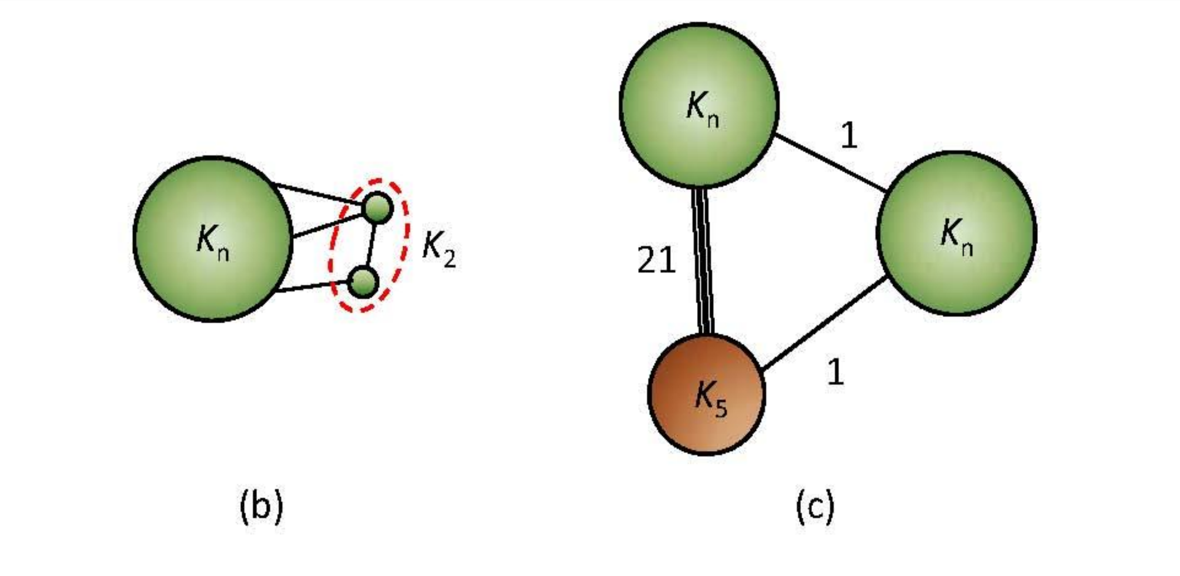
Fortunato and Barthe´lemy, 2007

Fortunato, S., Barthelemy, M. (2007) ***Proc. Natl. Acad. Sci. USA*** 104, 36-41.

Rosvall, M., Bergstrom, C.T., (2007) ***Proc. Natl. Acad. Sci. USA*** 104, 7327-331.

产生精度局限是由于Q的有效定义区域与团的密度和个数有关

错分的例子



- **X. S. Zhang**, ***et al***., Modularity optimization in community detection of complex networks
- ***EPL***, 87 (2009) 38002 (**EPL 2009 BEST PAPER**)

Optimization-based reverse-engineering

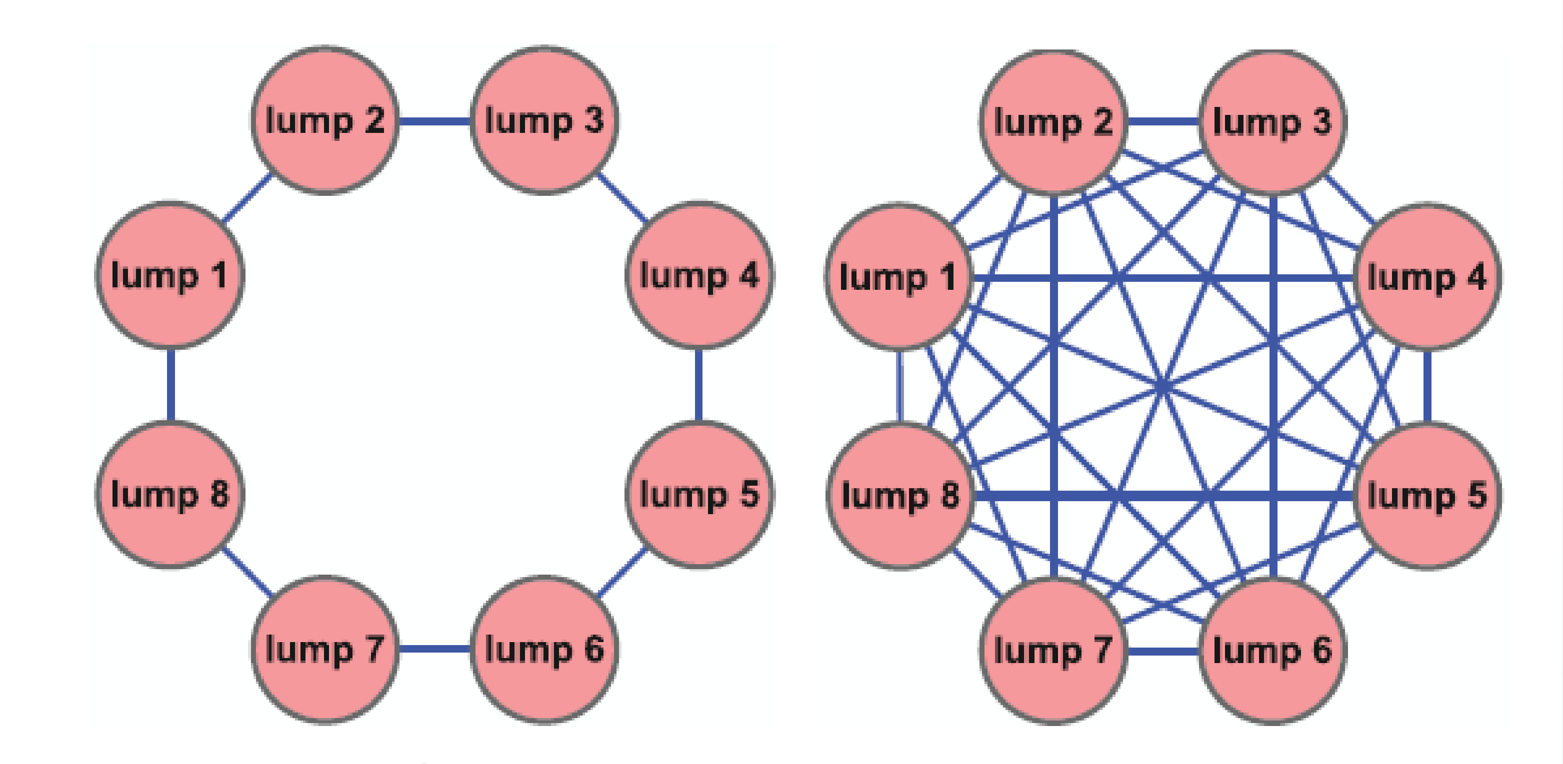
- ***Reverse-engineering*** 指对网络的一些重要属性，我们并不知道产生这些属性的真正机理和演化过程，但试着用优化的原理和方法去解释产生这些属性的可能机理、模拟复杂网络的组织过程。

- ***Reverse-engineering*** 意义在于问题分析的数学化和定量化。这对复杂网络的研究极为重要，因为至今为止，对复杂网络的研究是基于数据和实证方法的。

- 对使用***Q***时会产生 ***Resolution limit*** 现象的问题进行 ***Optimization-based reverse-engineering.***

- 为了定量化，我们要选取一些特殊的网络来进行 ***Q-optimization***

两类示例性网络



Ring of lumps *ad hoc*

网络的参数，***N***：图中**lump**的数目；l_{bw}：两个**lump**之间的连接边数；l_{in}：为**lump**中的边数。

Optimization-based reverse-engineering （续）

- $\max_{K} \max_{V_1 \cup \bullet\bullet\bullet \cup V_K} \sum_{s=1}^{K} Q_s$ 是离散凸规划/凹规划。

  ----------------这一结果解释了为何Q非常有效。

- 解的数学显式：

对 *ring of lumps*,

$$k^* = \left\langle \sqrt{\frac{l_{in} + l_{bw}}{l_{bw}}} \sqrt{N} \right\rangle_F$$

对 *ad hoc* 网，

$$k^* = \begin{cases} N, & l_{bw} < 2l_{in} \\ 1, & l_{bw} > 2l_{in} \end{cases}$$

------------- 这一结果说明Resolution limit 的出现所产生的精度局限是由于***Q***的有效定义区域对于团的密度和个数有关, 还同网络的结构有关。

Optimization-based reverse-engineering(续)

以上结果发表在论文

***X. S. Zhang**, R. S. Wang, Y. Wang, J. Wang, Y. Qiu, L. Wang and L. Chen*

"Modularity optimization in community Detection of complex networks"

(***Europhycs Letter, 2009 Best Paper***)

为解决盲分问题，我们建立了第一个"社团识别的精确优化模型"

***X.-S. Zhang**, Z. Li, R.-S. Wang, Y. Wang,*

A combinatorial model and algorithm for globally searching community structure in complex networks,

***J. Comb. Optim.**,* **Volume 23, Number 4, 425-442, 2012.**

这是第一篇由组合图论的角度来研究社团结构的论文

社团识别问题的优化定义

将一个网络划分为尽可能多的相互不重叠且满足社团结构定义 (强定义、弱定义或最弱定义) 的子图。

这句话可以用一个整数规划来加以描述：

设有一有L条边、n个点的网络，定义0-1整数变量：

$x_{ik} = 1$，如果点v_i分在社团k中，否则$x_{ik} = 0$，$k = 1, 2, \dots N$

$z_{lk} = 1$，如果边l在社团k中，否则$z_{lk} = 0$

$y_k = 0$，如果社团k是空的，否则$y_k = 1$

M 为一大于 n 的整数

我们有以下的整数规划

$$
\begin{aligned}
\max \quad & \sum_{k=1}^{n} y_k \\
\text{s.t.} \quad & \sum_{k=1}^{n} x_{ik} = 1 \\
& z_{l,k} \le x_{ik} \\
& z_{l,k} \le x_{jk} \\
& x_{ik} + x_{jk} - 1 \le z_{l,k} \\
& \sum_{i=1}^{n} x_{ik} \ge y_k \\
& \sum_{i=1}^{n} x_{ik} \le M y_k \\
& 2\sum_{l=1}^{L} z_{lk} \ge \sum_{j=1}^{n}\sum_{i=1}^{n} x_{ik} a_{ij} - 2\sum_{l=1}^{L} z_{lk} + y_k \\
& x_{ik} \in \{0, 1\},\ y_k \in \{0, 1\},\ z_{lk} \in \{0, 1\} \\
& i = 1, 2, \ldots, n,\ k = 1, 2, \ldots, n,\ l = 1, 2, \ldots, L
\end{aligned}
$$

论文的主要结果

- 证明了这是一个 NP-hard 的问题

- 设计了一个基于图的极小割的启发式算法，复杂度小于 $O(n^3)$.

- 由 ***M.Girvan*** 和 ***M.E.Newman*** 所建立的算法 (*PNAS* 99, 2002) 的复杂度为 $O(n^3 \log n)$

我们近年来发表的有关复杂网络的论文：

- ***X.-S. Zhang****, Z. Li, R.-S. Wang, Y. Wang,*

  A combinatorial model and algorithm for globally searching community structure in complex networks,

  J. Comb. Optim*., DOI 10.1007/s10878-010-9356-0, 2010*
- *J.Zhang, Y.Qiu,* ***X.-S. Zhang****,*

  Detecting community structure: from parsimony to weighted parsimony,

  J. Syst. Sci. Complex 23: 1024-1036, 2010
- ***X.-S. Zhang****, R.-S. Wang, Y. Wang, J. Wang, Y. Qiu, L. Wang, and L.Chen,*

  Modularity optimization in community detection of complex networks,

  Europhysics Letters, 87:38002(6pp), doi:10.1029/0295-5075/87/38002, 2009
- *Z.Li, S.Zhang, R.Wang,* ***X.-S. Zhang*** *and L.Chen,*

  Quantitative function for community detection,

  Physical Review E, 77, 036109, 2008, selected for the March 15, 2008 issue of Virtual Journal of Biological Physics Research

我们近年来发表的有关复杂网络的论文(续):

- *J. Wang, Y. Qiu, R.-S. Wang, **X-S Zhang**,*
  Remarks on network community,
  J. Syst Sci & Complexity, 21: 637-644, 2008
- *J.Zhang, S.Zhang, **X.-S. Zhang***, Detecting community structure in complex networks based on a measure of information discrepancy reference,
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- *S.Zhang, R.-S. Wang, **X.-S. Zhang***, Identification of overlapping community structure in complex networks using fuzzy c-means clustering,
  Physica A, 374, pp.483-490, 2007
- *S.-H.Zhang, X.Ning, **X.-S.Zhang***, Graph kernels, hierarchical clustering, and network community structure: experiments and comparative analysis, ***European Physical J. B***, 57, 67-74, 2007
- *S.Zhang, R.-S.Wang and **X.-S. Zhang**,*
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Comment

- 社团结构的研究还有许多问题要做
  1. ***Fuzzy community structure***
  2. ***Community structure dynamics***

- 复杂网络研究中的 ***Optimization-based reverse-engineering*** 还刚刚开始，其中一个重要的研究方向是复杂网络的生成机制。

最近“***Nature***”的一篇论文： ***Popularity versus similarity in growing networks***，**F. Papadopoulos**等用优化的框架来说明了***Scale free*** 网的生成， 是***Optimization-based reverse-engineering*** 研究的又一范例。

Comment（续）

Optimization-based reverse-engineering在系统生物学上有重要的应用

重要生物问题：	*用到的运筹模型*
1. 基因调控网络重建	*a.整数规划、线性规划、二次规划*
2. 蛋白相互作用网络重建	*b.动态规划*
3. 生物分子网络保守模块探测	*c.组合优化*
4. 复杂疾病的调控机理	*d. 马氏过程*

我们研究组最近十年在运筹学与生物医学的交叉研究方面做了大量的探索，希望中国运筹学界的同仁们加以关注

谢谢!

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