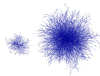


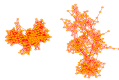


Mean Field Analysis of Algorithms Generating Scale-free Networks

S Konini and EJ Janse van Rensburg
Mathematics & Statistics, York University
Toronto, Ontario



Barabasi-Albert



Vazquez

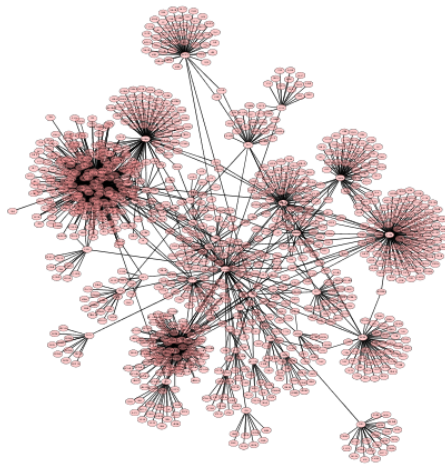


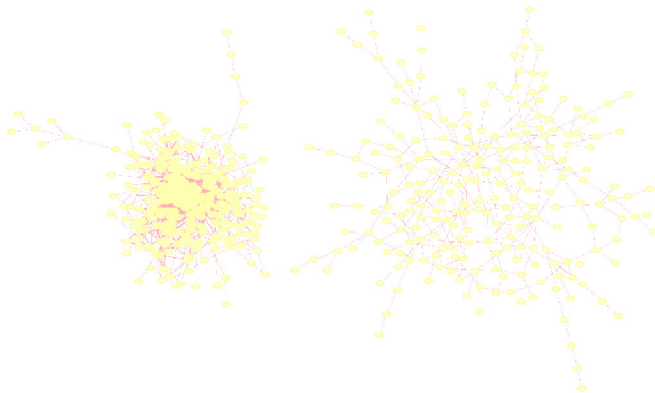
Solé



iSite

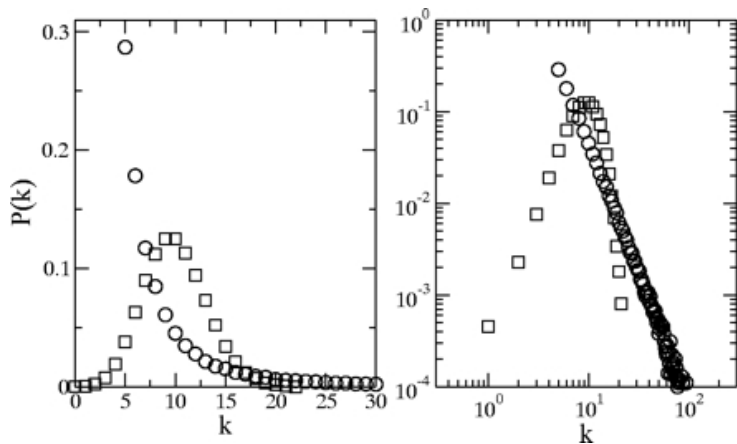
— Protein interaction network





- Growing a cluster using a recursive algorithm

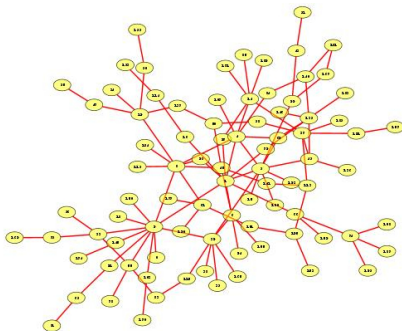
Growing a Random Network or Cluster



Source: Albert *Scale-free networks in cell biology*
(Journal of Cell Science 2005 118: 4947-4957; doi: 10.1242/jcs.02714)

Plotting the degree distribution $P(k)$

— Scale-free networks



- Degree distribution $P(k) = \text{Prob}(\text{degree of node is } k)$
- Normally $P(k)$ is binomially distributed (eg Erdős-Rényi model)
- Said to be Scale-free if $P(k)$ obeys a power law:

$$P(k) \sim k^{-\gamma}$$



A large but finite network of n nodes has degree probability

$$P(k) \sim k^{-\gamma}$$

- $P(k)$ is not integrable if $\gamma \leq 1$ as $n \rightarrow \infty$
- However $\sum_{k=0}^n P(k) \simeq \int_1^n P(k) dk \sim \frac{1-n^{1-\gamma}}{\gamma-1}$
- That is, if $\gamma > 1$, then this is finite as $n \rightarrow \infty$



Measurable quantities associated with networks:

- Average number of nodes of degree k : $\{\langle d_k \rangle\}_n$

$$\langle d_k \rangle = n P(k)$$



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- Average degree: $\{\langle k \rangle\}_n$

$$\langle k \rangle = \sum k P(k)$$

- Average number of edges (Size): E_n

$$E_n = \frac{n}{2} \langle k \rangle$$

The average degree (*connectivity*) for networks of size n grows as

$$\langle k \rangle_n = \sum_{k=1}^n k P(k) \simeq \frac{\int_1^n k k^{-\gamma} dk}{\int_1^n k^{-\gamma} dk} \simeq \left(\frac{\gamma-1}{\gamma-2} \right) \frac{n^\gamma - n^2}{n^\gamma - n}$$

$$\sim \begin{cases} \left(\frac{1-\gamma}{2-\gamma} \right) n, & \text{if } \gamma < 1; \\ \frac{n}{\log n}, & \text{if } \gamma = 1; \\ \left(\frac{\gamma-1}{2-\gamma} \right) n^{2-\gamma}, & \text{if } 1 < \gamma < 2; \\ \log n, & \text{if } \gamma = 2; \\ \left(\frac{\gamma-1}{\gamma-2} \right), & \text{if } \gamma > 2. \end{cases}$$

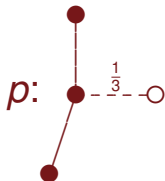
- The number of edges grows as

$$E_n = \frac{1}{2} n \langle k \rangle_n$$

$$E_n \sim \begin{cases} \left(\frac{1-\gamma}{2(2-\gamma)} \right) n^2, & \text{if } \gamma < 1 \text{ (dense);} \\ \frac{n^2}{2 \log n}, & \text{if } \gamma = 1 \text{ (marginally dense);} \\ \left(\frac{\gamma-1}{2(2-\gamma)} \right) n^{3-\gamma}, & \text{if } 1 < \gamma < 2 \text{ (super linear);} \\ \frac{1}{2} n \log n, & \text{if } \gamma = 2 \text{ (marginally sparse);} \\ \left(\frac{\gamma-1}{2(\gamma-2)} \right) n, & \text{if } \gamma > 2 \text{ (linear or sparse).} \end{cases} \quad (1)$$

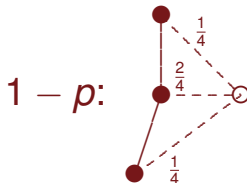
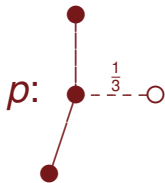
— Barabasi-Albert clusters

- Barabasi & Albert in *Science*; **286**:509–512 (1999)
- Attach new nodes to existing nodes:



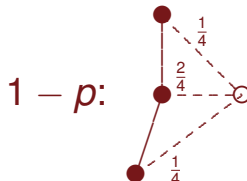
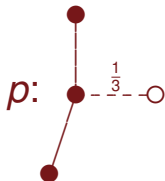
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- Attach new nodes to existing nodes:



- Preferential attachment of nodes to vertices of high degree

— Modified Barabasi-Albert clusters

Bonds are added in two ways:

- p : Select x_j uniformly and attach x_n by inserting $\langle x_j \sim x_n \rangle$;

- $1 - p$: Attach x_n by adding $\langle x_j \sim x_n \rangle$ with probability $P_{jn} = \frac{k_j}{\sum_j k_j}$

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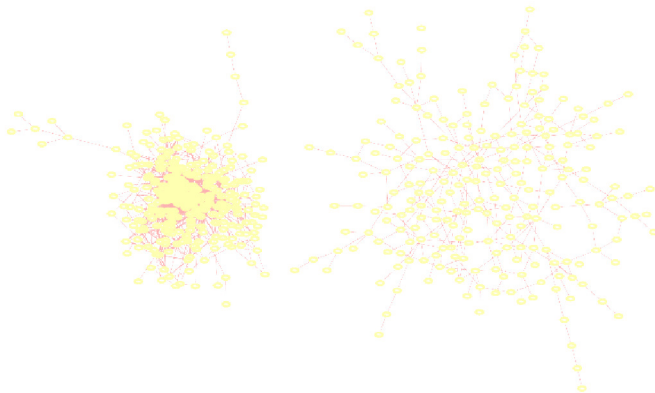
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Modification:

Attach x_n by adding $\langle x_j \sim x_n \rangle$ with probability

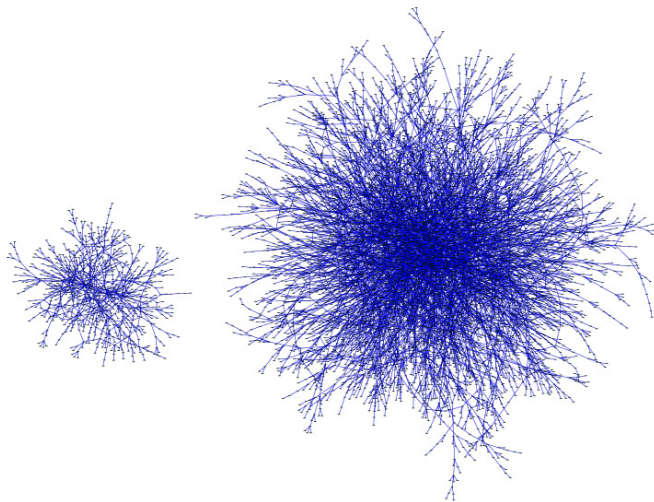
$$P_{jn} = \min \left\{ \frac{\lambda k_j + A}{\sum_j k_j}, 1 \right\}$$

Recover the canonical algorithm when $\lambda = 1$ and $A = 0$

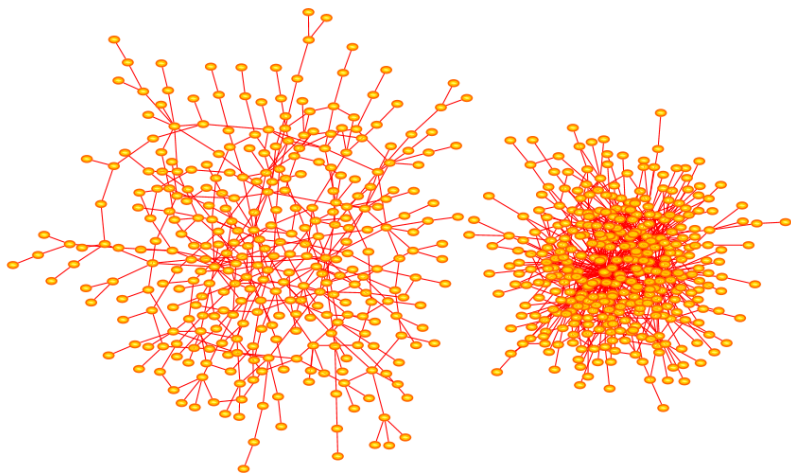


- Growing a cluster with $p = 0.5$ and of order $n = 100000$

Barabasi-Albert Cluster with $p = 0.5$



Barabasi-Albert clusters ("Dendritic appearance")



Modified Barabasi-Albert Clusters ($\lambda = 0.1$ left, and $\lambda = 1.5$ right)



— Mean field theory for the Modified Barabasi-Albert algorithm

Barabasi-Albert clusters are relatively sparse networks

- $k_j(n)$ = degree of node j after n iterations
- Mean field: $k_j(n) = \langle k \rangle$



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 - 1 Probability p append a random edge and node
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- Elementary move of the algorithm:
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$$\text{Probability} = p$$

- 2 Default: append edges $\langle x_j \sim x_n \rangle$ with probability

$$\text{Probability} = (1 - p) \times \frac{\lambda k_j(n) + A}{\sum_j k_j(n)}$$



- Bonds added:

- 1 With probability p one bond is appended



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- ② With probability $1 - p$ for each j add $\langle j \sim n \rangle$ with $\text{Pr} = \frac{\lambda k_j(n) + A}{\sum_j k_j(n)}$

$$(1 - p) \sum_j \frac{\lambda k_j(n) + A}{\sum_j k_j(n)} = \left(\lambda + \frac{nA}{\sum_j k_j(n)} \right) = (1 - p) \left(\lambda + \frac{nA}{2E_n} \right)$$

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- Change in the size $\Delta E_n = p + (1 - p)\lambda + (1 - p)\frac{nA}{2E_n}$

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- Solve:

$$E_n = \frac{n}{2}((p + (1 - p)\lambda) + \sqrt{(p + (1 - p)\lambda)^2 + 2(1 - p)A}) = Cn$$

- $\gamma > 2$ (the network is sparse)

Scaling exponent γ for Barabassi-Albert clusters

$$k_j(n) = \text{Degree of vertex } j \text{ at time } n$$

- Recurrence for $k_j(n)$:

$$k_j(n+1) = k_j(n) + \frac{p}{n} + \frac{(1-p)(\lambda k_j(n) + A)}{2E_n}$$

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- DE approximation (j -th node is added at time $t = j$)

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Solve the equation

$$k_j(n) = \left(1 + \frac{Q}{P}\right) (n/j)^P - \frac{Q}{P}, \quad \text{where } Q = p + \frac{(1-p)A}{2C} \text{ and } P = \frac{(1-p)\lambda}{2C}$$



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- Fixed $\kappa > 0$
- The probability that $k_j(n) < \kappa$ is given by

$$P(k_j(n) < \kappa) \gtrsim P\left(\frac{j}{n} > \left(\frac{Q/P + \kappa}{1 + Q/P}\right)^{-1/P}\right) \quad \text{for } 0 \leq j \leq n$$



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- Mean Field: j is uniform in $\{1, 2, \dots, n\}$
- The RHS evaluates to

$$P(k_j(n) < \kappa) \gtrsim 1 - \left(\frac{Q/P + \kappa}{1 + Q/P}\right)^{-1/P}$$

Take the derivative to find (for $1 \ll \kappa \ll n$)

$$P(\kappa) = P[k_j(n) = \kappa] = \frac{\partial}{\partial \kappa} P[k_j(n) < \kappa] \simeq \frac{(P+Q)^{1/P}}{(P\kappa+Q)^{1+1/P}} \sim \kappa^{-1-1/P}$$

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This gives the following expression for γ :

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- Canonical Barabasi-Albert clusters ($\lambda = 1$ and $A = 0$) are sparse

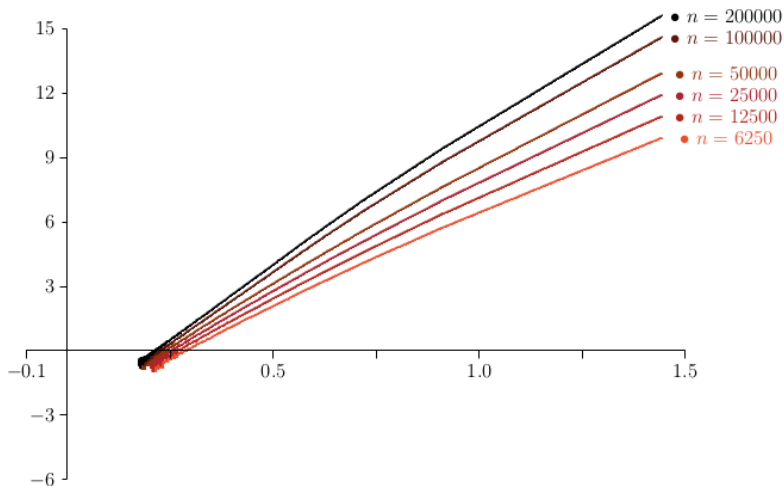
$$\gamma = 3 + \frac{2p}{1-p} \geq 3$$

- If $A = 0$ then

$$\gamma = 3 + \frac{2p}{(1-p)\lambda} \geq 3$$

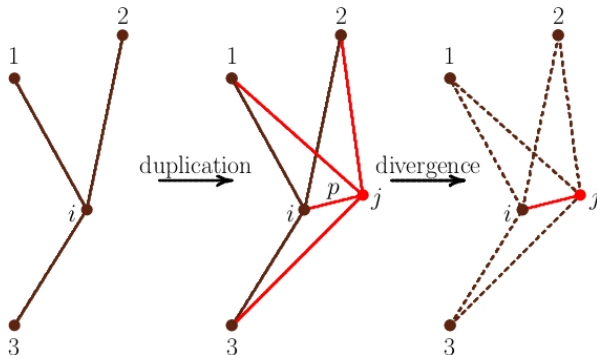
- If $\lambda = 1$ then

$$\gamma = 1 + \frac{1}{1-p} + \frac{\sqrt{1+2(1-p)A}}{1-p} \geq 3$$



- If $p = 0$ then $\gamma = 3.026$
- $\langle k \rangle_n \rightarrow \text{Constant}$ and the clusters are sparse

— Duplication-Divergence clusters



- Vazquez *etal* in *ComplexUS 2003*; 1:38–44 (2003)
- Parameters

p = add bond between duplicated vertices;

q = delete predecessor and duplicated bonds

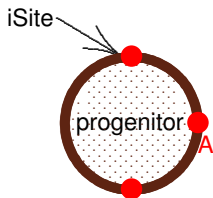


— iSite evolutionary clusters

- Gibson & Goldberg in *BioInformatics*; **27**:376–382 (2011)

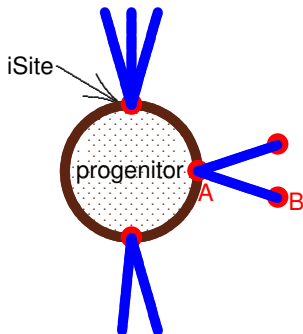
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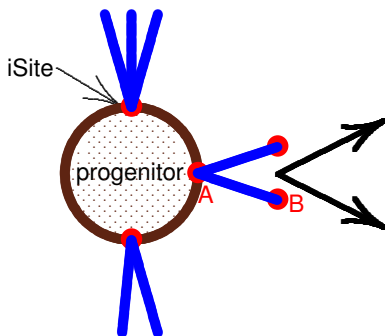
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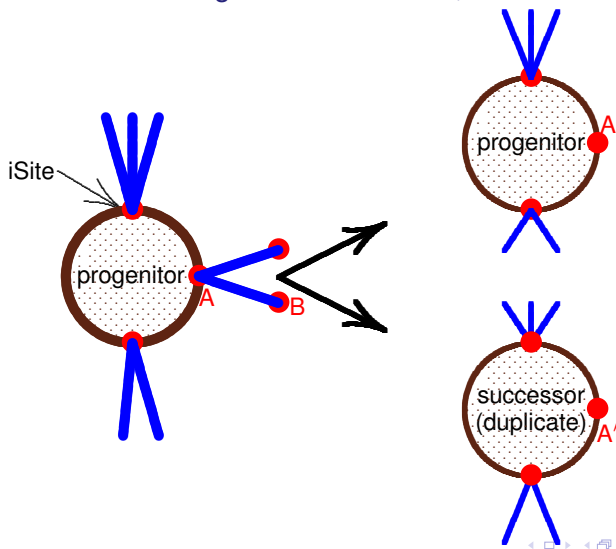
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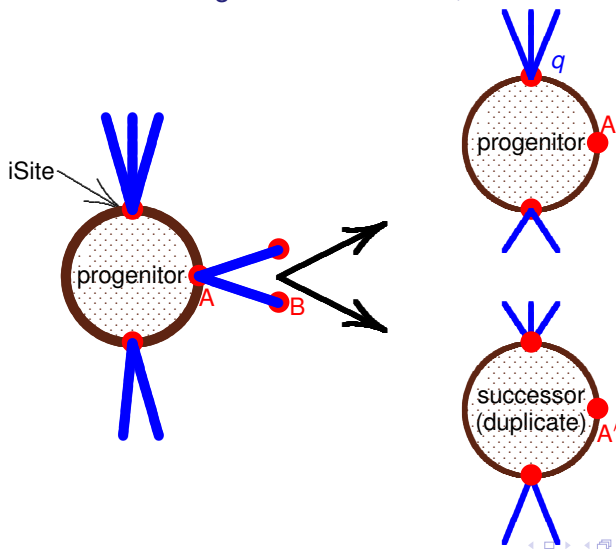
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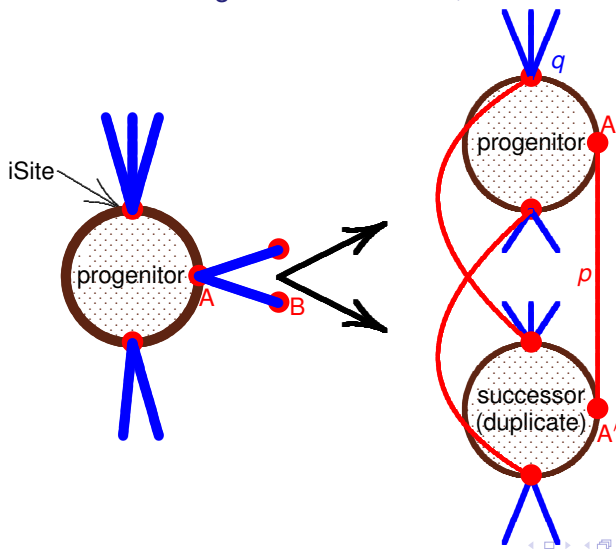
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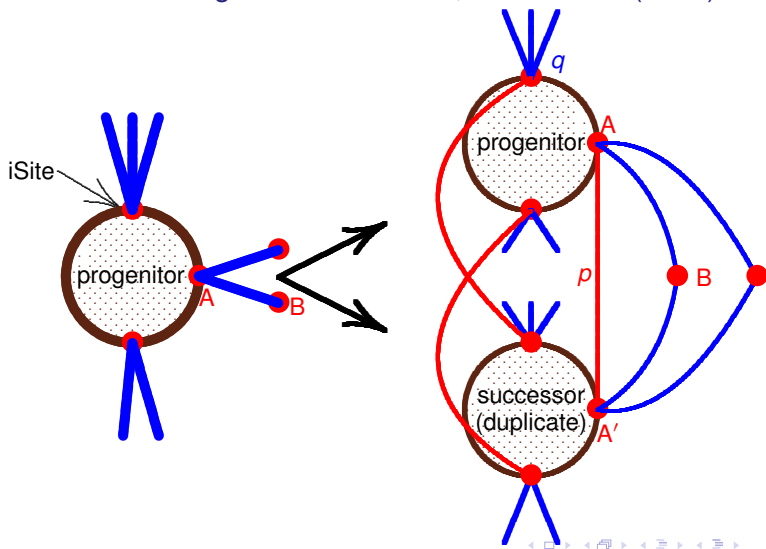
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-
- The diagram illustrates the evolution of a site from a single progenitor to a duplicated state with two successors. On the left, a single circular node labeled "progenitor" is shown. It has a dotted interior and a brown border. A red dot labeled "A" is on its right boundary. Two blue lines extend from "A" to two red dots labeled "B". A black arrow points from the "progenitor" node to the right. On the right, two circular nodes are shown, stacked vertically. The top node is labeled "progenitor" and the bottom node is labeled "successor (duplicate)". Both have a dotted interior and a brown border. The top node has a red dot labeled "A" on its right boundary. The bottom node has a red dot labeled "A'" on its right boundary. A red line connects "A" and "A'", labeled "p". A green curved line connects "A" and "A'", labeled "1-r". Blue lines extend from "A" and "A'" to a red dot labeled "B" on the right. A black arrow points from the "progenitor" node to the "successor (duplicate)" node.



The iSite evolutionary algorithm:
Isites are **self-interacting** with probability p



The iSite evolutionary algorithm:

Isites are **self-interacting** with probability p
and are **active** with probability q



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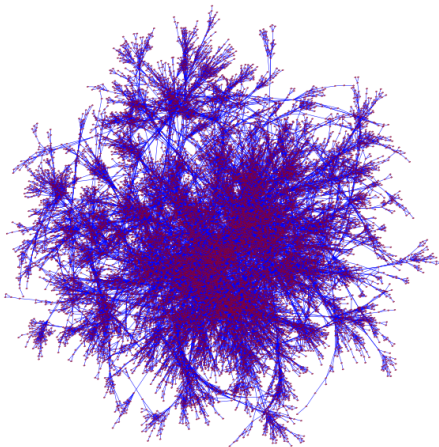
Isites are **self-interacting** with probability p

and are **active** with probability q

Interactions are **lost** with probability r

- 1 Initiate the network with one node x_0 with l active iSites;
- 2 Choose a progenitor protein v uniformly and duplicate it to a successor protein v' :
 - A duplicated iSite $A' \in v'$ is *active* with probability q ;
 - A duplicated iSite $A' \in v'$ is *self-interacting* with probability p ;
- 3 Add new interactions as follows if A' is active:
 - If iSite $A' \in v'$ is self-interacting then add the edge $\langle A \sim A' \rangle$;
 - If $\langle A \sim B \rangle$ is an interaction, then duplicate it to $\langle A' \sim B \rangle$ with probability $1-r$;
- 4 Iterate the algorithm until a network of order N is grown.

— iSite clusters





— Mean field theory for iSite clusters

- $i_j(n)$ = # active iSites on node j after n iterations
- The average number of iSites per protein is

$$i(n) = \frac{1}{n} \sum_j i_j(n)$$

- $k_j(n)$ = degree of node j after n iterations

$$2 E_n = \sum_j k_j(n)$$

- Mean field: $i(n)$ iSites are created and $q i(n)$ are silenced
- Recurrence for $i(n)$:

$$(n + 1) i(n + 1) = n i(n) + (1 - q) i(n)$$

since $n i(n) = \# \text{ iSites}$ and $(1 - q) i(n)$ are added in the mean field



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- Exact solution

$$i(n) = \frac{i(0) \Gamma(1-q+n)}{n! \Gamma(1-q)} \simeq \frac{I n^{-q}}{\Gamma(1-q)}$$

if $i(0) = I$



- The number of edges increases in the mean field

$$\Delta E_{n+1} = \frac{2(1-r)}{n} E_n + p i(n)$$

since $\langle k_j(n) \rangle = \frac{2}{n} E_n$ edges are duplicated with probability $1 - r$
and $p i(n)$ edges are created by self-interacting iSites

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and $p i(n)$ edges are created by self-interacting iSites

- Approximate this with a DE

$$\frac{d}{dn} E_n = \frac{2(1-r)}{n} E_n + \frac{pl}{\Gamma(1-q)} t^{-q}$$

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- Approximate this with a DE

$$\frac{d}{dn} E_n = \frac{2(1-r)}{n} E_n + \frac{pl}{\Gamma(1-q)} t^{-q}$$

- Solve this with IC $E_1 = 0$:

$$E_n = \frac{pl}{(1+q-2r)\Gamma(1-q)} \left(n^{2-2r} - n^{1-q} \right).$$

Mean field connectivity of iSite clusters

$$\langle k \rangle_n = \frac{2}{n} E_n \simeq \frac{2pl}{(1+q-2r)\Gamma(1-q)} \left(n^{1-2r} - n^{-q} \right)$$

- $\langle k \rangle_n$ is dominated by the larger of $-q$ and $1 - 2r$

Mean field connectivity of iSite clusters

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- $\langle k \rangle_n$ is dominated by the larger of $-q$ and $1 - 2r$
- The γ exponent is

$$\gamma = \begin{cases} 1 + 2r, & \text{if } r < \frac{1}{2}(1 + q); \\ 2 + q, & \text{if } r > \frac{1}{2}(1 + q). \end{cases}$$

Mean field connectivity of iSite clusters

$$\langle k \rangle_n = \frac{2}{n} E_n \simeq \frac{2pl}{(1+q-2r)\Gamma(1-q)} \left(n^{1-2r} - n^{-q} \right)$$

- $\langle k \rangle_n$ is dominated by the larger of $-q$ and $1 - 2r$
- The γ exponent is

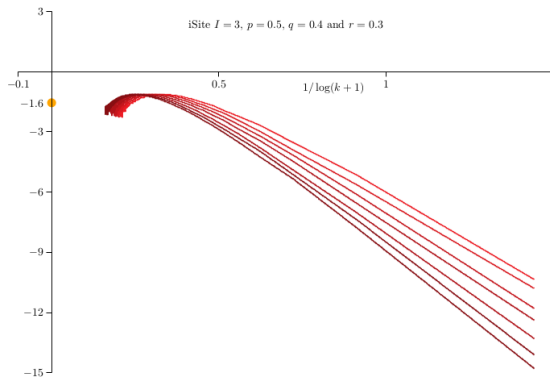
$$\gamma = \begin{cases} 1 + 2r, & \text{if } r < \frac{1}{2}(1 + q); \\ 2 + q, & \text{if } r > \frac{1}{2}(1 + q). \end{cases}$$

- If $2r = (1 + q)$ then a different solution is obtained

$$\langle k \rangle_n = \frac{pl}{\Gamma(1-q)} n^{-q} \log n$$

so $\gamma = 2 + q$ with a $\log n$ correction

— iSite clusters



- Plot of $\log P(k)/\log(k+1)$ against $1/\log(k+1)$
- $I = 3$, $p = 0.5$, $q = 0.4$, $r = 0.3$
- For these parameters, $\gamma = 1 + 2r = 1.6$

— Average degree data for iSite Clusters

n	Column 2	Column 3	Column 4	Column 5
3125	22.385	20.701	4.756	6.648
6250	26.524	25.752	4.770	6.556
12500	31.395	29.137	4.677	6.579
25000	37.808	35.308	4.733	6.358
50000	45.931	42.244	4.579	6.299
100000	54.830	50.035	4.584	6.204
200000	64.668	59.284	4.649	6.071
Column 2: $l = 3, p = 0.5 \quad q = 0.4, r = 0.3$				
Column 3: $l = 5, p = 0.5 \quad q = 0.4, r = 0.3$				
Column 4: $l = 3, p = 0.5 \quad q = 0.05, r = 0.8$				
Column 5: $l = 5, p = 0.5 \quad q = 0.05, r = 0.8$				

- $\langle k \rangle_n = \frac{\gamma-1}{2-\gamma} n^{2-\gamma}$

- Columns 2 & 3:

Least squares: $\gamma = 1.74$ and $\gamma = 1.74$ (MF $\gamma = 1.6$)

- Columns 4 & 5: $\gamma = 2.1$ and $\gamma = 2.02$ (MF $\gamma = 2.05$)

— Computational Time Complexity of Implemented Algorithms

- Time complexity $\sim n^\tau$

Algorithm	$n = 6250$	$n = 12500$	$n = 25000$	$n = 50000$	τ
Bar-Alb ($p = 0$)	0.602	2.51	9.03	38.0	1.97
Mod Bar-Alb ($\lambda = 2, p = A = 0$)	0.618	2.55	10.1	36.3	1.96
Dupl-Div ($p = 1, q = 0.4$)	0.349	0.862	2.04	5.01	1.28
Dupl-Div ($p = 1, q = 0.6$)	0.155	0.319	0.635	1.31	1.02
Solé ($\delta = 0.25, \alpha = 0.005$)	4.84	20.5	91.0	436.0	2.16
Solé ($\delta = 0.75, \alpha = 0.005$)	6.10	20.0	79.5	323.2	1.92
iSite ($p = 0.5, q = 0.01, r = 0.8, l = 1$)	0.114	0.234	0.454	0.925	1.00
iSite ($p = 0.5, q = 0.01, r = 0.8, l = 2$)	0.110	0.216	0.458	0.878	1.01
iSite ($p = 0.5, q = 0.01, r = 0.8, l = 3$)	0.106	0.217	0.432	0.857	1.00
iSite ($p = 0.5, q = 0.01, r = 0.8, l = 4$)	0.107	0.231	0.422	0.848	0.98
iSite ($p = 0.25, q = 0.01, r = 0.8, l = 4$)	0.104	0.249	0.415	0.844	0.98
iSite ($p = 0.75, q = 0.01, r = 0.8, l = 4$)	0.108	0.216	0.437	0.867	1.00



— Conclusions

- Variety of algorithms in the mean field
- Mixed success, in some cases good, other cases perhaps not
- Also considered the Solé model – the clusters are not scale-free, but do exhibit a distribution which scales
- Also introduced variants of the models, and considered their properties
- S Konini and EJJvR PLoSOne 12(12):e0189866 (2017)

Thank you for the invitation to speak here!