

Hyperparameters used to build the AE, AEC, scMEDAL-FE, scMEDAL-FEC, and scMEDAL-RE models

In Tables 1-3 there are described the Hyperparameters and variables for data loading, model construction, compilation, and training were applied across the AE, AEC, scMEDAL-FE, scMEDAL-FEC, and scMEDAL-RE models in three datasets: Healthy Heart, the Autism Spectrum Disorder (ASD), and Acute Myeloid Leukemia (AML) datasets.

Settings	Hyperparameter/variable	AE	AEC	scMEDAL-FE	scMEDAL-FEC	scMEDAL-RE
Compile model	optimizer 1	Adam(lr=0.0001)				
	optimizer 2 (adversarial)	-		Adam(lr=0.0001)		-
	reconstruction loss (X)	MSE				
	adversarial loss (z)	-		CCE	CCE	-
	classification loss (y)	-	CCE	-	CCE	-
	classification loss (z)/ λ_L	-				CCE
	reconstruction loss_weights (X): λ_{recon}	1	81	5400	9450	110
	classification loss_weights (y): λ_y	-	0.1	-	1	-
	adversarial loss weights (z): λ_A	-	-	1	1	-
Build model	cluster loss weight (z): λ_L	-				0.1
	kl_weight (z): λ_K	-				1.00E-05
	post_loc_init_scale (z)	-				0.1
	prior_scale (z)	-				0.25
	n_latent_dims	2				
	layer_units	[512,132]				
	layer_units_latent_classifier	-	[2]	-	[2]	[5]
	n_clusters	-	-	147	147	147
	n_pred (y)	-	13	-	13	-
	last_activation	linear				
	use_batch_norm	TRUE				default in RE layers
	dense hidden layers activation	selu				
	classifier activation	softmax				
Load data	use_z	FALSE	FALSE	TRUE	TRUE	TRUE
	get_pred (y)	FALSE	TRUE	FALSE	TRUE	FALSE
	scaling	min_max				
	batch_size	512				
Train model	epochs	500				
	monitor_metric	val_loss	val_loss	val_total_loss	val_total_loss	val_total_loss
	patience	30				
	stop_criteria	early_stopping				

Settings	Hyperparameter/variable	AE	AEC	scMEDAL-FE	scMEDAL-FEC	scMEDAL-RE
Compile model	optimizer 1	Adam(lr=0.0001)				
	optimizer 2 (adversarial)	-		Adam(lr=0.0001)		-
	reconstruction loss (X)	MSE				
	adversarial loss (z)	-		CCE	CCE	-
	classification loss (y)	-	CCE	-	CCE	-
	classification loss (z)	CCE				
	reconstruction loss_weights (X): λ_{recon}	1	1	1000	1000	110
	classification loss_weights (y): λ_y	-	0.1	-	1	-
Build model	adversarial loss weights (z): λ_A	-		1	1	-
	cluster loss weight (z): λ_L	-				
	kl_weight (z): λ_K	-				
	post_loc_init_scale (z)	-				
	prior_scale (z)	-				
	n_latent_dims	2				
	layer_units	[512,132]				
	layer_units_latent_classifier	NA	[2]	-	[2]	[5]
	n_clusters	-	-	31	31	31
	n_pred (y)	NA	17	-	17	17
	last_activation	linear				
	use_batch_norm	TRUE				default in RE layers
	dense hidden layers activation	selu				
	classifier activation	softmax				
	Load data	use_z	FALSE	FALSE	TRUE	TRUE
get_pred (y)		FALSE	TRUE	FALSE	TRUE	FALSE
scaling		min_max				
batch_size		512				
Train model	epochs	500				
	monitor_metric	val_loss	val_loss	val_total_loss	val_total_loss	val_total_loss
	patience	30				
	stop_criteria	early_stopping				

Table 3. Hyperparameters and variables for data loading, model building, compilation, and training in the AML dataset.

Settings	Hyperparameter/variable	AE	AEC	scMEDAL-FE	scMEDAL-FEC	scMEDAL-RE
Compile model	optimizer 1	Adam(lr=0.0001)				
	optimizer 2 (adversarial)	-		Adam(lr=0.0001)		-
	reconstruction loss (X)	MSE				
	adversarial loss (z)	-		CCE	CCE	-
	classification loss (y)	-	CCE	-	CCE	-
	classification loss (z)	-			-	CCE
	reconstruction loss_weights (X): λ_{recon}	1	100	4000	1500	110
	classification loss_weights (y): λ_y	-	0.1	-	1	-
	adversarial loss weights (z): λ_A	-	-	1	1	-
Build model	cluster loss weight (z): λ_l	-				0.1
	kl_weight (z): λ_k	-				1.00E-05
	post_loc_init_scale (z)	-				0.1
	prior_scale (z)	-				0.25
	n_latent_dims	2				
	layer_units	[512,132]				
	layer_units_latent_classifier	-	[2]	-	[2]	[5]
	n_clusters	-		19	19	19
	n_pred (y)	-	21	-	21	-
	last_activation	linear				
	use_batch_norm	TRUE				default in RE layers
	dense hidden layers activation	selu				
	classifier activation	softmax				
Load data	use_z	FALSE	FALSE	TRUE	TRUE	TRUE
	get_pred (y)	FALSE	TRUE	FALSE	TRUE	FALSE
	scaling	min_max				
	batch_size	512				
Train model	epochs	500				
	monitor_metric	val_loss	val_loss	val_total_loss	val_total_loss	val_total_loss
	patience	30				
	stop_criteria	early_stopping				