Pseudo-Differential Relaxation Equations and Semi-Markov Processes

Enrico Scalas

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CTRWs

Let $\{J_i\}_{i=1}^{\infty}$ be a sequence of i.i.d. positive random variables with the meaning of waiting times between events. Let $N(t)$ be the corresponding renewal counting process and $\{X_i\}_{i=1}^{\infty}$ a sequence of i.i.d. random variables. Define

$$X(t) = \sum_{i=1}^{N(t)} X_i$$

Then the density $f_{X(t)}(x,t)dx = \mathbb{P}(X(t) \in dx | X(0) = 0)$ obeys the following equation (1):

$$\int_0^t dt' \, \Phi(t - t') \frac{\partial f_{X(t)}(x, t')}{\partial t'} = -p(x,t) + \int_{-\infty}^{+\infty} dx' \, f_X(x - x') f_{X(t)}(x', t')$$

where (using Laplace transforms)

$$\mathcal{L}(\Phi(t))(s) = \frac{\mathcal{L}(\bar{F}_J(t))(s)}{\mathcal{L}(f_J(t))(s)}$$

and $\bar{F}_J(t) = 1 - F_J(t)$.

Two-state Markov chain I

A clear and simple relation between relaxation and semi-Markov processes is in (2). Consider a two-state system existing in states A and B. Assume that state A is transient and state B absorbing. The deterministic embedded chain has the following transition probabilities $q_{A,A} = 0$, $q_{A,B} = 1$, $q_{B,A} = 0$, and $q_{B,B} = 1$. This means that if the system is prepared in state A, it will jump to state B at the first step and it will stay there forever. Suppose that the inter-event time J is random and follows an exponential distribution with rate $\lambda = 1$ for the sake of simplicity. Let $Y(t)$ denote the state of the time-changed chain at time t, then

$$p_{i,j}(t) = \mathbb{P}(Y(t) = j | Y(0) = i) = \bar{F}_J(t)\delta_{i,j} + \sum_{n=1}^{\infty} q_{i,j}^{(n)} \mathbb{P}(N(t) = n).$$

Then $p_{A,A}(t) = \overline{F}_J(t) = \exp(-t)$: the probability of finding the system in the initial state decays exponentially towards zero.

Two-state Markov chain II

The relaxation function $\exp(-t)$ is the solution of

$$\frac{d}{dt} p_{A,A}(t) = -p_{A,A}(t), \;\; p_{A,A}(0) = 1.$$

The response function is defined as $\xi_D(t) = -dp_{A,A}(t)/dt$ and its Laplace transform is $1/(1+s)$. For $s = -i\omega$ this is the Debye model (2). If inter-event times follow the Mittag-Leffler distribution, we get $p_{A,A}(t) = \overline{F}_J(t) = E_\beta(-t^\beta)$. This is the solution of (3)

$$\frac{d^\beta}{dt^\beta} p_{A,A}(t) = -p_{A,A}(t), \;\; p_{A,A}(0) = 1.$$

In this case, the Laplace transform of the response function $\xi_{CC}(t) = -dp_{A,A}(t)/dt$ is $1/(1+s^\beta)$ and for $s = -i\omega$, we get the Cole-Cole model (2). For a general renewal time change $N(t)$ one gets

$$\int_0^t dt' \, \Phi(t-t') \frac{dp_{A,A}(t')}{dt'} = -p_{A,A}(t), \;\; p_{A,A}(0) = 1.$$

Meerschaert and Toaldo

Meerschaert and Toaldo in (4) consider non-local abstract Cauchy problems on Banach and Hilbert spaces of the form introduced above

$$\Phi_t q(t) = Aq(t), \;\; q(0) = u.$$

as well as related time-changed processes as in the previous examples.
Our recent examples belong to this class of problems. We are interested in applications.

- Can we find explicit expressions for cumulative distribution function, etc. of the time-changed processes?
- How this is related to the solution of relaxation problems?
- Is numerical work possible?
- What can we say on mixing and stability of time-changed processes?

Statistics

Let $\{X_i\}_{i=1}^n$ be a sequence of n independent and identically distributed positive random variables with cumulative distribution function $F_{X_1}(u) = \mathbb{P}(X_1 \leq u)$. A *statistic* is a function from $\mathbb{R}^n$ to $\mathbb{R}$ that summarizes some characteristic behavior of the random variables:

$$S_n = G_n(X_1, \ldots X_n).$$

Examples:

1. $S_n^{(1)} = \sum_{i=1}^n X_i$;
2. $S_n^{(2)} = \max\{X_1, \ldots, X_n\}$;
3. $S_n^{(3)} = \prod_{i=1}^n X_i$.

Renewal process

Introduce another set of positive independent and identically distributed random variables (independent from the X_is) $\{J_i\}_{i=1}^{\infty}$ with the meaning of sojourn times. Let $F_J(t) = \mathbb{P}(J \leq t)$ denote the cumulative distribution function of the J_is and $f_J(t) = dF_J(t)/dt$ denote their probability density function. The epochs at which events occur are

$$T_n = \sum_{i=1}^{n} J_i,$$

and the counting process $N(t)$ giving the number of events that occur up to time t is

$$N(t) = \max\{n : \; T_n \leq t\}.$$

Continuous-time statistics

The continuous-time statistic $S(t)$ corresponding to S_n is

$$S(t) = S_{N(t)} = G_{N(t)}(X_1, \dots, X_{N(t)}).$$

Examples:

1. $S^{(1)}_{N(t)} = \sum_{i=1}^{N(t)} X_i$;
2. $S^{(2)}_{N(t)} = \max\{X_1, \dots, X_{N(t)}\}$;
3. $S^{(3)}_{N(t)} = \prod_{i=1}^{N(t)} X_i$.

Convolution-type statistics-1

To connect continuous-time statistics and relaxation equations, consider a special class of statistics of *convolution* type (as in the examples above). Denote these statistics with the following symbol

$$S_n = \bigoplus_{i=1}^{n} X_i.$$

Further assume the existence of a linear transform $\mathcal{L}_{\bigoplus}$ such that

$$\mathcal{L}_{\bigoplus}(F_{S_n}(u))(w) = [\mathcal{L}_{\bigoplus}(F_{X_1}(u))(w)]^n.$$

Now consider a continuous-time statistic of convolution time

$$S(t) = S_{N(t)} = \bigoplus_{i=1}^{N(t)} X_i,$$

and compute its cumulative distribution function.

Convolution-type statistics-2

One has

$$F_{S(t)}(u) = \mathbb{P}(S(t) \leq u) = \sum_{n=0}^{\infty} F_{S_n}(u)\mathbb{P}(N(t) = n).$$

Let $Q(w,s)$ denote the Laplace-$\mathcal{L}_{\bigoplus}$ transform of $F_{S(t)}(u)$

$$Q(w,s) = \mathcal{L}\mathcal{L}_{\bigoplus}(F_{S(t)}(u))(w,s).$$

Under suitable conditions, one gets

$$Q(w,s) = \mathcal{L}(\bar{F}_J(t))(s)\frac{1}{1 - \mathcal{L}(f_J(t))(s)\mathcal{L}_{\bigoplus}(F_{X_1}(u))(w)},$$

where $\bar{F}_J(t) = 1 - F_J(t)$ is the complementary cumulative distribution function of the time intervals $\{J_i\}_{i=1}^{\infty}$.

Anomalous relaxation and convolution-type statistics

Following Mainardi *et al.* (1), Meerschaert and Toaldo (4), Georgiou *et al.* (5), the above Laplace transform can be inverted to get

$$\mathcal{Q}(w,t) = \mathcal{L}_{\bigoplus}(F_{S(t)}(u))(w) = \mathcal{L}^{-1}(Q(w,s))(t),$$

the solution of the Cauchy problem ($\mathcal{Q}(w,t=0)=1$) for the following pseudo-differential relaxation equation

$$\int_0^t \Phi(t-t') \frac{\partial \mathcal{Q}(w,t')}{\partial t'}\, dt' = -[1-\mathcal{L}_{\bigoplus}(F_{X_1}(u))(w))]\mathcal{Q}(w,t),$$

where

$$\mathcal{L}(\Phi(t))(s) = \frac{\mathcal{L}(\bar{F}_J(t))(s)}{\mathcal{L}(f_J(t))(s)}.$$

A simple example-1

Consider the continuous-time sum statistic

$$S^{(1)}(t) = \sum_{i=1}^{N(t)} X_i.$$

where $N(t)$ is the Poisson process.
In this case, $\bigoplus$ is the usual convolution and the operator $\mathcal{L}_{\bigoplus}$ coincides with the usual Laplace transform $\mathcal{L}$. As the J_is are exponentially distributed, one can see that the kernel $\Phi(t)$ in the relaxation equation coincides with Dirac's delta $\delta(t)$.

A simple example-2

As $\Phi(t) = \delta(t)$, one gets an ordinary relaxation equation

$$\frac{\partial \mathcal{Q}^{(1)}(w,t)}{\partial t} = -(1 - \mathcal{L}(F_{X_1}(u))(w))\mathcal{Q}^{(1)}(w,t).$$

The solution of the Cauchy problem for the above relaxation equation is

$$\mathcal{Q}^{(1)}(w,t) = \exp(-(1 - \mathcal{L}(F_{X_1}(u))(w))t)$$

leading to (rate $\lambda = 1$)

$$F_{S^{(1)}(t)}(u) = \exp(-t) \sum_{n=0}^{\infty} F_{X_1}^{\star n}(u) \frac{t^n}{n!},$$

where $F_{X_1}^{\star n}(u)$ denotes the n-fold convolution and $F_{X_1}^{\star 0}(u) = \theta(u)$.

A non-trivial example-1

Take the maximum continuous-time statistic

$$S^{(2)}_{N(t)} = \max\{X_1, \dots, X_{N(t)}\}.$$

Assume that sojourn times J_i are independent and identically positive random variables following a Mittag-Leffler distribution; in other words, the cumulative distribution function of J_1 is given by

$$F_{J_1}(t) = 1 - E_\alpha(-t^\alpha), \quad (2.1)$$

where

$$E_\alpha(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(n\alpha + 1)}$$

with $\alpha \in (0, 1)$.

A non-trivial example-2

In this case, $\bigoplus$ is the usual product and the operator $\mathcal{L}_{\bigoplus}$ is the identity. The kernel is

$$\Phi(t) = \frac{t^{-\alpha}}{\Gamma(1-\alpha)},$$

and the non-local relaxation equation becomes

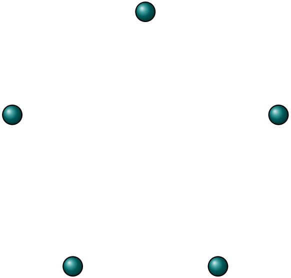
$$\frac{\partial^{\alpha} \mathcal{Q}^{(2)}(u,t)}{\partial t^{\alpha}} = -(1 - F_{X_1}(u))\mathcal{Q}^{(2)}(u,t),$$

where $\partial^{\alpha}/\partial t^{\alpha}$ is the Caputo derivative. The solution of the Cauchy problem for the relaxation equation is

$$F_{S^{(2)}(t)}(u) = \mathcal{Q}^{(2)}(u,t) = E_{\alpha}(-(1 - F_{X_1}(u))t^{\alpha}).$$

Model for "Human" Dynamics?

As an example from (5), consider a population of 5 and let X_n be the number of links at discrete time n.



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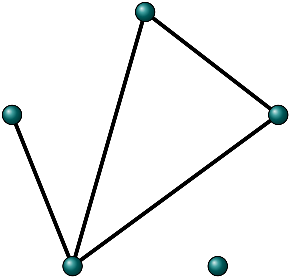

1. Initial state of the number of links is $X_0 = 4$.

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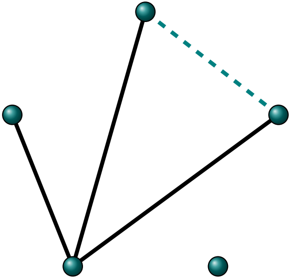

1. Initial state of the number of links is $X_0 = 4$.
2. A link is chosen uniformly, and if present...

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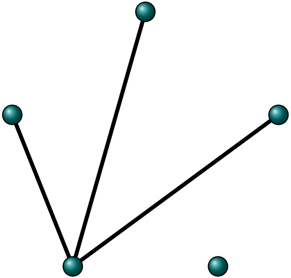

1. Initial state of the number of links is $X_0 = 4$.
2. A link is chosen uniformly, and if present...
3. ...it is deleted. $X_1 = 3$.

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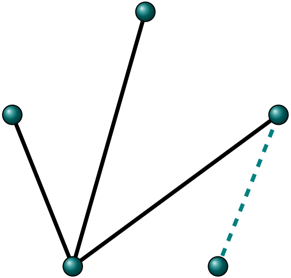

1. Initial state of the number of links is $X_0 = 4$.
2. A link is chosen uniformly, and if present...
3. ...it is deleted. $X_1 = 3$.
4. Otherwise...

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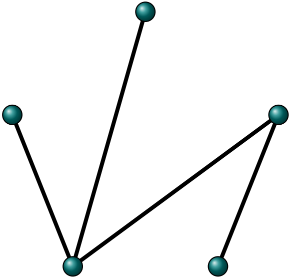

1. Initial state of the number of links is $X_0 = 4$.
2. A link is chosen uniformly, and if present...
3. ...it is deleted. $X_1 = 3$.
4. Otherwise...
5. ... it is added. $X_2 = 4$.

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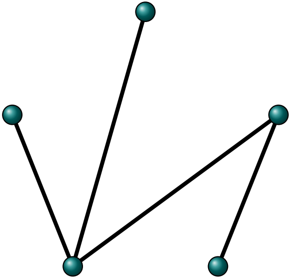


1. Initial state of the number of links is $X_0 = 4$.
2. A link is chosen uniformly, and if present...
3. ...it is deleted. $X_1 = 3$.
4. Otherwise...
5. ... it is added. $X_2 = 4$.

Human interactions are generally 'slow' in evolution. Add Mittag-Leffler dynamics.

Embedded Ehrenfest Chain

$X_n, n \geq 1$, is the number of links after n events. Initially $X_0 = i$, as we start with i present links and the number of links in the network increases, remains or decreases according to the following transition probabilities

$$q_{k,k-1} = \mathbb{P}_i\{X_{j+1} = k-1|X_j = k\} = \begin{cases} 0, & k=0, \\ 1-\alpha, & k=M, \\ (1-\alpha)\frac{k}{M}, & \text{otherwise,} \end{cases}$$

$$q_{k,k} = \mathbb{P}_i\{X_{j+1} = k|X_j = k\} = \alpha,$$

$$q_{k,k+1} = \mathbb{P}_i\{X_{j+1} = k+1|X_j = k\} = \begin{cases} 1-\alpha, & k=0, \\ 0, & k=M, \\ 1-\alpha-\frac{k(1-\alpha)}{M}, & \text{otherwise.} \end{cases}$$

Bottom-up derivation with semi-Markov dynamics-1

Mittag-Leffler again!

1. Mittag-Leffler i.i.d. waiting times $\{J_i\}_{i\geq 1}$ of order $\beta \in (0,1)$, scaling $\gamma > 0$ and c.d.f.

$$F_T^{(\beta,\gamma)}(t) = \mathbb{P}\{J \leq t\} = 1 - E_\beta(-(t/\gamma)^\beta).$$

   where $E_\beta(z)$ is the Mittag-Leffler function, defined by

$$E_\beta(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(1+\beta n)}.$$

   In this talk $\gamma = 1$ unless explicitly said otherwise.

2. Counting process

$$N_\beta(t) = \max\left\{n : \, S_n = \sum_{i=1}^{n} J_i \leq t\right\}.$$

   counts the number of M-L events up to time t.

Bottom-up derivation with semi-Markov dynamics-2

1. The number of links in the fractional network is given (via the embedded chain) by
$$X(t) = X_{N_\beta(t)} = X_n \mathbb{1}\{S_n \le t < S_{n+1}\}.$$
In words, at every M-L event, the chain jumps according to the discrete transition probabilities.
2. All information about $X(t)$ is encoded in $\{(X_n, J_n)\}_{n\ge 1}$ which are a discrete Markov renewal process, satisfying
$$\mathbb{P}\{X_{n+1} = j, J_{n+1} \le u \,|\, (X_0, S_0), \ldots, (X_n = i, S_n)\} \\ = \mathbb{P}\{X_{n+1} = j, J_{n+1} \le u | X_n = i\}.$$
$X(\cdot)$ is then a semi-Markov process subordinated to $N_\beta(t)$ and satisfies the forward equations
$$p_{i,j}(t) = \overline{F}_J^{(\beta)}(t)\delta_{ij} + \sum_{\ell\in\mathcal{S}} q_{\ell,j} \int_0^t p_{i,\ell}(u) f_J^{(\beta)}(t-u)\, du.$$
Here $p_{i,j}(t) = \mathbb{P}\{X(t) = j | X(0) = i\}$, c.c.d.f. $\overline{F}_J^{(\beta)}(t) = 1 - F_J^{(\beta)}(t)$ and $f_t^{(\beta)}(t)$ the M-L(β) density.

Fractional Kolmogorov Equations

Theorem (Georgiou, Kiss, Scalas 2015 (5))

The probabilities $p_{i,j}(t)$ satisfy the following pseudo-differential equations

$$\frac{d^\beta p_{i,j}(t)}{d\,t^\beta} = -(1-\alpha)\; p_{i,j}(t) + (1-\alpha)\left(\frac{M-j+1}{M} p_{i,j-1}(t) + \frac{j+1}{M} p_{i,j+1}(t)\right)$$

Similarly, the equations of the boundary terms are

$$\frac{d^\beta p_{i,0}(t)}{d\,t^\beta} = (1-\alpha)\left(-p_{i,0}(t) + \frac{1}{M} p_{i,1}(t)\right)$$

$$\frac{d^\beta p_{i,M}(t)}{d\,t^\beta} = (1-\alpha)\left(-p_{i,M}(t) + \frac{1}{M} p_{i,M-1}(t)\right).$$

Solution to the fractional equations

$$
\begin{aligned}
p_{i,j}(t) &= \mathbb{P}_i\{X(t) = j\} \\
&= \sum_{k=0}^{\infty} \mathbb{P}_i\{X(t) = j, N_\beta(t) = k\} = \sum_{k=0}^{\infty} \mathbb{P}_i\{X(t) = j | N_\beta(t) = k\} \mathbb{P}\{N_\beta(t) = k\} \\
&= \mathbb{P}_i\{X(t) = j | N_\beta(t) = 0\} \mathbb{P}\{N_\beta(t) = 0\} \\
&\quad + \sum_{k=1}^{\infty} \mathbb{P}\{X(t) = j | N_\beta(t) = k, X(0) = i\} \mathbb{P}\{N_\beta(t) = k\} \\
&= \mathbb{P}_i\{X(t) = j | T_1 \geq t\} \mathbb{P}\{T_1 \geq t\} + \sum_{k=1}^{\infty} \mathbb{P}_i\{X(t) = j | N_\beta(t) = k\} \mathbb{P}\{N_\beta(t) = k\} \\
&= \delta_{ij} \overline{F}_T^{(\beta)}(t) + \sum_{k=1}^{\infty} \mathbb{P}_i\{X_k = j | \mathbb{1}\{S_k \leq t < S_{k+1}\}\} \mathbb{P}\{N_\beta(t) = k\} \\
&= \delta_{ij} \overline{F}_T^{(\beta)}(t) + \sum_{k=1}^{\infty} \mathbb{P}_i\{X_k = j\} \mathbb{P}\{N_\beta(t) = k\},
\end{aligned}
$$

Monte-Carlo simulations

where it finally leads to

$$p_{i,j}(t) = \delta_{ij}\overline{F}_T^{(\beta)}(t) + \sum_{k=1}^{\infty} q_{ij}^{(k)}\mathbb{P}\{N_\beta(t) = k\}.$$

Here,

$$\mathbb{P}\{N_\beta(t) = k\} = \frac{t^{\beta n}}{n!}E_\beta^{(n)}(-t^\beta).$$

Scalas, Gorenflo, Mainardi (2004) (3).

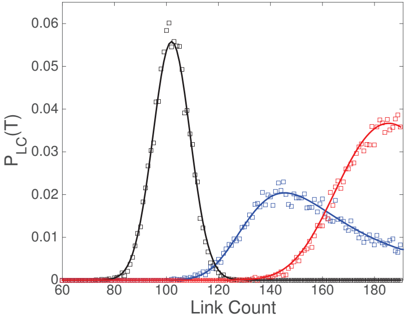
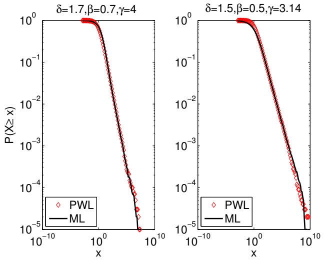


Figure: Discrete markers are the estimated probabilities $p_{190,j}(250)$, averaged over 10000 MC simulations starting from a fully connected network with $N = 20$ nodes and for $\beta = 1, 0.7, 0.5$, as we move from left to right.

Approximation to power law distributions.



Pareto density:

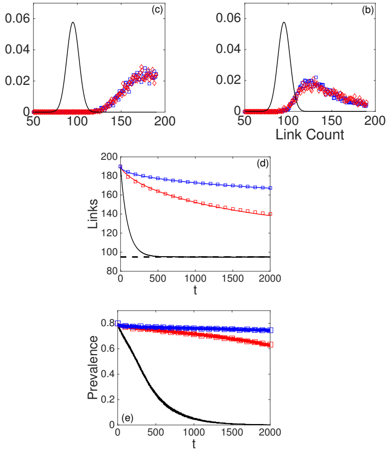
$$f_{\mathcal{P}(\delta)}(s) = \frac{\delta - 1}{(1+s)^{\delta}}, s > 0.$$

- Can we use the analytical fractional network as a rigorous approximation to others?
- Main idea: For a fixed finite time horizon T, the value of the r.v. N_T is (severely) restricted by the long inter-event times that are not "uncommon" because of the fat tails.
- Match the survival functions (c.c.d.f), at least up to T, by playing with scaling γ.

$$\frac{\sin(\beta\pi)}{\pi}\frac{\Gamma(\beta)}{(t/\gamma)^{\beta}} = \frac{1}{t^{\delta-1}} \iff \gamma = \left(\frac{\pi}{\sin(\beta\pi)\Gamma(\beta)}\right)^{1/\beta}$$

Three Monte Carlo tests for the approximation

1. Finite time horizon T, link distributions $\mathbb{P}\{X_T = k\}$.
2. The evolution of $\mathbb{E}(X_t)$, $0 \leq t \leq T$.
3. The prevalence of a Markovian S-I-S epidemic on the dynamical network.



Equilibrium via the discrete embedding

1. Network of N nodes and maximum possible number of links $M = \frac{N(N-1)}{2}$.
2. Order the links and encode the state of the network by a $0-1$ (M-dimensional) vector. Possible states are the 2^M vertices of the hypercube.
3. Discrete Ehrenfest chain defines a random walk on the hypercube, therefore the equilibrium distribution on graphs is, by symmetry, uniform.
4. Moreover, we have Erdös-Rényi(1/2) network selection:

$$\mathbb{P}\{L_1 = x_1, L_2 = x_2, \ldots, L_k = x_k\} = \frac{2^{M-k}}{2^M} = \prod_{i=1}^{k} \mathbb{P}\{L_i = x_i\}$$

   and binomial degree distribution.
5. Recall: Markov Chains tend a.s. (empirically) to their invariant limit (ergodic theorem). Renewal counting processes satisfy SLLN and $\mathcal{L}^1$ convergence (renewal theorems). Versions of MCMC work well because of this fact.

Equilibrium via the discrete embedding

1. The fat tails destroy several of these properties (including the appropriate scaling) for all the good theorems because of the considerable time delay.
2. Monte-Carlo simulations need to be treated with care. E.g FRT fails to give meaningful information

$$\mathbb{E}(N_\beta(t)) = Ct^\beta \Longrightarrow \lim_{t\to\infty} t^{-1}\mathbb{E}(N_\beta(t)) = 0.$$

3. Main idea: Utilise the mixing time of the discrete chain to decide whether you are studying near-equilibrium behaviour or not.
4. We say the chain is well mixed at time T (in the total variation distance), up to some tolerance ε if

$$\sup_j |\mathbb{P}_i\{X(T) = j\} - \pi(j)| \leq \varepsilon.$$

The mixing time $t_{\text{mix}}(\varepsilon)$ is the infimum over all times such that the chain is well-mixed.

Numerical approximation of the equilibrium

Theorem (Diakonis, Chen - Sallof-Coste, ...)

For the discrete Ehrenfest Markov chain on M states,

$$t_{mix}(\varepsilon) \leq C\varepsilon^{-2} M^2 \log M.$$

1. Same bound will hold for the continuous MC because of the law of large numbers. Thus, what is essential for mixing, is to have $t_{\text{mix}}(\varepsilon)$ many jumps.
2. For a finite time horizon T, the expected number of jumps of the fractional chain is CT^{β}. Therefore, for the chain to be well-mixed at time T we must at least have that
$$T = C\varepsilon^{-2/\beta} M^{2/\beta} (\log M)^{1/\beta}.$$
3. This horizon becomes forbidding/unrealistic for large networks (or small β) so quite likely we are away from equilibrium.
4. This argument is not quite rigorous, but it can be made.

Numerical approximation of the equilibrium

Let $\alpha < \eta < \beta$. Also let $s = -t^{-\eta} < 0$. Then

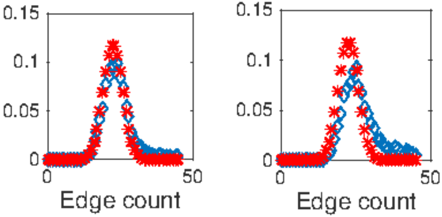
$$\begin{aligned}\mathbb{P}\{N_\beta(t) \le t^\alpha\} &= \mathbb{P}\{e^{sN_\beta(t)} \ge e^{st^\alpha}\} \le e^{|s|t^\alpha}\mathbb{E}(e^{-|s|N_\beta(t)}) \\ &= e^{t^{\alpha-\eta}}E_\beta(-t^\beta(1-e^{-t^{-\eta}})) \\ &\sim e^{t^{\alpha-\eta}}E_\beta(-t^{\beta-\eta})) = Ce^{t^{\alpha-\eta}}t^{-\beta+\eta} \\ &\sim C(1+t^{\alpha-\eta})t^{-\beta+\eta} = C(t^{-\beta+\eta}+t^{-\beta+\alpha}) \to 0.\end{aligned}$$

Therefore, with probability near 1, for a sufficiently large time horizon, the counting process $N_\beta \ge t^\alpha$ so the sufficient condition for mixing is

Lemma (2015+)

For any $\delta > 0$,

$$T > C(\varepsilon)M^{(2+\delta)/\beta}(\log M)^{(1+\delta)/\beta}$$



To do

We have preliminary answers to our questions

- Can we find explicit expressions for cumulative distribution function, etc. of the time-changed processes?
  Indeed!
- How this is related to the solution of relaxation problems?
  Probabilities turn out to be solutions of relaxation problems!
- Is numerical work possible?
  It is possible. We use Monte Carlo simulations, but other methods are welcome!
- What can we say on mixing and stability of time-changed processes?
  We are working on that, stay tuned!

And there is no limit to modelling. For instance, we are now working on more refined time-changed network dynamical models related to percolation models.

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Thank You

Thank You
Questions & Comments ?