Re-estimation of a transition matrix

In this project, goal is to start with a specified transition matrix, generate a continuous trajectory out of it and then after rotating it into high-dimensional space and adding some noise, try to retrieve it again by msm/hmm.

(i) Generation of the continuous trajectory data:

a) Construct a transition matrix P of three meta-stable states with one intermediate state and generate a discrete trajectory s_t with a minimum length of 10000 frames. Such a transition matrix might look like

$$P = \begin{pmatrix} 0.97 & 0.03 & 0 \\ 0.015 & 0.97 & 0.015 \\ 0 & 0.03 & 0.97 \end{pmatrix}.$$

b) Define a two-dimensional output probability distribution for each state i of P, e.g., Gaussians with mean μ_i and covariance matrix C_i. Then, for each time t, generate an output $x(t) \sim G(\mu_i, C_i)$. The means of the Gaussians should span a plane.

c) Rotate the data into 5-dimensional space, translate it by a constant vector and add some noise.

(ii) Reconstruction of the transition matrix:

Apply tica/pca, k-means/regspatial and msm/hmm. Do the transition matrices agree? What happens if the Gaussians do not span a plane?