Coarse-graining the dynamics of (and on) evolving graphs:

Algorithms and Computation.

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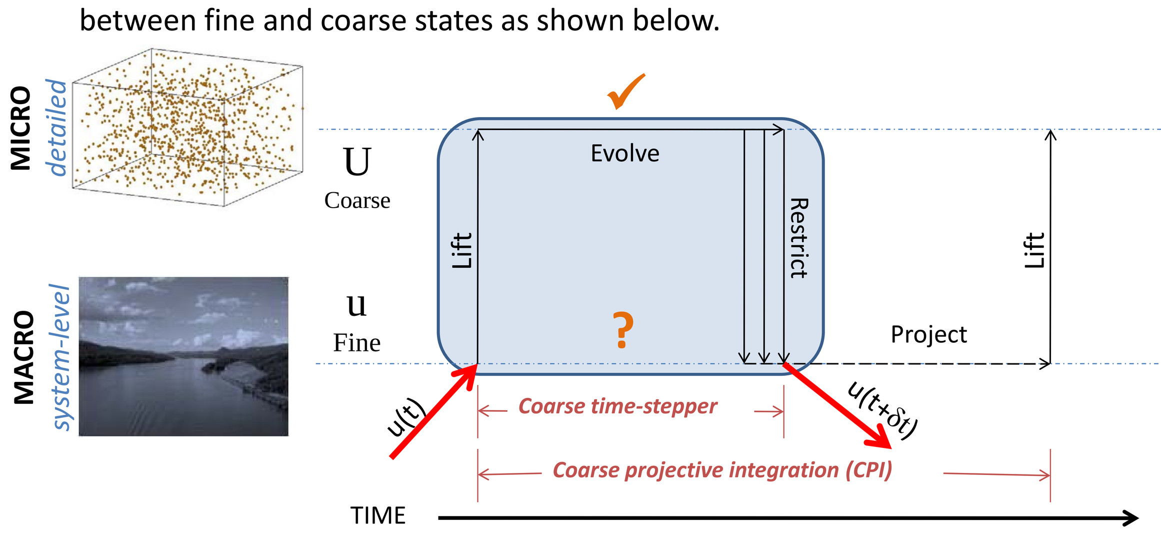
Dynamical models and coarse-graining

Dynamical models of networks

- Usually presented in terms of nodes and edges (i.e., using ***detailed***, "microscopic" rules of evolution).
- Macroscopic "system-level" description is usually NOT available
- OBJECTIVE: Find coarse models (macroscopic descriptions) for the evolutionary network problems.

Equation-free modeling for coarse-graining multi-scale systems

- The key step is to define suitable *coarse* variables (observables); e.g., the network degree distribution.
- Then, *lifting* and *restriction* operators are constructed to translate between fine and coarse states as shown below.



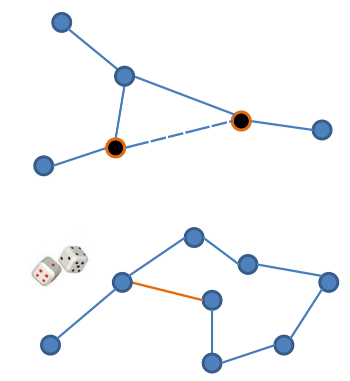
- This is a "coarse time-stepper", which ACTS AS A SUBSTITUTE FOR UNAVAILABLE MACROSCOPIC EQUATIONS.
- A primary focus is on the identification of "suitable" coarse variables.

A simple example: random evolution of networks

A random evolution model of networks

Dynamics at each time step:

- Choose 2 random nodes and connect them if not already connected
- Remove an edge with probability '*p*'

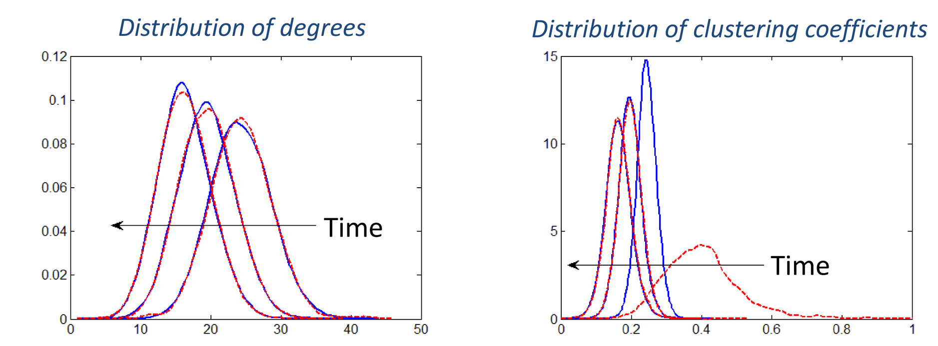


Simulations

- 100 networks with 100 nodes each
- p = 0.9
- Degree distribution evolves smoothly
- But, do we need other statistics (*like triangles*) to predict this evolution?

Direct simulation with the same degree distribution

but two different distributions of clustering coefficients



- Blue curves : initial graph was an Erdos-Renyi random graph
- Red curves : initial graph was created using the Havel-Hakimi algorithm to match the degree distribution of the previous case

*To explain this **slaving of triangles**, some tools from the theory of convergent graph sequences will be used.*

Limits of dense graph sequences

L. Lovász and B. Szegedy, J. Comb. Theory Ser. B 96, 933 (2006)

- **Definition:** homomorphism density of F onto G

  t(F,G) = probability that a random mapping from ("small" test subgraph) F to ("big" graph) G, V(F) → V(G)) is a homomorphism
- Consider a graph, G, in '*n*' vertices and a test subgraph, F, in '*k*' vertices

$$t(F,G) := \frac{1}{n^k} \sum_{\varphi:[k]\to[n]} \mathbb{1}\left[\forall\, i,j \in [k] \,:\, F(i,j) = G(\varphi(i),\varphi(j))\right]$$

- Now, consider a sequence of graph $\{G_n\}$ in n vertices $\lim_{n\to\infty} t(F,G_n) = \ ?$
- If the limit exists, the graph sequence is said to be 'convergent'
- In the limit of number of nodes going to infinity, the limit object of G_n is a graphon *W(x,y)* on which *homomorphism densities* of small *test subgraphs* F can be found using:

$$\lim_{n\to\infty} t(F,G_n) = t(F,W) = \int_0^1 \dots \int_0^1 \prod_{1\le i<j\le k} W(x_i,x_j)^{F(i,j)}\, \mathrm{d}x_1 \dots \mathrm{d}x_n.$$

Results for our example using these concepts:

As, t →∞, convergence rate for

$$\frac{\mathrm{d}}{\mathrm{d}t} W_t(x,y) = 1 - \boxed{\left(1 + \frac{p}{\rho(t)}\right)} W_t(x,y)$$

Graphon ~ 1/(1-p)

10 for p = 0.9

cherry

$$t(\text{cherry}, W_t) = \int_0^1\int_0^1\int_0^1 W_t(x,y)W_t(y,z)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z$$

$$\frac{\mathrm{d}}{\mathrm{d}t} t(\text{cherry}, W_t) = 2\rho(t) - \boxed{2\left(1 + \frac{p}{\rho(t)}\right)} t(\text{cherry}, W_t)$$

Cherry density ~ 2/(1-p)

20 for p = 0.9

K_3

$$t(K_3, W_t) = \int_0^1\int_0^1\int_0^1 W_t(x,y)W_t(y,z)W_t(z,x)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z$$

$$\frac{\mathrm{d}}{\mathrm{d}t} t(K_3, W_t) = 3\ t(\text{cherry}, W_t) - \boxed{3\left(1 + \frac{p}{\rho(t)}\right)} t(K_3, W_t)$$

Triangle density ~ 3/(1-p)

30 for p = 0.9

Additional results and coarse-graining

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = (1-p) - \rho(t)$$

Edge density
Convergence rate = 1

Decoupled from other quantities

$$\frac{\mathrm{d}}{\mathrm{d}t}\bar{D}(t) = 1 - \boxed{\left(1 + \frac{p}{\rho(t)}\right)} \bar{D}(t)$$

*(Mean of) Normed degree**
Convergence rate (as t →∞) = 1/(1-p)

Does not depend on higher order information (like triangles)

Equations for the degree distribution

**Normed degree = (degree/number of nodes)*

$$\mathrm{d}D(t) = \left(1 - D(t) - p\frac{D(t)}{\rho(t)}\right)\mathrm{d}t + \sqrt{1 - D(t) + p\frac{D(t)}{\rho(t)}} \cdot n^{-1/2}\mathrm{d}W_t$$

SDE for the normed degree of the nodes

$$X(t) := n^{1/2}(D(t) - \bar{D}(t))$$ (definition)

$$\frac{\partial}{\partial t}P(t,x) = \frac{1}{1-p}\frac{\partial}{\partial y}(x \cdot P(t,x)) + p\frac{\partial^2}{\partial x^2}P(t,x)$$

P – probability density function of *X*

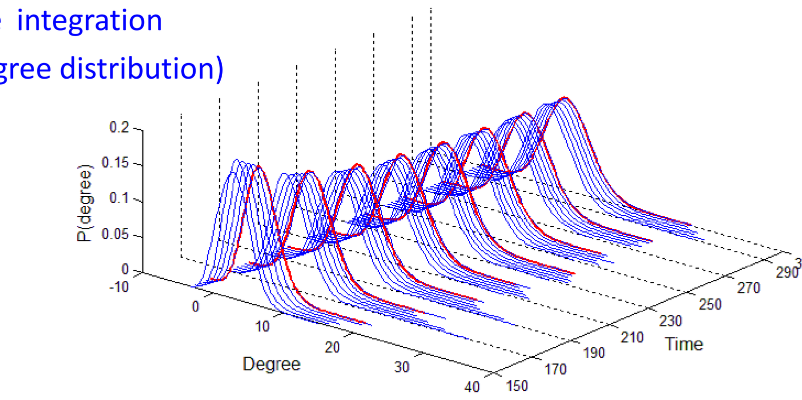
Eigenvalues	$\lambda = 0$	$\lambda = -\frac{1}{1-p}$	$\lambda = -\frac{2}{1-p}$
Eigenfunctions	$\exp\left(-\frac{1}{2}\frac{x^2}{p(1-p)}\right)$	$\exp\left(-\frac{1}{2}\frac{x^2}{p(1-p)}\right).x$	$\exp\left(-\frac{1}{2}\frac{x^2}{p(1-p)}\right).(p(1-p)-x^2)$

Coarse graining using (discretized) degree distribution as the coarse variable

Blue - Coarse projective integration (using just the degree distribution)

Red - Direct simulation (detailed model)

Heal 150;
Evolve 10;
Project 10



Kuramoto model on a static network

Synchronization of coupled oscillators on a network

- General coupled oscillator model

$$\dot{\theta}_i = \omega_i + F(\theta_{\forall j\neq i} - \theta_i).$$

- Phases, θ_i of oscillators
- Heterogeneous frequencies, ω_i
- Kuramoto model on a network:

$$\frac{d\theta_i}{dt} = \omega_i + K\sum_j A_{ij}\sin(\theta_j - \theta_i).$$

- A is the adjacency matrix of the network; A_{ij} is 1 if there is a link between nodes *i* and *j*.
- K is the coupling strength
- Networks constructed to facilitate separation of timescales

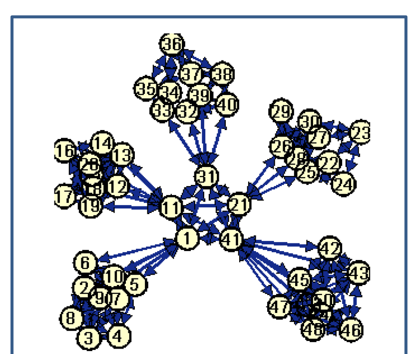


Figure: Sample 5 x 10 network
5 communities with 10 members each

Heterogeneous communities
Watts-Strogatz model
(Varying average degrees, Varying rewiring probabilities)

Leaders are connected by a complete network

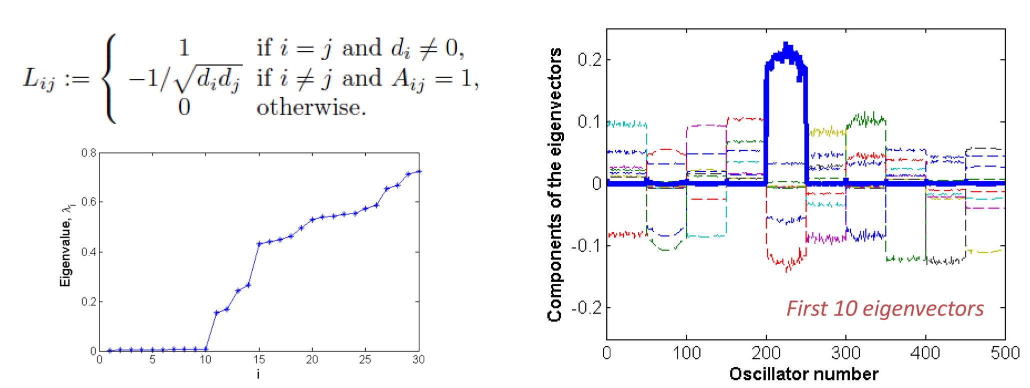
Define: Order parameter (r) as a measure of synchronization

$$r = \left\|\frac{1}{N}\sum_{j=1}^{N} e^{i\theta_j}\right\|.$$

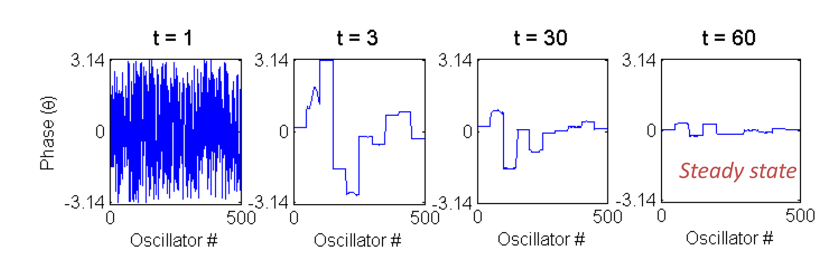
Using the Graph Laplacian

Define: Normalized graph Laplacian *L* of the network (A)

$$L_{ij} := \begin{cases} 1 & \text{if } i = j \text{ and } d_i \neq 0, \\ -1/\sqrt{d_i d_j} & \text{if } i \neq j \text{ and } A_{ij} = 1, \\ 0 & \text{otherwise.} \end{cases}$$



500 oscillators
10 x 50 network
K = 0.5
w ~ N(0,1/15)



$\Theta_j = e^{i\theta_j}$ Complex phase

$L\mathbf{v}_j = \lambda_j\mathbf{v}_j$ Laplacian eigenbasis, $\{v_j\}$

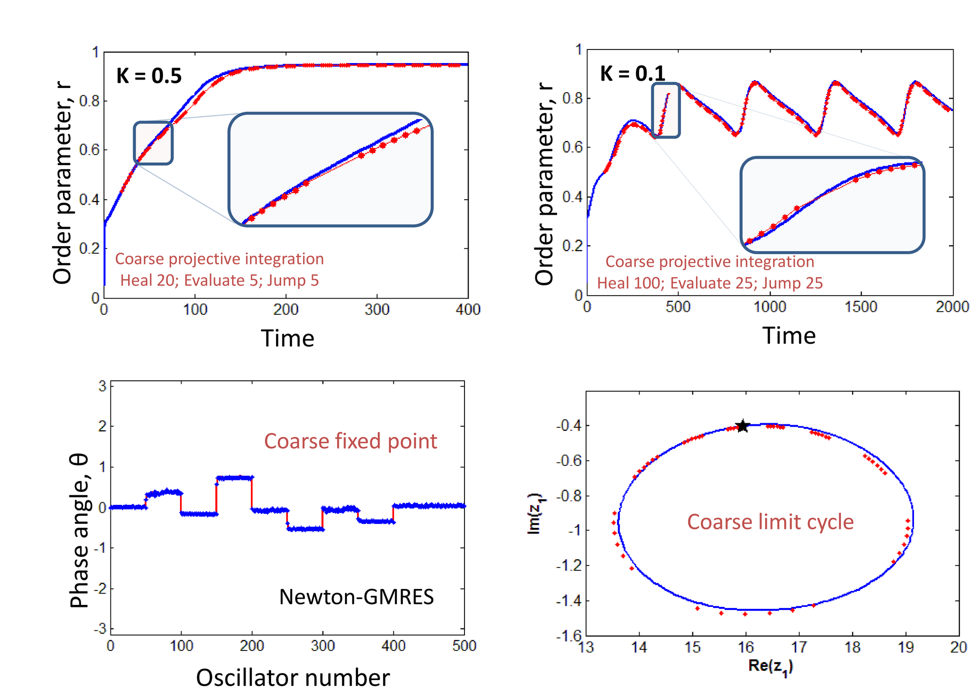
$z_{j\in[1,m]} = \mathbf{v}_j^T\Theta$ Projection onto Laplacian eigenbasis

Coarse variables, z_j

Coarse integration, coarse fixed points

Blue – From direct simulations; Red – From coarse model

500 Phases → 10 Projection coefficients; **50 % Simulation, 50% Projection**



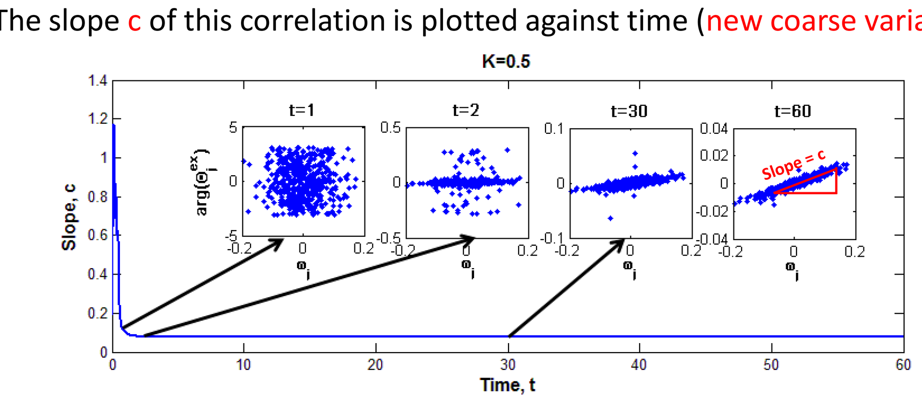
Heterogeneity and the coarse-grained model

$\Theta_j = e^{i\theta_j}$ Complex phase

$L\mathbf{v}_j = \lambda_j\mathbf{v}_j$ Laplacian eigenbasis, $\{v_j\}$

$\Theta^{ex} = \Theta - \sum_{j=1}^{m}\mathbf{v}_j^T\Theta\mathbf{v}_j$ DEFINE: Excess phase

- Correlations develop between this "excess" phase and the heterogeneity (intrinsic oscillator frequency).
- The slope c of this correlation is plotted against time (new coarse variable)



Coarse model

STEP 1:
Accounting for correlation
Coarse variable, c

$\tilde{\Theta}_j = e^{i(\theta_j - c\omega_j)}$

(Corrected phase angles)

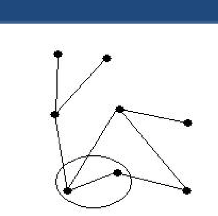
STEP 2:
Projection onto Laplacian eigenbasis
Coarse variable, z_j

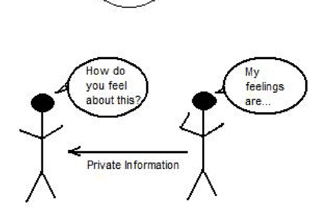
$z_{j\in[1,m]} = \mathbf{v}_j^T\tilde{\Theta}$

Opinion propagation on a static network

Every person has an emotional state, x ∈ [-1,1]

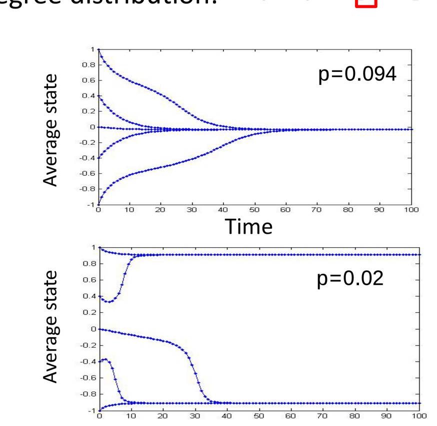
In the absence of information	$x(t) = x(0)\cdot\exp(-\gamma t)$
Arrival of public information	$x(t) = x(t) + \varepsilon^{\pm}$
Arrival of private information	$x(t) = x(t) + e^{\pm}$

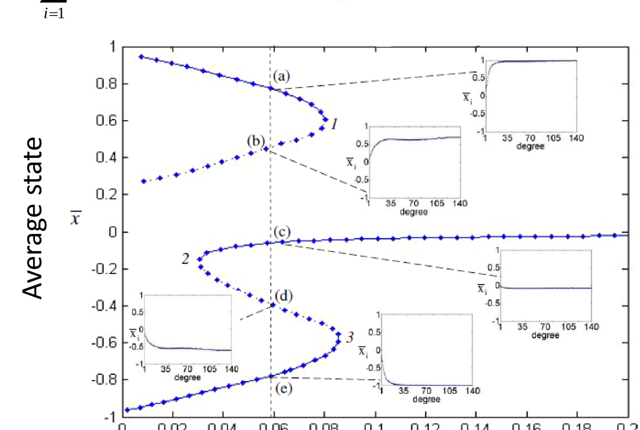




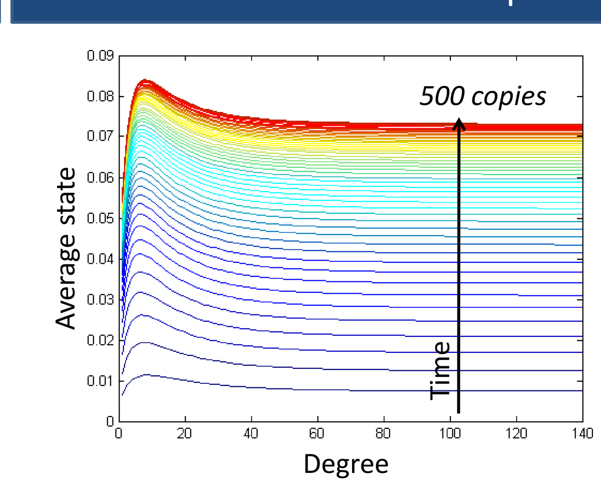
Social network provides the private information

Degree distribution: $y = y(k;p) = p(1-p)^k \Big/ \sum_{i=1}^{\max Deg} p(1-p)^i$





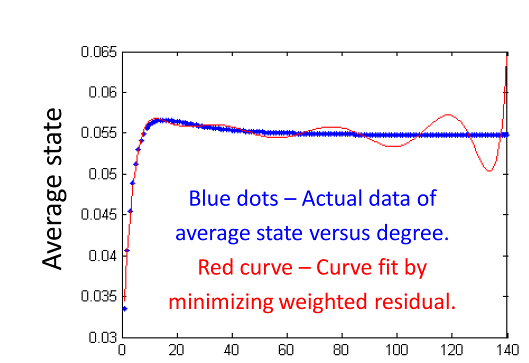
Development of correlations

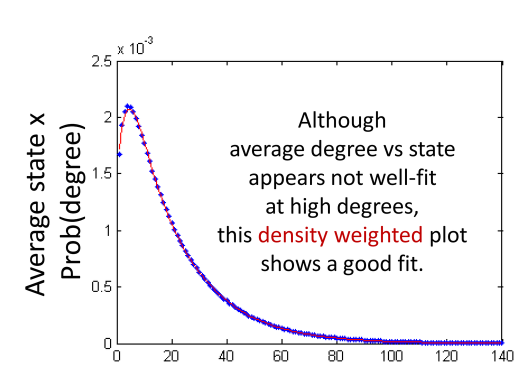


- Geometric degree distribution
- p = 0.5 (Truncated at 140)

Coarse variables: Average state as a function of degree.

We should weigh this function according to the relative density of nodes in different degree classes.





Polynomial chaos

D. Xiu and G. E. Karniadakis, SIAM Journal on Scientific Computing 24, 619 (2002).

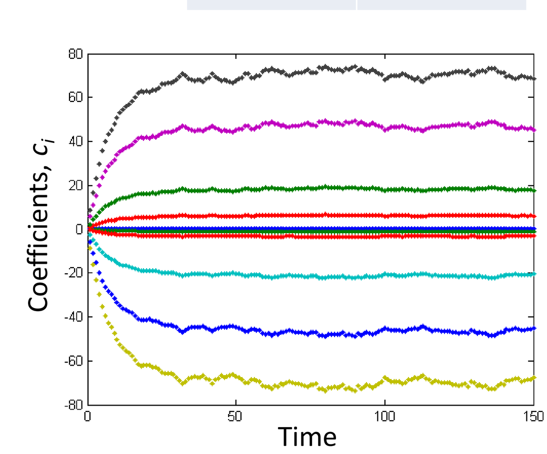
- In UQ, uncertainty parameters have an associated probability distribution.
- Here, DEGREES have an associated probability distribution.
- IDEA: Represent the solution to the problem *(state as a function of degree)* with the help of orthogonal polynomial basis functions i.e., polynomials that are orthogonal with respect to w(d)

  $< p_i , p_j >_{w(d)} = \delta_{ij}$

Distribution	Orthogonal polynomial
Gaussian	Hermite
Poisson	Charlier
Gamma	Laguerre
Binomial	Krawtchouk

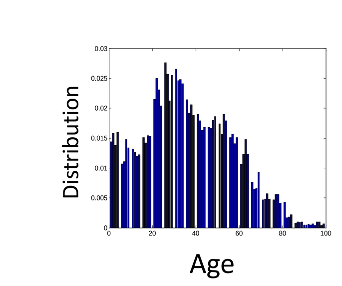
- The coefficients can then be found as: $c_i = < p_i , f >_{w(d)}$
- Appropriate orthogonal polynomials using the Wiener-Askey scheme for some distributions (weight functions) are shown in the table (right).

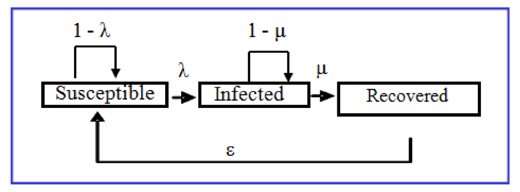
The evolution of the function *f(d)* now becomes the evolution of the coefficients, c_i.
These coefficients are our coarse variables.

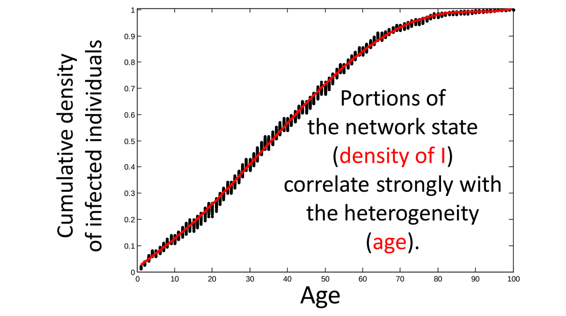


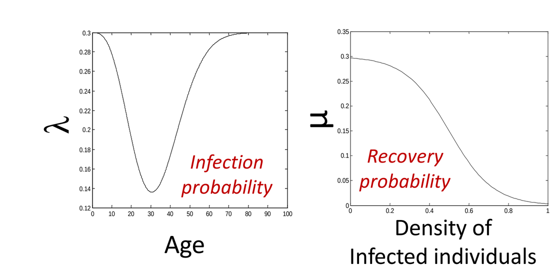
One more illustration: SIR on a *heterogeneous* social network

- N = 10,000 individuals
- Regular random graph (fixed degree)
- Age distribution from empirical distribution
- States: *S – Susceptible; I – Infected; R – Recovered*
- Transition Probabilities :
- λ : Infection (S to I) (depends on age)
- μ : Recovery (I to R) (depends on density of I)
- ε : R to S









Again, state is written as a function of heterogeneity, in terms of basis functions *inspired by the heterogeneity distribution*

EQUATION-FREE AND VARIABLE FREE MODELING FOR COMPLEX/MULTISCALE SYSTEMS: Coarse-grained computation in science and engineering using fine-grained models; R.R.Coifman, Yale, co-PI