

S4 Hyperparameter search results

Tables A, B and C section summarises the optimal model parameters for MCPC, PC, and DLGMs found during the hyperparameter search to maximise the FID, the marginal likelihood $-\ln p(y_{eval})$, and the reconstruction MSE.

Table A. Results of the hyperparameter search to maximize the FID for MCPC, PC, and DLGMs.

	MCPC	PC	DLGM
Architecture			
input dimension	748	748	748
number of hidden layers	3	3	3
hidden layers dimension	(128, 128, 20)	(128, 128, 20)	(256,256,20)
activation function	ReLU	ReLU	ReLU
PC Inference			
optimizer	Adam	Adam	-
lr	0.7	0.1	-
max_steps	250	250	-
MCPC Inference			
optimizer	SGD	-	-
lr	0.1	-	-
mixing steps	50	-	-
sampling steps	100	-	-
Learning			
optimiser	Adam	Adam	Adam
lr	0.01	0.01	0.001
decay	0.0	0.1	0.01
num_epochs	50	50	50
batch_size	256	128	128

Table B. Results of the hyperparameter search to maximize the marginal likelihood for MCPC, PC, and DLGMs.

	MCPC	PC	DLGM
Architecture			
input dimension	748	748	748
number of hidden layers	3	3	3
hidden layers dimension	(128, 128, 20)	(128, 128, 25)	(128, 128, 10)
activation function	ReLU	Tanh	ReLU
PC Inference			
optimizer	Adam	Adam	-
lr	0.1	0.3	-
max_steps	250	250	-
MCPC Inference			
optimizer	SGD	-	-
lr	0.03	-	-
mixing steps	50	-	-
sampling steps	100	-	-
Learning			
optimiser	Adam	Adam	Adam
lr	0.003	0.001	0.001
decay	0.1	0.01	0.01
num_epochs	50	50	50
batch_size	64	256	256

Table C. Results of the hyperparameter search to maximize the reconstruction MSE for MCPC, PC, and DLGMs.

	MCPC	PC	DLGM
Architecture			
input dimension	748	748	748
number of hidden layers	3	3	3
hidden layers dimension	(256, 256, 20)	(256, 256, 30)	(256, 256, 20)
activation function	ReLU	Tanh	ReLU
PC Inference			
optimizer	Adam	Adam	-
lr	0.7	0.7	-
max_steps	250	250	-
MCPC Inference			
optimizer	SGD	-	-
lr	0.03	-	-
mixing steps	50	-	-
sampling steps	100	-	-
Learning			
optimiser	Adam	Adam	Adam
lr	0.001	0.003	0.003
decay	0.01	0.1	0.1
num_epochs	50	50	50
batch_size	64	256	128