

Some math on $C_f(n, m)$

We wish to show how $C_f(n, m)$ can be related to the transition matrix P . We will use the same notations we used in the previous addendum, where we presented a mathematical proof that the bias is of order $1/N$ and obtained an exact expression in terms of the transition matrix.

In terms of the transition matrix we can write (for $n < m$)

$$C_f(n, m, X_0) = \langle (f(X_n) - F)(f(X_m) - F) \rangle_{MC,0} = \sum_{xy} (f(x) - F)(f(y) - F) P_{0x}^n P_{xy}^{m-n}.$$

where we set $F = \langle f(x) \rangle_{\pi}$.

Now we assume that **we start in equilibrium**. Rigorously, this means that we pick the starting point X_0 with probability π and average over the initial conditions. In practice, it corresponds to consider a **typical** configuration X_0 . Indeed, if we choose X_0 with probability π , we will only obtain typical configuration. Therefore, the equilibrium autocorrelation function is

$$C_{f,\text{eq}}(n, m) = \sum_x \pi_x C_f(n, m, x)$$

We obtain

$$C_{f,\text{eq}}(n, m) = \sum_z \pi_z \sum_{xy} (f(x) - F)(f(y) - F) P_{zx}^n P_{xy}^{m-n} = \sum_{xy} \pi_x (f(x) - F)(f(y) - F) P_{xy}^{m-n},$$

In the last step we have used repeatedly the stationarity condition:

$$\sum_z \pi_z P_{zx}^n = \sum_{zy} \pi_z P_{zy} P_{yx}^{n-1} = \sum_y \left(\sum_z \pi_z P_{zy} \right) P_{yx}^{n-1} = \sum_y \pi_y P_{yx}^{n-1} = \dots = \pi_x$$

The dependence on the starting time disappears, so that the autocorrelation function depends only on the difference $m - n$.

We obtain

$$\begin{aligned}
 & \sum_{xy} \pi_x f(x)(f(y) - F) P_{xy}^{m-n} - F \sum_{xy} \pi_x P_{xy}^{m-n} (f(y) - F) \\
 &= \sum_{xy} \pi_x f(x)(f(y) - F) P_{xy}^{m-n} - F \sum_y \pi_y (f(y) - F) \\
 &= \sum_{xy} \pi_x f(x)(f(y) - F) P_{xy}^{m-n} \\
 &= \sum_{xy} \pi_x f(x) f(y) P_{xy}^{m-n} - F \sum_x \pi_x f(x) \sum_y P_{xy}^{m-n} = \sum_{xy} \pi_x f(x) f(y) P_{xy}^{m-n} - F^2
 \end{aligned}$$

Let us comment on the different steps.

a) The second line is obtained from the first using the relation derived above

$$\sum_x \pi_x P_{xy}^{n-m} = \pi_y.$$

b) The last term in the second line vanishes, since $\sum_y \pi_y f(y) = F$ and $\sum_y \pi_y F = F$.

c) In the last line we use $\sum_y P_{xy}^{m-n} = 1$.

Defining the projector $\Pi_{xy} = \pi_y$ we have

$$\begin{aligned} \sum_{xy} \pi_x f(x) f(y) P_{xy}^{m-n} - F^2 &= \sum_{xy} \pi_x f(x) f(y) P_{xy}^{m-n} - \sum_{xy} \pi_x \pi_y f(x) f(y) = \\ &= \sum_{xy} \pi_x f(x) f(y) [P_{xy}^{m-n} - \Pi_{xy}] \\ &= \sum_{xy} \pi_x f(x) f(y) [P - \Pi]_{xy}^{m-n} \end{aligned}$$

The derivation of the relation $P^{m-n} - \Pi = (P - \Pi)^{m-n}$ is given in the notes on the bias.

As we already discussed all eigenvalues of $P - \Pi$ lie in the unit circle (this is correct for a finite system; for an infinite one some caveats are needed). Hence, the autocorrelation function decays exponentially as $|\lambda_2|^{m-n}$ as $m - n \rightarrow \infty$, where λ_2 is the second largest (in absolute value) eigenvalue of P .