

# ERGM Algorithms

Peng Wang

# Simulation: Technical details

Using the *Metropolis algorithm*:

- random starting graph on fixed number of nodes
- many iterations (e.g. 1,000,000)
- sample every 1000th graph (for example)

The algorithm sets up a Markov Chain on the space of all possible nondirected networks that has  $\Pr(\mathbf{X}=\mathbf{x})$  as its stationary distribution

- at each step, we consider changing the value of the  $(i,j)$  tie (from 1 to 0 or 0 to 1) for a randomly selected pair (and relation):  $\mathbf{x} \rightarrow \mathbf{x}'_{ij}$
- the change is made with probability

$$\min[1, \exp(\{\sum_Q \lambda_Q (z_Q(\mathbf{x}'_{ij}) - z_Q(\mathbf{x}))\})]$$

# Simulation: Intuitively

Fixed number of nodes; fixed parameter values

1. Start from a random graph
2. For each step, propose to change one edge at a time
  - If the probability of the graph increases, make the change
  - If the probability decreases, don't make the change (EXCEPT SOMETIMES – this makes it a proper statistical distribution)
3. Throw away the early iterations so the starting graph has no effect on the distribution – “burn-in”
4. Sample as many graphs as needed
5. Stop after a suitable number of iterations

# MCMC: important points

- To draw a distribution of graphs we have to rely on iteratively generating graphs using a random walk
- You have to make sure
  - Process has forgotten about the past (burn-in)
  - Chain is “moving freely”
- The “multiplication factor” controls this
  - Large  $\rightarrow$  more iterations for exploring
  - Large  $\rightarrow$  more iterations means longer time

# Exercise: Illustrate burn-in

Use PNet to simulate a Bernoulli distribution of non-directed 50 node graphs

Edge parameter =  $-2$

Take 1,000 samples from a simulation of run of 100,000.

Set the *burn-in* to be zero

Do the simulation twice

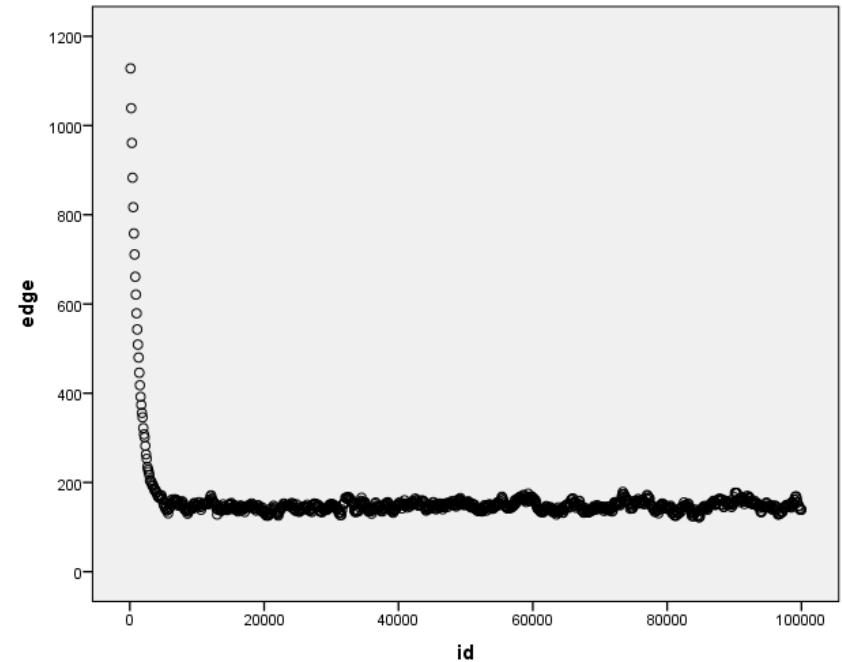
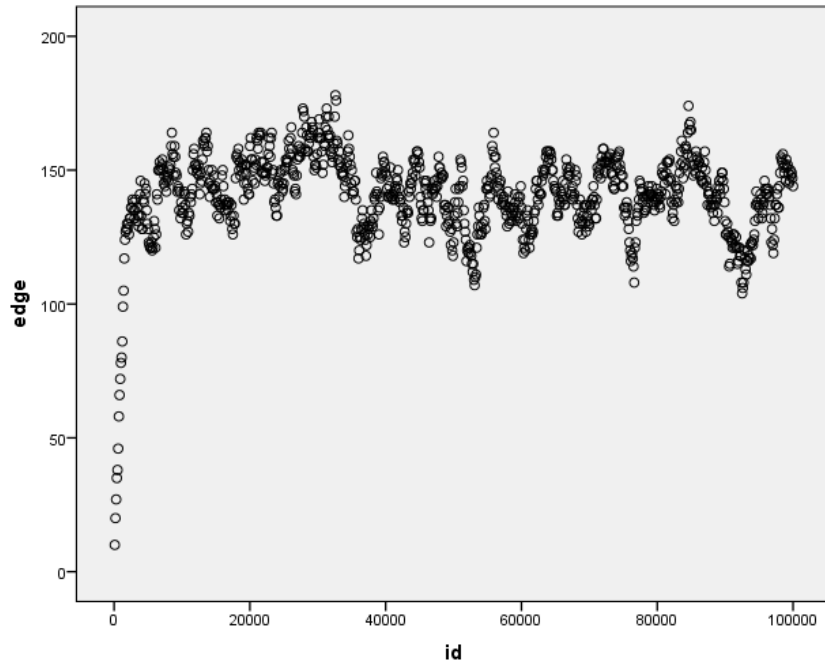
1. Starting density = 0 (empty graph)

2. Starting density = 1 (complete graph)

The *simulation\_(session name).txt* file contains the number of edges of each sampled graph against the simulation number (ID). Draw a scatterplot for each simulation.

Notice how each distribution ends up in the same way (same mean number of edges), although starting from a different graph.

# Burn-in



Start simulation from empty or complete graph, end up in same place.  
Remove the first few simulations that depend on the starting point – *burn-in*

# Exercise: Markov vs Social circuit

(Chapter 13.1.1, Lusher et al, 2013)

- ❑ 30 nodes;
- ❑ Undirected graph
- ❑ **fix density** 0.10;
- ❑ burnin 100,000;
- ❑ Number of iterations 1,000,000
- ❑ Number of samples 1,000

# Exercise: Markov vs Social circuit

(Chapter 13.1.1, Lusher et al, 2013)

## 1. Run three simulations with Markov triangle parameter

- ☐ Triangle = 0.5
- ☐ Triangle = 1.0
- ☐ Triangle = 1.5

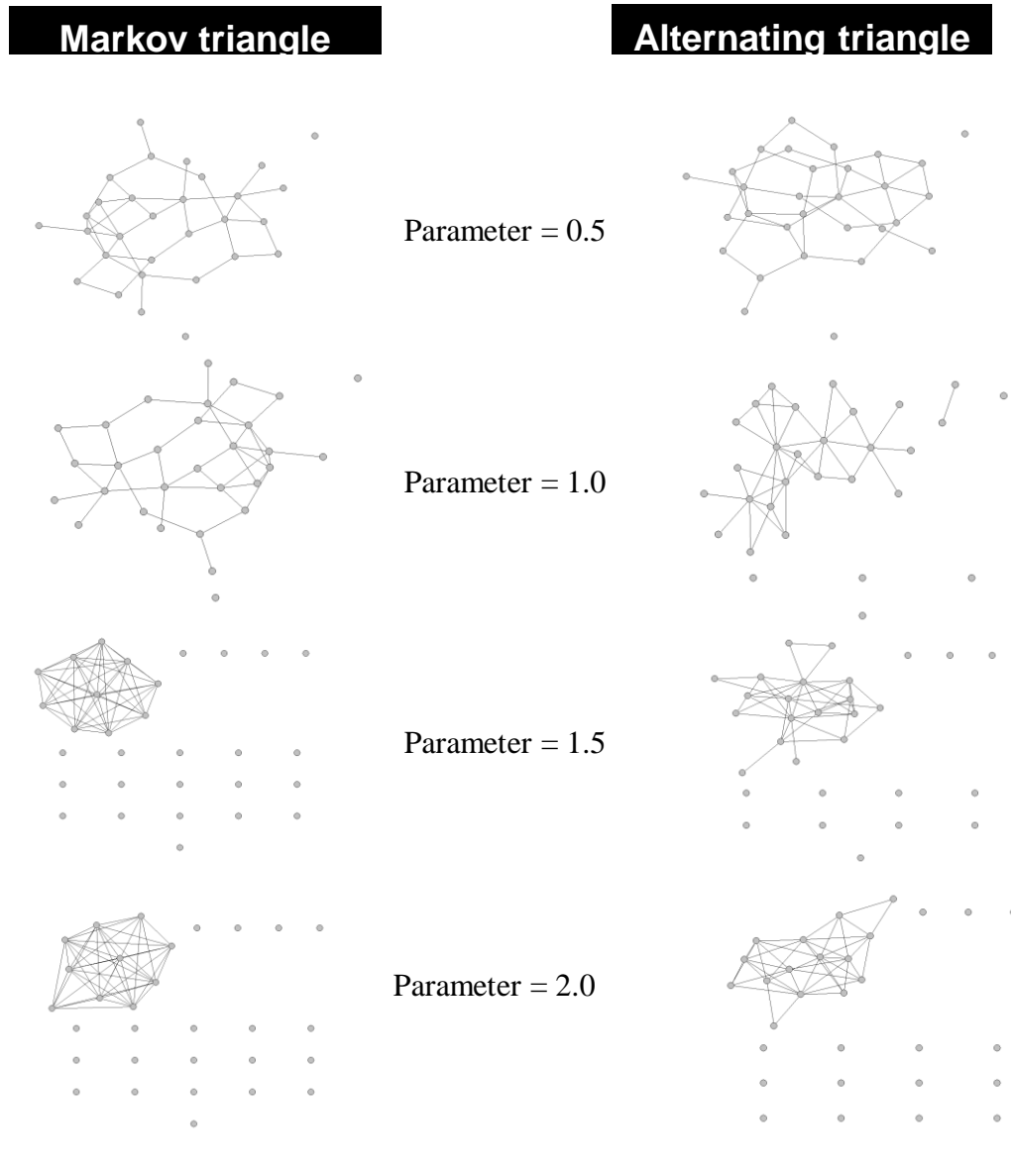
In each case, draw the final graph. Note a sudden jump to a full clique as the triangle parameter increases

## 2. To compare, run three simulations with alt. triangle parameter ( $\lambda = 2$ )

- ☐ AT = 0.5
- ☐ AT = 1.0
- ☐ AT = 1.5



# Figure 13.2, Lusher et al



## Exercise: Positive and negative stars parameters (Chapter 13.1.2, Lusher et al, 2013)

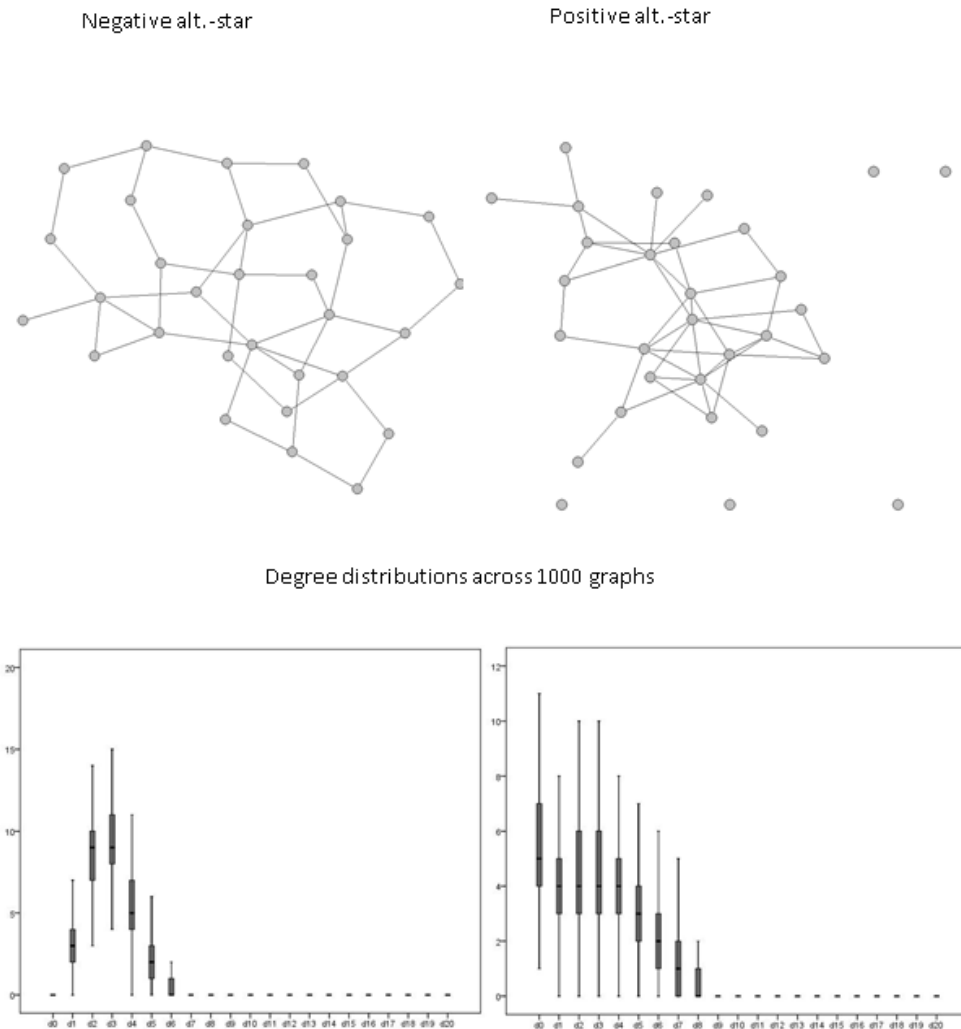
### 1. Run two simulations with only alternating star parameters ( $\lambda = 2$ )

☐ AS = - 1.0

☐ AS = + 1.0

In each case, draw the final graph. Note that the positive star parameter graph is more centralized with some higher degree nodes. The negative star graph has degrees more evenly spread among nodes.

# Figure 13.5, Lusher et al (2013)

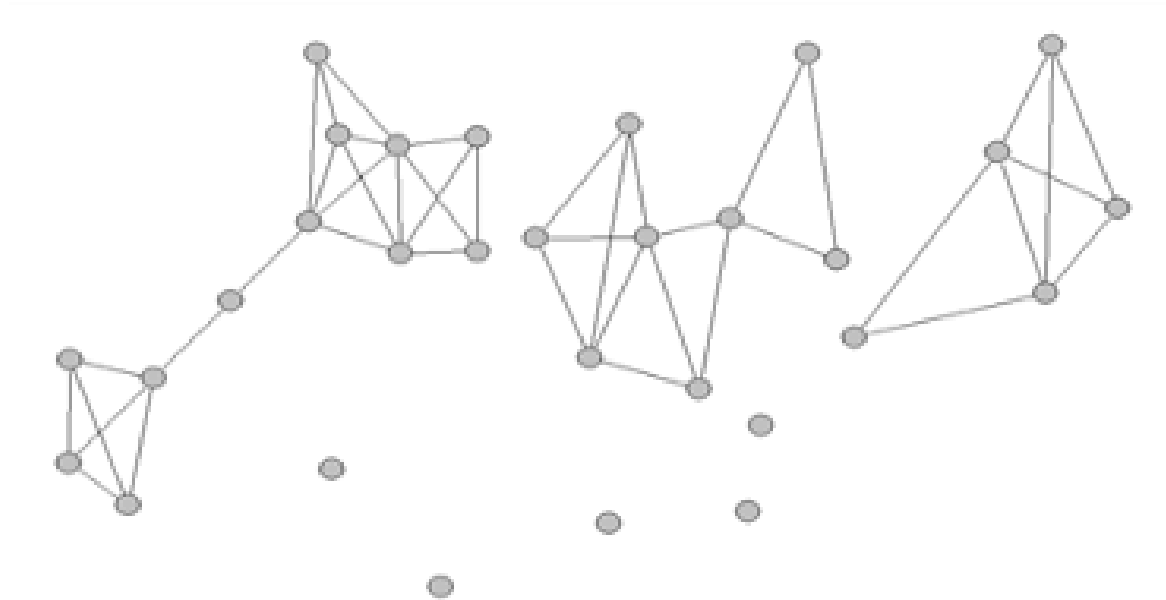


# Exercise: Star and triangle parameters together

(Chapter 13.1.3, Lusher et al, 2013)

1. Run a simulation with alternating star and triangle parameters together ( $\lambda = 2$ )
  - ☐ AS = - 1.0
  - ☐ AT = + 2.0

Figure 13.7, Lusher et al

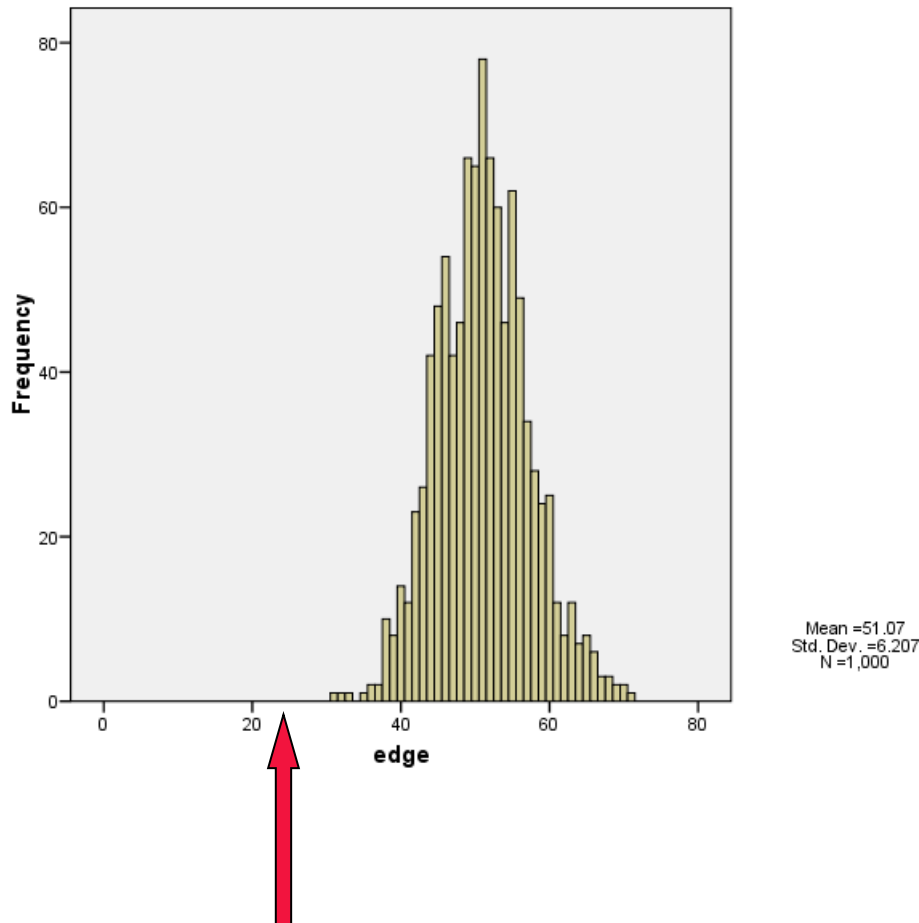


# Markov Chain Monte Carlo Maximum Likelihood Estimation (MCMCMLE)

Simulation of a distribution of random graphs from a starting set of parameter values, and subsequent refinement of the parameter values by comparing the distribution of graphs against the observed graph, with this process repeated until the parameter estimates stabilize. (**convergence**)

# Fit a Bernoulli model to a network

## First guess at parameter : $\theta = -1$



Suppose the observed graph  
on 20 nodes has 23 edges

Simulate distribution using  $\theta = -1$

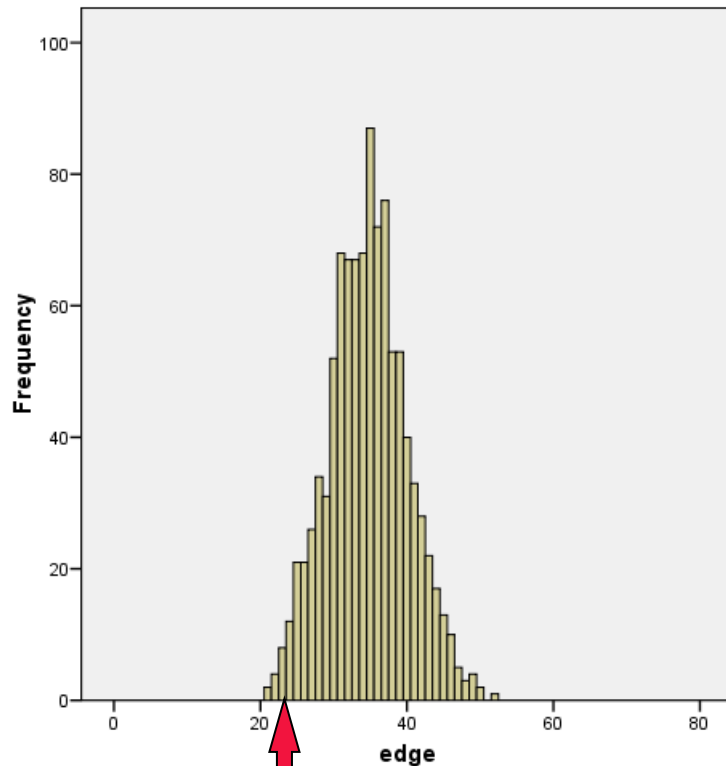
t-value for observed graph  
=  $-4.52$

**ADJUST PARAMETER GUESS**

Observed graph is OFF THE SCALE!!  $\theta = -1$  is not a good estimate

# Fit a Bernoulli model to a network

## Second guess at parameter : $\theta = -1.5$



Mean = 34.69  
Std. Dev. = 5.337  
N = 1,000

t-value for observed graph  
= - 2.19

**Still not good!**

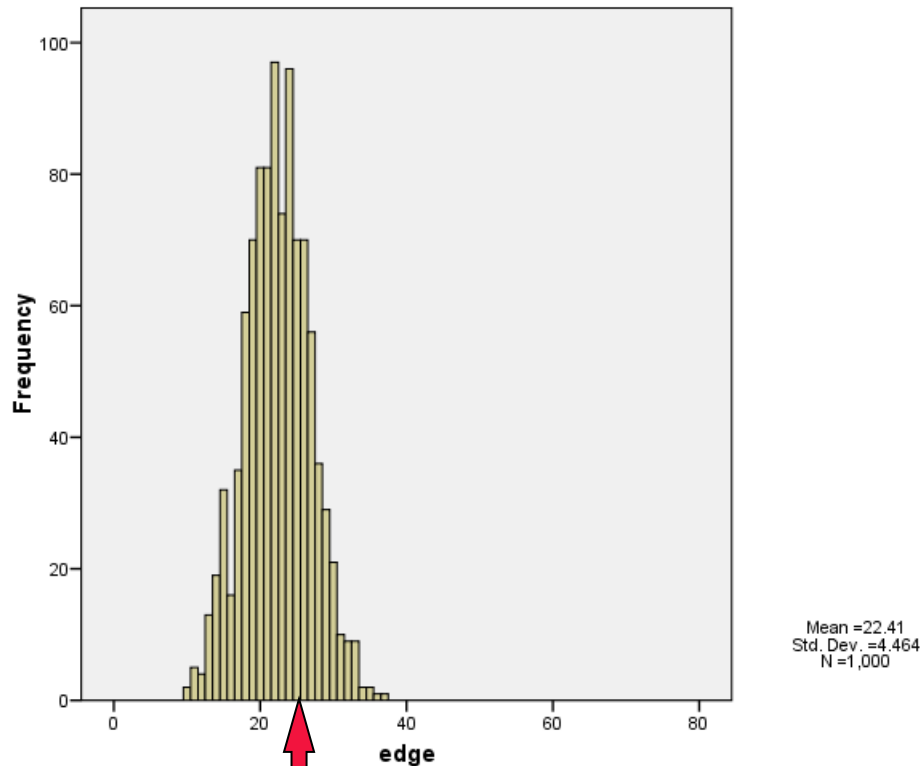
**ADJUST PARAMETER GUESS**

Observed graph



# Fit a Bernoulli model to a network

## Third guess at parameter : $\theta = -2$



Observed graph

t-value for observed graph  
= + 0.13

**A pretty good result!**  
 **$\theta = -2$  is a plausible estimate for  
this observed graph**

If the estimation can find such a good result for  
ALL parameters simultaneously, the model  
**converges**

# MCMCMLE - “Method of moments”

Snijders (2002): **Polyak-Ruppert variant of the Robbins-Monro procedure to solve the moment equation  $E_{\lambda}\{z(X)\} = z(x)$  for  $\lambda$ :**

- **Phase 1:** estimate a diagonal matrix  $D_0$  to be used in Phase 2:

$D_0 = \text{diag}(d_{kk})$  where  $d_{kk} = \partial E_{\lambda} z_k(X) / \partial \lambda_k$  evaluated at initial value of  $\lambda$

- **Phase 2:** Over several subphases:
  - generate network statistics according to current estimate  $\lambda^{*(n)}$  of  $\lambda$  at step  $n$
  - use update step  $\lambda^{*(n+1)} = \lambda^{*(n)} - \alpha_n D_0^{-1} z(X_n)$ , where  $X_n$  are generated from  $P_{\lambda}(X)$  for  $\lambda = \lambda^{*(n)}$ , gain sequence  $\alpha_n = n^{-c}$ , for  $.5 < c < 1.0$
  - at end of subphase, set new  $\lambda^{*(n+1)}$  as average value over subphase
- **Phase 3:** estimate the covariance matrix of the estimator as the inverse of the covariance matrix of statistics (and check convergence)

## More intuitively - “Method of moments” as implemented in PNET

- **Phase 1:** Essentially gets the process started to reach some very rough and ready parameter “guesses”
- **Phase 2:** Several subphases:
  - In each subphase we simulate from the current parameter estimates and take a sample of graphs. The size of the simulation is determined by the “Multiplication factor”.
  - Check the observed graph against the simulation
  - Change the parameter estimate multiple times within each subphase – for every subphase, the size of the changes permitted get smaller and smaller – hopefully more and more precise (the “Gaining factor”)
  - Stop at the end of the specified number of subphases
- **Phase 3:** Simulates from the final parameter estimates, checks convergence and estimates standard error.

# Main aim of ML- “Method of moments”

□ Find those parameter values such that

$$E_{\hat{q}}\{z(X)\} = z(x_{obs})$$

...as we have  
observed

We get the same  
number of  
configurations (in  
expectation)

NOTE: CONVERGENCE IS NOT GUARANTEED!!

- So:
  - If hard to get convergence, try with bigger multiplication factor (longer simulations mean more of the possible graph space covered, but of course it takes longer)
  - If close to convergence, can use a smaller gaining factor (already quite precise)
  - Results differ slightly from run to run – this is a stochastic algorithm

MPNet-comms

File

Number of nodes:  
A: 30  
B: 0

☐ Simulation ☒ Estimation ☐ GOF ☐ Bayesian estimation

☐ Attribute file:  Browse...

Model specification

A B X (two-mode) A X B

☒ Include ☐ Directed ☐ Fixed ☐ Fix density Starting density: 0.000

Network file: Pete\datafiles\corporation\comm\_undirected.txt Browse...

☐ Structural zero file:  Browse...

☐ Missing indicators:  Browse...

Select parameters...

Attribute/Dyadic covariates

<input type="checkbox"/> Binary:	0	Attribute file:	<input type="text"/>	Browse...	Select...
<input type="checkbox"/> Continuous:	0	Attribute file:	<input type="text"/>	Browse...	Select...
<input checked="" type="checkbox"/> Categorical:	1	Attribute file:	D:\My Documents\	Browse...	Select...
<input type="checkbox"/> Dyadic:	0	Attribute file:	<input type="text"/>	Browse...	Select...

Simulation/GOF Estimation

Subphases: 5

Gaining factor: 0.010

Multiplication factor: 10

Iterations in phase 3: 500

Max. estimation runs: 1

☐ Do GOF at convergence 500

☐ Generate GCD at convergence

Bayesian estimation options

Maximum lag (SACF): 1

☒ Scaled identity matrix

☐ Combined simulation

☐ Nonconditional simulation

☐ Covariance file:  Browse...

Update Start

Ready

# The important part of the PNet output

effects	estimates	stderr	t-ratio
edge	-3.219886	0.69602	-0.07846 *
2-star	0.196034	0.26175	-0.06178
3-star	-0.200038	0.12604	-0.04406
Triangle	1.886621	0.27807	-0.05492 *

Asterisk indicates  
absolute value of  
estimate more than  
twice standard error

Parameter estimate  
(strength of effect:  
positive usually means  
more of the  
configurations are  
observed; negative  
means fewer)

Standard error  
(If the value of the  
parameter estimate is  
more than twice the  
standard error, the  
parameter is significant)

Convergence statistic  
(If this value is less than  
0.1, then there is good  
evidence that the  
estimation has converged.  
You can increase this for a  
very large network.)

# What happens if I can't get convergence statistics less than 0.1?

Click the “update” button on pnet

This updates the starting parameter values to those you last estimated.

Run it again.

If the model is well-behaved, you should eventually get convergence.

If you still have troubles, try increasing the “Multiplication factor”.

**Badly behaved models will not converge!!**

You then need to specify the model in a different way.

The screenshot shows the 'Estimation' tab of the pnet software interface. The 'Simulation/GOF' tab is also visible. The 'Multiplication factor' is set to 10, which is circled in red. Other settings include 'Subphases: 5', 'Gaining factor: 0.010', 'Iterations in phase 3: 500', 'Max. estimation runs: 1', 'Do GOF at convergence: 500', and 'Generate GCD at convergence'. Under 'Bayesian estimation options', 'Maximum lag (SACF): 1' is set, and 'Scaled identity matrix' is selected. The 'Update' button is circled in red at the bottom left, and the 'Start' button is at the bottom right.



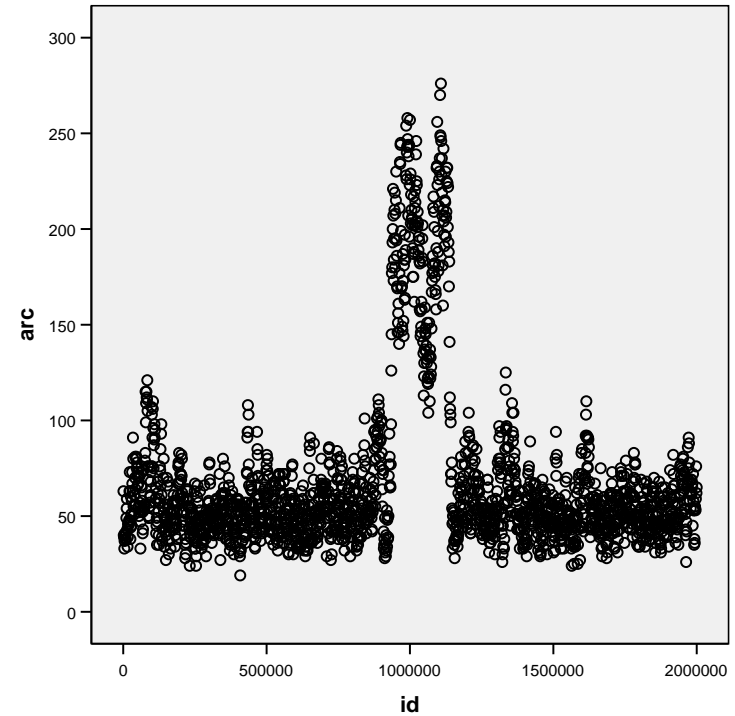
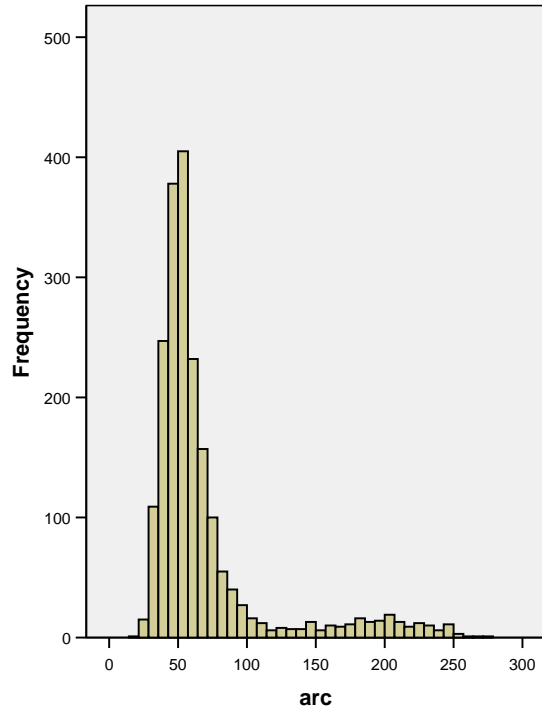
# What happens if I can't get convergence statistics less than 0.1?

If it looks like you have converged parameter estimates – congratulations!

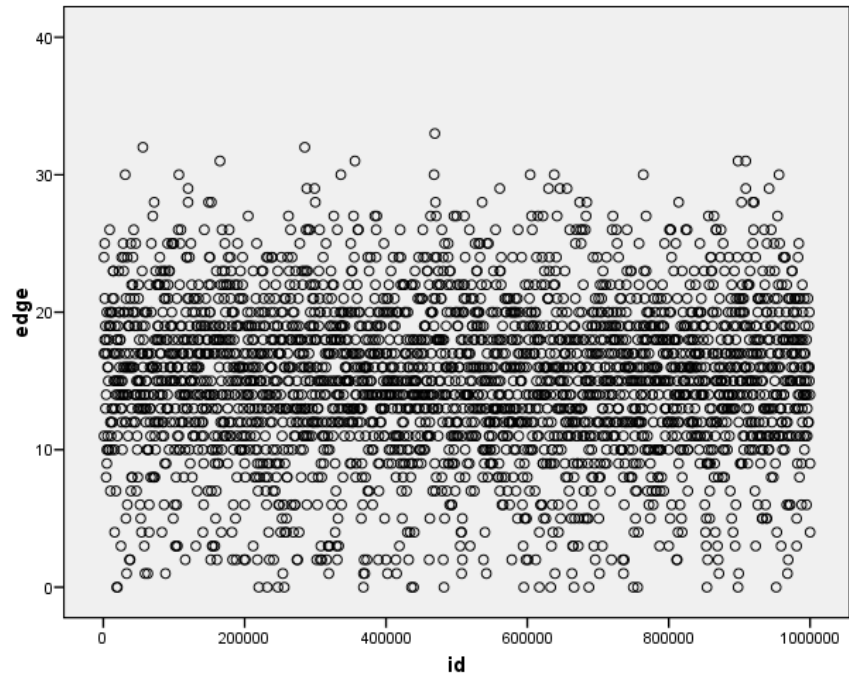
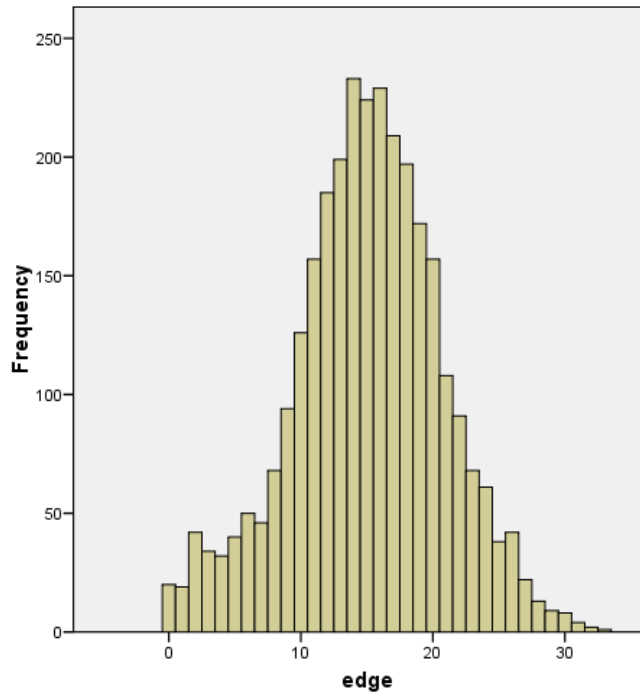
BUT you can't be entirely sure – good to do a long simulation using your good looking estimates.

Sometimes a long simulation run reveals two (or more) REGIONS of graphs

This is called a “near degenerate” model, and is NOT GOOD



What we DON'T want to see:  
the model exhibits two regions!  
This would indicate a bad model.



What we DO want to see:  
the model exhibits only one region for all parameters  
This suggests a well-behaved model.