A simple model for aging and the dynamic glass transition: the trap model

We consider a phenomenological model for the dynamics of a spin glass which we will show to reproduce the aging phenomenon typical of these systems. Aging means that the dynamics, or typical response times, get slower the longer the system has been in the glassy phase. Each valley in configuration space (a cluster of low energy configurations that are connected by low energy moves) is represented as a trap, of which there are N in total.

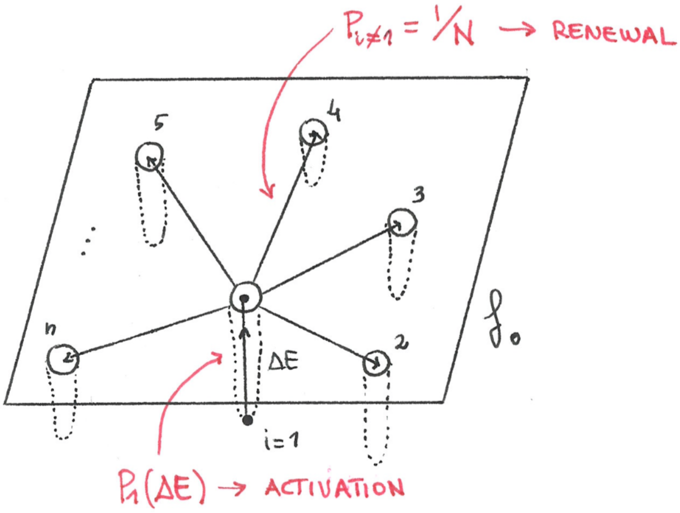

FIG. 1: Schematic representation of the configuration space of the trap model. The threshold free energy f_0 is the *minimal* energy required to go from one metastable state to another one. In general, to reach more distant states, or taking different routes between two states, one may encounter higher threshold values for f. The present model neglects such subtleties. Moreover, there is no geometry or notion of phase space distance between the traps. The traps represent valleys of low energy around a local minimum. These are considered the possible states visited in the course of a stochastic activated evolution in a high-dimensional phase space. The traps are like energy holes, drilled from f_0, their depths representing the free energy difference between the local minimum and the threshold f_0. This model emphasizes the activation/exiting step: the probability to jump to a new trap depends only on the energy of the trap from which the system exits, but not on the energy of the trap into which it falls.

The dynamics is described by jumps from trap to trap. We suppose that once the system reaches a given trap it stays there for a time which is exponentially distributed, with a characteristic time τ_i, that depends on the trap i. This is equivalent to assuming a rate $1/\tau_i$ of exiting the trap i. That is, if the system is still in the trap at time t, the probability of exiting from it between t and $t + dt$ is dt/τ_i. Once the system exits trap i, it jumps towards another trap j, which is chosen uniformly at random among all N traps (for simplicity we assume that one may fall back into the same trap as well). In order to model the heterogeneity of the system and the fact that the dynamics is activated, we suppose that, in order to exit from a trap, an activation energy $E_i > 0$ is necessary to reach a threshold energy where large rearrangements become possible, and that these activation energies are distributed according to

$$P(E) = \frac{1}{E_0} \exp(-E/E_0), \quad E \geq 0. \tag{1}$$

Thus, deeper traps with larger E_i are exponentially less abundant, on the other hand they trap the system for exponentially longer times

$$\tau_i = \tau_0 \exp(E_i/T). \tag{2}$$

Here τ_0 is a microscopic time representing the minimal time to move between very shallow traps. An exponential decrease of the abundance of "metastable states" (configuration valleys) is indeed found in mean field models, especially in structural glasses (while spin glasses have usually a more complex valley structure). It is particularly relevant at temperatures close to the 'dynamical glass temperature' T_d where relatively long-lived metastable configurations (i.e. traps) start appearing. To be more precise, T_d is reached when the resulting dynamics gets slow, which, as we will see, requires that $T \leq E_0 \equiv T_d$. We saw that 1-step replica symmetry breaking predicts a family of pure states whose number grows exponentially with energy. We are now interested in the threshold states that are barely stable. Now we assume that there is a maximal energy, which we take as reference, $E = 0$, above which there are no stable states, and such that once the system reaches that level of energy, it can pretty freely explore phase space before it falls into a local minimum again. The distribution of minima with energy close to $E = 0$ is then exponential with $1/E_0$ given by $d\Sigma(f)/f|_{f=f_{\rm th}}$.

1. Derive the distribution of trapping times τ_i, $\rho(\tau)$, from the above distribution of activation energies E_i.

   Solution: We have to set $\rho(\tau)d\tau = P(E(\tau))dE$, with $E(\tau) = T\ln(\tau/\tau_0)$.

$$\rho(\tau) = P(E(\tau))dE/d\tau = \frac{T}{E_0}\frac{1}{\tau}\left(\frac{\tau_0}{\tau}\right)^{T/E_0} = \mu\frac{\tau_0^\mu}{\tau^{1+\mu}} \tag{3}$$

   where $\mu = T/E_0$.

2. After the first escape the system chooses a new trap randomly. What is the expected time it spends in the next trap? What happens for $\mu \equiv T/E_0 \leq 1$, i.e., for $T < E_0$? From your result, argue that the temperature $T_d = E_0$ marks a dynamical glass transition.

   Solution: The expected time spent in a trap is

$$\overline{\tau} = \int_{\tau_0}^{\infty} d\tau\tau\rho(\tau) = \begin{cases} \frac{\mu}{\mu-1}\tau_0 & \text{for } \mu > 1 \\ \infty & \text{for } \mu \leq 1. \end{cases} \tag{4}$$

   Thus for $\mu > 1$ the expected time is finite and the system jumps steadily from trap to trap, the number of traps visited per unit time being proportional to $1/\tau_0$. Instead for $\mu \leq 1$ the expected trapping time diverges. The system tends to spend increasingly long times in deep traps. It actually does not reach the stationary state in a time proportional to the number of traps, N. The time to reach the stationary state thus becomes exceedingly long in the large N limit. More precisely: The time to reach stationarity in a system of N traps grows faster than N. In that case the sum over all trap times $\sum_{i=1}^{N}\tau_i$ is not governed by the central limit theorem (but rather tends to a Lévy distribution). It is dominated by the largest time τ_M which can be estimated from

$$\int_{\tau_M}^{\infty} d\tau\rho(\tau) = 1/N \to \tau_M = \tau_0 N^{1/\mu}, \tag{5}$$

   which grows super-linearly with N indeed.

3. Write down a differential equation for the time evolution of the probability P_i to find the system in trap i, and find the stationary distribution P_i.

   Solution: The time evolution of probabilities follows the differential equation

$$dP_i/dt = -\frac{P_i}{\tau_i} + \frac{1}{N}\sum_{j=1}^{N}\frac{P_j}{\tau_j}. \tag{6}$$

   The stationary state requires $dP_i/dt = 0$, and thus $P_i \propto \tau_i$, with a proportionality constant which is equal for all states. Normalizing the probabilities yields

$$P_i = \frac{\tau_i}{\sum_{j=1}^{N}\tau_j} \tag{7}$$

4. Compute the probability that at any given time, when the system has reached a stationary state, the system is found in a trap of escape time τ. What happens in the limit of an infinite number of traps, when $\mu \leq 1$?

   Solution: In the stationary state, the probability to find the system in a trap with $\tau_i = \tau$ is

$$P_{\rm stat}(\tau) = \sum_i P_i\delta(\tau - \tau_i) = \frac{\sum_i \tau_i\delta(\tau - \tau_i)}{\sum_j \tau_j}. \tag{8}$$

Since $\rho(\tau)$ is the pdf of trap times, in the limit of a large number of traps we may replace $\sum_i \to N \int d\tau \rho(\tau)$, and obtain

$$P_{\text{stat}}(\tau) = \frac{\rho(\tau)\tau}{\int_{\tau_0}^{\infty} \rho(\tau')\tau' d\tau'} \tag{9}$$

$$= \frac{\tau^{-\mu}}{\int_{\tau_0}^{\infty} \tau^{-\mu} d\tau}. \tag{10}$$

Note that the denominator becomes divergent for $\mu \leq 1$, as we saw in point 2. The probability distribution $P_{\text{stat}}(\tau)$ for an infinitely large system is thus not normalisable, which in turn means that no stationary state is reached. In contrast, the system gets trapped for increasingly long times as time progresses. In the case of a finite number of traps, as the system eventually reaches a stationary state, the system spends the largest fraction of the time in the deepest trap with $\tau \sim \tau_M \sim N^{1/\mu}$ determined above.

For a system with a large number of traps $N \to \infty$ one can say that for $\mu > 1$, the distribution of trap times encountered in the dynamics will soon converge to P_{stat}. In contrast, for $\mu \leq 1$, the tail of the distribution of encountered trap times continues to grow and never becomes stationary: The rare traps with trapping times $\tau \gg \tau_0$ will typically only be visited at times of order τ itself.

5. Consider the dynamical evolution starting from one of the traps chosen uniformly at random at $t = 0$. What is the statistics (mean and variance) of the time elapsed after M jumps,

$$T_M = \sum_{a=1}^{M} \tau_a, \tag{11}$$

in the limit $M \gg 1$? What is the difference between the cases $\mu \leq 1$, $2 \leq \mu > 1$ and $\mu > 2$? Explain why for $\mu \leq 1$ aging is displayed. **Hint:** Determine first how the largest term in the sum scales with M. Then use this as an effective cut-off on $\rho(\tau)$, and estimate mean and variance of the sum for T_M by using the thus truncated $\rho(\tau)$.

Solution: The variable T_M is a sum of independent random variables. The outcome of the sum then depends on whether the mean of the distribution is finite or not. In the case where the mean is finite ($\mu > 1$) the mean of the sum of random variables is simply $M\langle\tau\rangle$. How much do values of T_M vary around this mean? If $\mu > 2$ the variance is also finite and therefore one can use the central limit theorem and conclude that the standard deviation scales as $M^{\frac{1}{2}}$. However, for $1 < \mu < 2$, while the distribution still has a finite mean, the variance is divergent! We can then estimate the variance of a sum of M random variables by computing it with $\rho(\tau)$, truncated at the largest value, $\tau_M \approx \tau_0 M^{1/\mu}$, as estimated in part 2. The variance of the sum can thus be estimated as

$$M\langle\tau^2 - \langle\tau\rangle^2\rangle \approx \int_{\tau_0}^{\tau_M} \rho(\tau)\left(\tau^2 - \langle\tau\rangle^2\right) d\tau \tag{12}$$

$$= M\mu\tau_0^{\mu}\left[\frac{1}{2-\mu}\left(\tau_M^{2-\mu} - \tau_0^{2-\mu}\right) - \langle\tau\rangle^2\right] \tag{13}$$

$$\approx \frac{\mu}{2-\mu}\tau_0^2 M^{\frac{2}{\mu}} \quad , \tag{14}$$

which is dominated by the cut-off. Therefore, we find the standard deviation to scale as $M^{\frac{1}{\mu}}$ and we can write

$$T_M \approx M\langle\tau\rangle + \mathcal{O}(M^{\frac{1}{\mu}}) \quad . \tag{15}$$

It is interesting to note that the standard deviation is proportional to τ_M and therefore is determined by the largest τ sampled. This is a characteristic of Lévy flights: the largest jumps remain visible on the scale of the standard deviation, even in the limit of a very large number of steps.

When the mean diverges ($\mu \leq 1$), using the same truncation method as above, the sum T_M can be estimated as

$$\langle T_M\rangle = M\langle\tau\rangle_{\text{trunc}} \approx \frac{\mu}{1-\mu}\tau_0 M^{\frac{1}{\mu}} \quad . \tag{16}$$

Therefore, in this case the sum T_M is proportional to τ_M and is thus dominated by the largest contribution

$$T_M \sim \mathrm{Max}_{1\leq i\leq M}[\tau_i] \quad . \tag{17}$$

Hence, the system spends more and more time in deeper and deeper traps as time progresses. At long times t, the trap with the longest τ_i visited scales as t itself. Moreover, with a probability $O(1)$ this deepest trap is the last trap that has been visited, and the remaining time to escape from it will still be of order $\tau_i \sim t$. This is the aging phenomenon: the age of the system, t, sets the time scale to be expected for the escape from the last trap the system fell into: The system's dynamics gets slower and slower as time progresses. This would also reflect on the autocorrelation function, which retains its large intra-valley value as long as the system remains in the trap, and only decays essentially to zero once the system manages to jump out. Note that all this phenomenology only occurs for $\mu \leq 1$, i.e. for $T \leq T_d$.

Solution: As in the aging case, the time remaining until the walker comes back scales like t, for the same reasons. In this case you would hardly say though that a random walk is "aging". It's just that the longer you wait, the longer walks the walker will undertake, and so the longer you will have to wait for him/her to come back, because it is rather likely that the longest walk undertaken is just the last one.

For a broader perspective on aging dynamics you may read the review by G. Biroli, https://www.arxiv-vanity.com/papers/cond-mat/0504681/.