A random graph model with duplication

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Random graphs

Erdős–Rényi graphs (E–R 1959, 1960)

$G_{n,m}$ – n vertices; m edges, each with equal probability

Random graph process

in discrete time: $\left(G_{n,t},\ t = 0, 1, \ldots, \binom{n}{2}\right)$
probabilistic version: $\left(G_{n,t},\ t > 0\right)$ – edges come according to a homogeneous Poisson process

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Very exciting mathematically, but real world networks often behave differently.

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Evolving random graphs

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More general, more complicated models of web graphs (e.g., Cooper and Frieze, RSA 2003)

Evolving random graphs

An evolving random graph process means that the probability spaces describing the graph at subsequent stages of evolution are embedded one in another, so the whole process can be defined in the same probability space. This makes it possible to prove almost sure theorems. When it makes sense, it is stronger than the corresponding whp result, the two notions are related like *convergence in probability* vs *a.e. convergence*.

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Asymptotic degree distribution: for every $d = 0, 1, \ldots$ the proportion of degree d vertices converges to a *constant* c_d with probability 1 as the size of the graph tends to infinity. The sequence (c_d) sums up to 1.
The asymptotic degree distribution is scale free, if $c_d \sim K\, d^{-\gamma}$ as $d \to \infty$, for some $\gamma > 0$ (characteristic exponent).

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E.g., for the PORT $c_d = \frac{4}{d(d+1)(d+2)}$, $\gamma = 3$.

Heuristic reasoning

In the beginning of the new millenium we saw an explosion of (mostly heuristic) results, which were proved rigorously later. It is always striking when heuristics and approximate computations fail.

Duplication

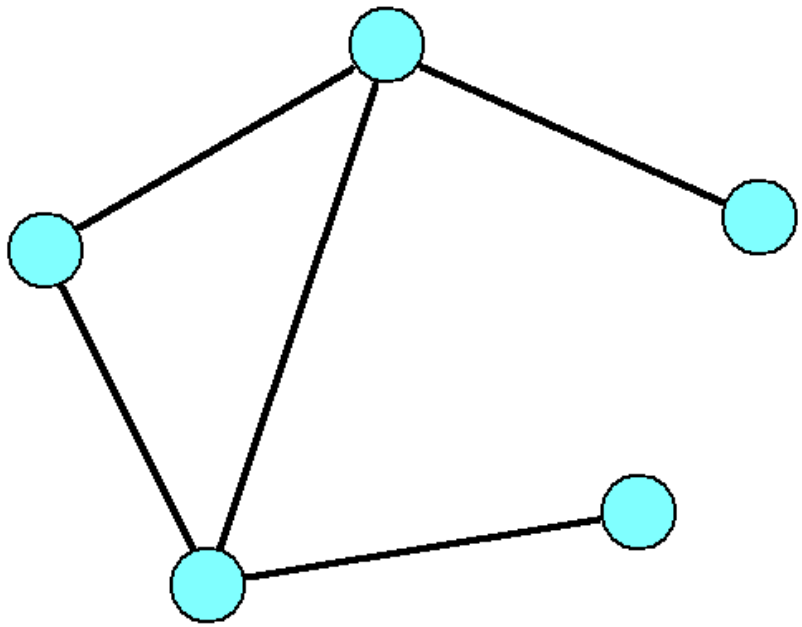
Biological networks within one cell (gene regulatory networks, protein-protein interaction networks, aka proteomes) are quite different from non-biological ones, e.g., $\gamma \in (1, 2)$. The central force of evolution is the duplication of the information in the genome.

Kim et al. (Phys. Rev. E, 2002)
Pastor-Satorras et al. (J. Theor. Biol., 2003)
Chung et al. (J. Comp. Biol., 2003)

Start from a set of connected vertices and at each time step

- select one vertex of the graph at random and duplicate: add a new vertex and connect it to the neighbors of the selected vertex;
- delete the new edges independently, with probability δ;
- connect the new vertex to each old one independently, with probability α/n; merge multiple edges.

Pastor-Satorras et al. model



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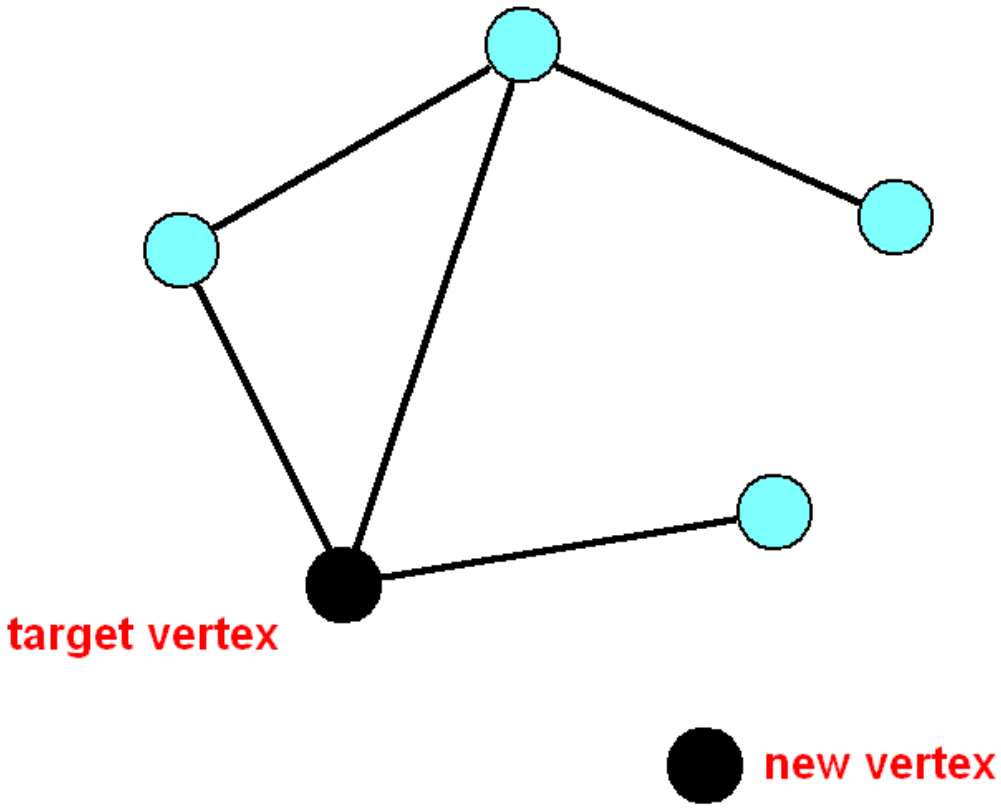

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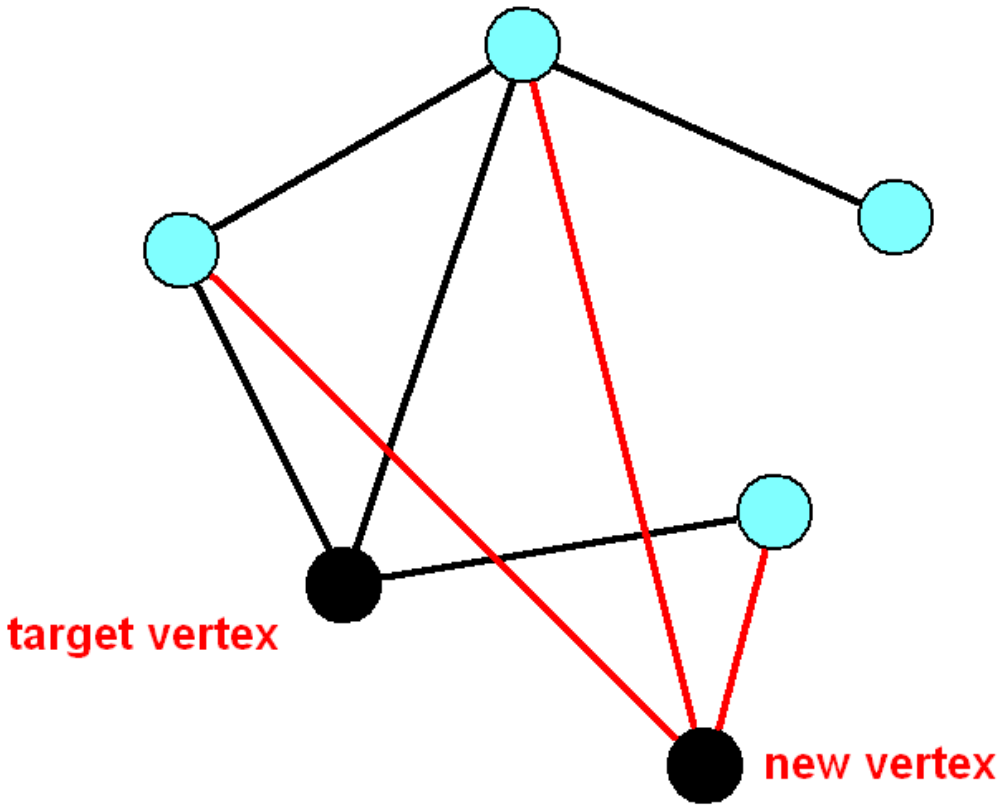

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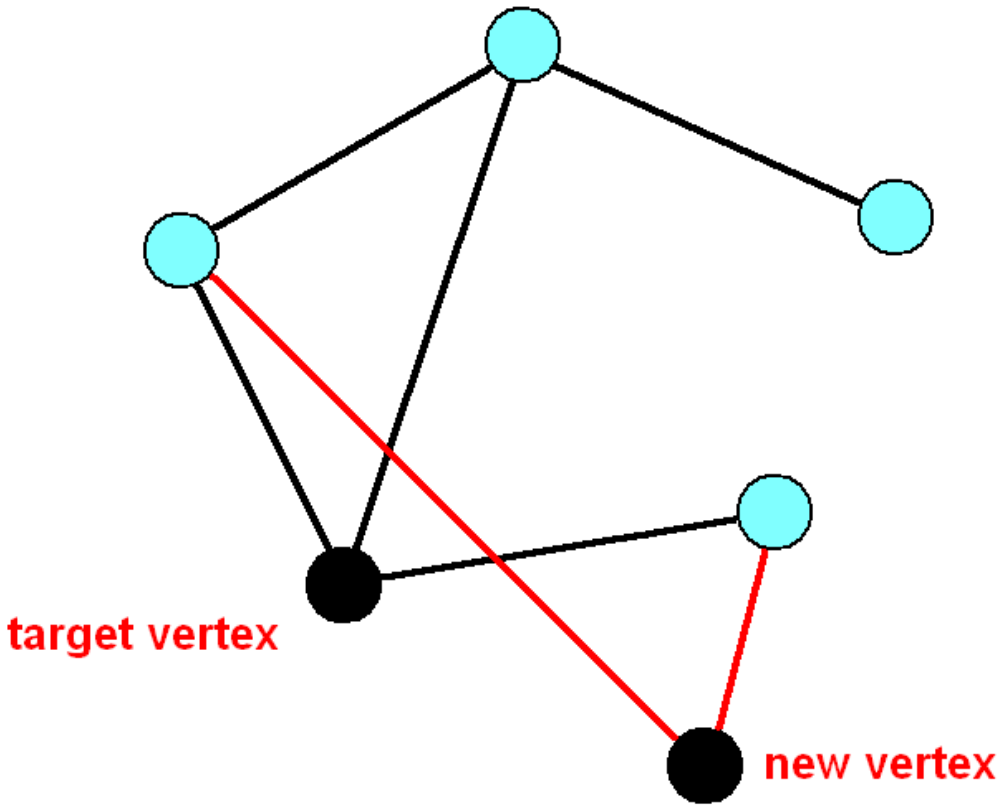

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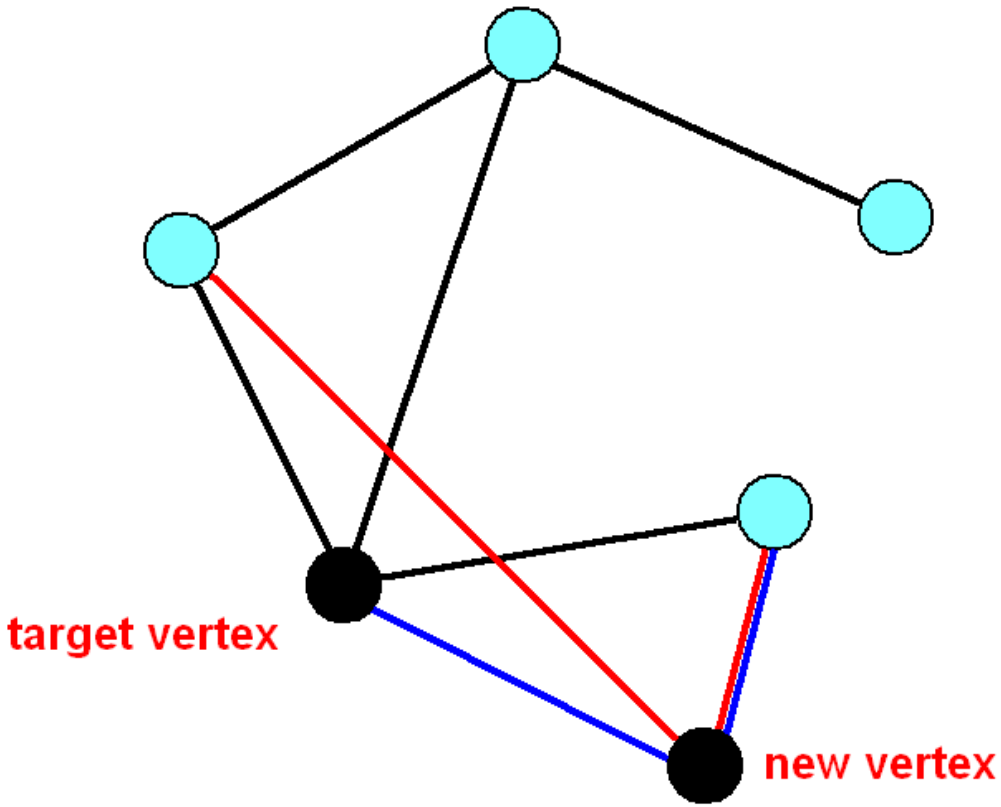

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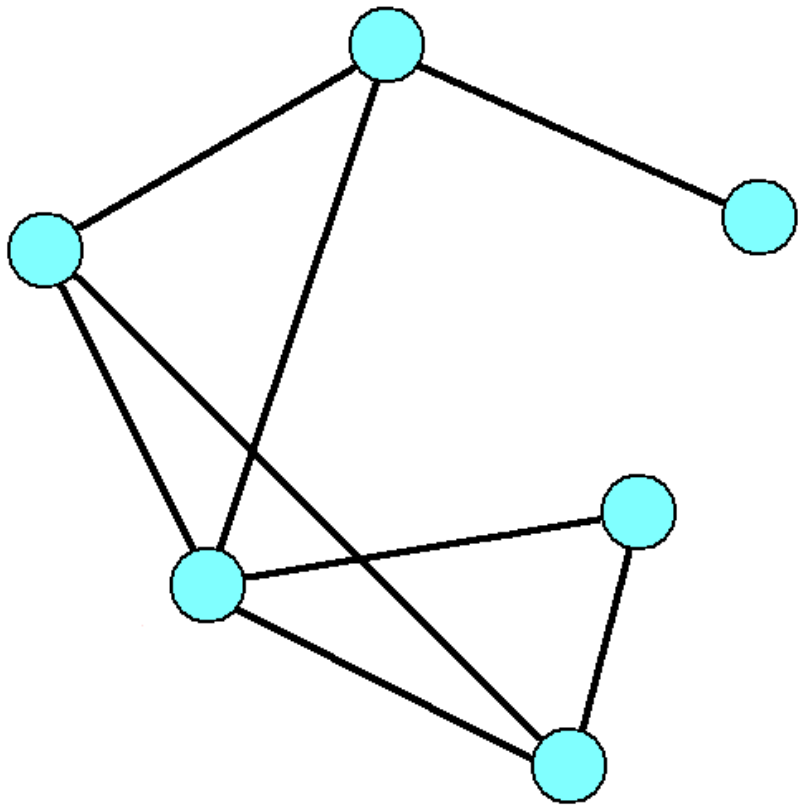

Pastor-Satorras et al. model

Results claimed

- The mean degree distribution is a power law with exponential cut-off, that is, $c_d \sim K\, d^{-\gamma} e^{-\lambda d}$ (Pastor-Satorras et al.)

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Modification: an extra step at the end of each turn. The new vertex is given a fixed number of additional edges, uniformly at random, so as to avoid singletons.

Then the expected number of degree d vertices, divided by n, converges, and the limits decrease polynomially (still a bit sketchy).

One more model with duplication and deletion

Inspired by these models we consider the following one.

Model 1

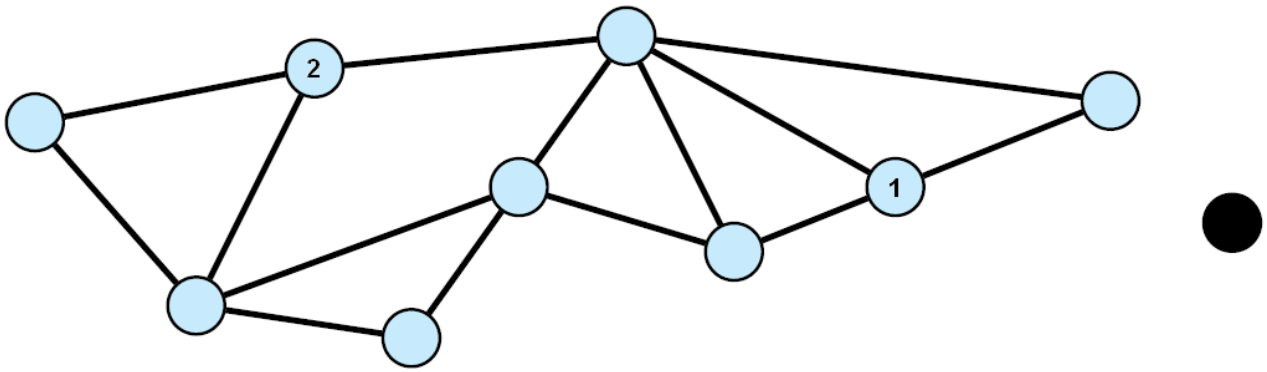
Start from a single vertex. The graph evolves in discrete time steps. At every step choose two (not necessarily different) vertices independently, uniformly at random.

- Duplication phase. Add a new vertex and connect it *to the first selected vertex* and to all of its neighbours.
- Deletion phase. Delete all *old* edges of the second selected vertex.

A kind of coagulation-fragmentation model. The presence of deletion causes intense fluctuation in the model's behavior, and makes it harder to access.

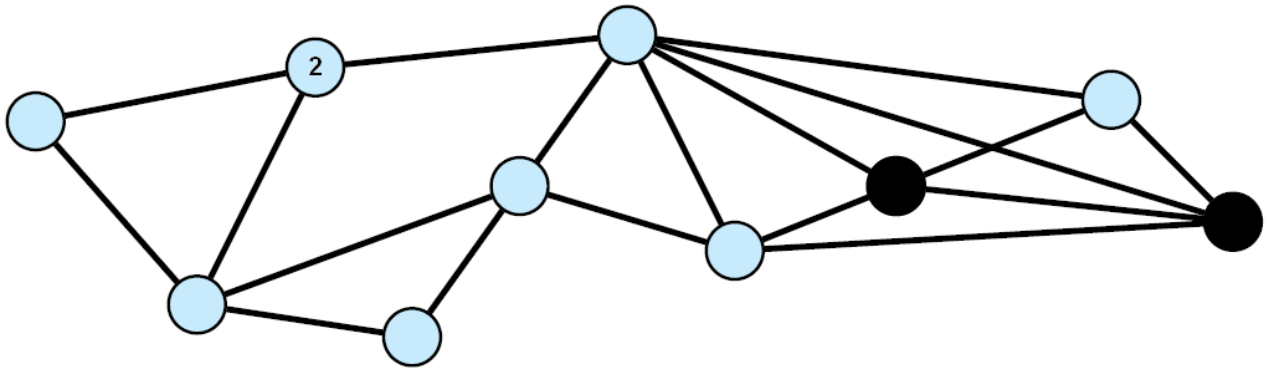
We do not claim that this model is biologically relevant.

One more model with duplication and deletion



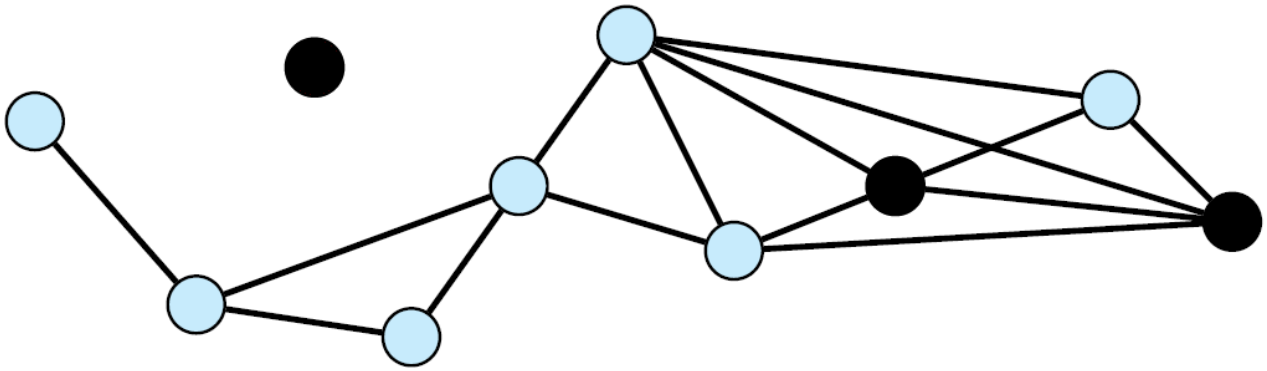
A new vertex is added (in black)

One more model with duplication and deletion



Duplication phase

One more model with duplication and deletion



Deletion phase

Properties

Linear growth

The number of vertices after step n is $n+1$, and the mean number of edges is equal to n — just like in a tree. However, in a recursive tree the individual degrees are increasing to infinity, while here they are regularly cut back to 0 due to deletion. In fact, individual degrees remain stochastically bounded, hence

- $\Rightarrow$ the asymptotic degree distribution (if exists) must have lighter tail;
- $\Rightarrow$ the maxdegree is of smaller order than any power of n;
- $\Rightarrow$ scale free property cannot be expected.

Asymptotic degree distribution

Theorem (Asymptotic degree distribution)

Let $X[n,d]$ denote the number of degree d vertices after step n. Then

$$\lim_{n\to\infty} \frac{X[n,d]}{n+1} = c_d, \quad d = 0, 1, \ldots,$$

with probability 1, where (c_d) is a sequence of positive numbers satisfying

$$c_0 = \frac{1+c_1}{3}; \quad c_d = \frac{(d+1)(c_{d-1}+c_{d+1})}{2d+3} \quad (d \geq 1);$$

$$c_0 + c_1 + \cdots = 1.$$

Not a recursion.

Method

A slight modification of the original model makes the analysis easier.

Model 2

The only point where Model 2 differs from Model 1 is that in the deletion phase the selected vertex loses *all of its edges* without any exceptions. That is, the new edges are protected in the erasure part of the same step in Model 1, but they might be deleted immediately in Model 2.

In Model 2, all connected components of the graph are cliques (including singletons). The number of d-cliques does not vary so vehemently as the number of degree d vertices: the fluctuation is bounded by 2.

Coupling

How to transfer the limit result from Model 2 to Model 1?

Coupling

We develop the two models simultaneously. The selected vertices are the same in both models. We color some of the edges and vertices of Model 1 red.

Edge coloring

- In the deletion phase, if a newborn edge is deleted in Model 2, color it red in Model 1.
- In the duplication phase, copies of red edges are also red in Model 1.
- All other edges are born to be black.

In this way, the edges in Model 1 are either black or red. The black subgraph is a realization of Model 2.

Coupling

Vertex coloring

- In the duplication phase, the new vertex becomes red if and only if the duplicated vertex is red.
- In the deletion phase, whenever an edge becomes red, color both endpoints red.
- If a red vertex is chosen to be deleted, and it loses all of its edges, color it back to black.

Black vertices can only have black edges, hence they have the same degree in both models. It is sufficient to show that the number of red vertices is $o(n)$. In fact, it is $o\left(n^{1/2+\varepsilon}\right)$.

A useful lemma

Lemma (simplified version)

Let $(\mathcal{F}_n)$ be a filtration, (ξ_n) a nonnegative adapted process. Suppose that

$$\mathbb{E}\big((\xi_n - \xi_{n-1})^2 \mid \mathcal{F}_{n-1}\big) = O\Big(n^{1-\delta}\Big)$$

holds with some $\delta > 0$. Let (u_n), (v_n) be nonnegative predictable processes such that $u_n < n$ for all $n \geq 1$.

(*a*) Suppose that $\mathbb{E}(\xi_n \mid \mathcal{F}_{n-1}) \leq \Big(1 - \dfrac{u_n}{n}\Big)\xi_{n-1} + v_n$, and $\lim_{n\to\infty} u_n = u$, $\limsup_{n\to\infty} v_n \leq v$ with some random variables $u > 0$, $v \geq 0$. Then

$$\limsup_{n\to\infty} \frac{\xi_n}{n} \leq \frac{v}{u+1} \quad \text{a.s.}$$

A useful lemma

Lemma (continued)

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$$\liminf_{n\to\infty} \frac{\xi_n}{n} \geq \frac{v}{u+1} \quad a.s.$$

Explicit form of the limits

Let $G(z)$ denote the generating function of the sequence (c_d), then

$$(1-z)^2 G'(z) = (3-2z)G(z) - 1, \quad G(0) = c_0.$$

This o.d.e can be solved.

$$G(z) = \frac{1}{(1-z)^2} \exp\Big(\frac{z}{1-z}\Big) \int_0^{1-z} \exp\Big(1 - \frac{1}{x}\Big)\, dx.$$

After some variable transformation we can expand it into Taylor series.

Theorem

$$c_d = (d+1) \int_0^{\infty} \frac{y^d e^{-y}}{(1+y)^{d+2}}\, dy, \quad d = 0, 1, \ldots .$$

Asymptotics

$$c_d = (d+1)\int_0^\infty \frac{y^d e^{-y}}{(1+y)^{d+2}}\, dy$$

In order to approximate the integral we first analyse the behavior of the integrand around the point where it attains its maximum. Second order Taylor approximation to the logarithm of the integrand turns the integral into a Gaussian one.

Theorem

$$c_d \sim (e\pi)^{1/2}\, d^{1/4}\, e^{-2\sqrt{d}}, \quad \text{as } d \to \infty.$$

Stretched exponential decay.

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