Ranking-based Convolutional Neural Network Models for Peptide-MHC Class I Binding Prediction (Supplementary Materials)

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APPENDIX

A1   ADDITIONAL EXPERIMENTAL RESULTS

A1.1   Hyperparameter Search Space

The search space of hyperparameters includes batch size $\{32, 128\}$, number of layers $\{1, 2\}$, filter size $\{1, 3, 5\}$, number of filters $\{8, 16, 64\}$ and the size of output layer $\{8, 16, 64\}$.

A1.2   Model Architecture Comparison

Table A1, A2, A3 and A4 present the average percentage improvement of our models over the baseline `MHCflurry` with MS. Models are trained with `BLOSUM` `+Onehot` `+Deep` and selected with respect to 4 different metrics (i.e., AR_{100}, HR_{100}, AUC and ROC_5, respectively).

A1.3   Encoding Method Comparison

Table A5, A6, A7, and A8 present the average percentage improvement of the 7 encoding methods over the baseline encoding method `BLOSUM`. We used `SpConvM` with H_v as the model to evaluate encoding methods and their combination. We trained the models and selected the hyper-parameters with respect to 4 different metrics (i.e., AR_{100}, HR_{100}, AUC and ROC_5, respectively).

Table A1. Performance Comparison over `MHCflurry` with MS (AR_{100}; `BLOSUM+Onehot+Deep`)

Model	loss	AR_{100}	HR_{100}	AR_{500}	HR_{500}	AUC	ROC_5	ROC_{10}
ConvM	H_v	8.08	4.79	3.56	5.93	6.36	9.92	10.01
	H_l	6.36	4.50	1.33	4.50	5.21	6.57	5.92
	H_i	6.58	3.49	1.36	3.26	5.63	7.25	6.05
	MS	-5.17	-7.93	-6.69	-1.93	1.24	-3.51	-3.36
SpConvM	H_v	10.75	7.58	**8.06**	**9.61**	**8.68**	**18.84**	**16.29**
	H_l	10.10	5.39	5.87	6.69	7.39	14.09	10.97
	H_i	10.59	**8.28**	5.32	7.47	7.35	14.66	11.56
	MS	7.36	7.54	3.27	5.74	5.16	15.66	11.68
MHCflurry	H_v	**10.95**	6.74	6.62	7.95	6.45	15.87	11.45
	H_l	8.61	7.32	5.37	6.08	5.71	10.75	9.39
	H_i	8.20	4.19	4.87	5.87	4.92	11.79	7.99
	MS	0.00	0.00	0.00	0.00	0.00	0.00	0.00

The values in the table are percentage improvement compared with the baseline `MHCflurry` with MS. Models are trained using `BLOSUM+Onehot+Deep` encoding methods, and selected with respect to AR_{100} and evaluated using the 7 evaluation metrics. The best improvement with respect to each metric is **bold**.

Table A2. Performance Comparison over `MHCflurry` with MS (HR_{100}; `BLOSUM+Onehot+Deep`)

Model	loss	AR_{100}	HR_{100}	AR_{500}	HR_{500}	AUC	ROC_5	ROC_{10}
ConvM	H_v	5.72	6.89	3.15	5.66	7.11	12.78	10.81
	H_l	4.89	5.54	2.47	3.50	6.27	7.34	8.35
	H_i	4.75	5.88	0.93	3.62	6.24	7.21	7.29
	MS	-8.57	0.21	-8.00	-1.23	1.65	-2.45	-2.47
SpConvM	H_v	9.86	**8.85**	**7.89**	8.59	**9.12**	**19.29**	**18.11**
	H_l	8.18	7.64	6.46	6.64	8.44	15.59	14.08
	H_i	7.35	8.5	5.02	6.41	7.96	13.21	14.04
	MS	7.10	8.05	2.49	4.95	6.30	15.17	12.5
MHCflurry	H_v	**10.11**	8.54	7.14	**9.21**	6.09	16.00	14.65
	H_l	8.78	6.60	5.55	5.95	5.50	13.19	11.30
	H_i	6.50	6.20	5.08	5.47	4.69	12.19	8.12
	MS	0.00	0.00	0.00	0.00	0.00	0.00	0.00

The values in the table are percentage improvement compared with the baseline `MHCflurry` with MS. Models are trained using `BLOSUM+Onehot+Deep` encoding methods, and selected with respect to HR_{100} and evaluated using the 7 evaluation metrics. The best improvement with respect to each metric is **bold**.

Table A3. Performance Comparison over `MHCflurry` with MS (AUC; `BLOSUM+Onehot+Deep`)

Model	loss	AR_{100}	HR_{100}	AR_{500}	HR_{500}	AUC	ROC_5	ROC_{10}
ConvM	H_v	6.83	2.28	5.03	7.34	3.44	9.69	8.55
	H_l	3.00	3.12	3.88	6.88	3.16	5.41	5.81
	H_i	3.66	-0.63	3.01	5.83	2.81	4.43	3.58
	MS	-9.12	-8.45	-5.46	-2.31	-0.52	-5.62	-5.45
SpConvM	H_v	**10.27**	**4.42**	**9.24**	**10.08**	**5.09**	**17.20**	**15.06**
	H_l	7.18	2.84	8.12	8.31	4.42	12.36	10.63
	H_i	7.54	2.98	7.69	7.25	4.44	11.57	10.04
	MS	4.31	2.49	5.28	4.78	2.86	11.68	9.47
MHCflurry	H_v	8.08	1.61	7.45	8.35	4.30	11.02	11.05
	H_l	7.64	3.96	6.31	7.61	3.56	8.63	7.63
	H_i	7.39	1.64	5.81	6.74	3.41	9.32	7.68
	MS	0.00	0.00	0.00	0.00	0.00	0.00	0.00

The values in the table are percentage improvement compared with the baseline `MHCflurry` with MS. Models are trained using `BLOSUM+Onehot+Deep` encoding methods, and selected with respect to `AUC` and evaluated using the 7 evaluation metrics. The best improvement with respect to each metric is **bold**.

Table A4. Performance Comparison over `MHCflurry` with MS (ROC_5; `BLOSUM+Onehot+Deep`)

Model	loss	AR_{100}	HR_{100}	AR_{500}	HR_{500}	AUC	ROC_5	ROC_{10}
ConvM	H_v	8.38	6.71	3.23	6.86	5.14	5.91	4.63
	H_l	3.33	5.16	0.96	5.52	4.22	5.22	2.56
	H_i	8.36	7.95	3.35	5.83	5.01	5.40	3.70
	MS	-11.59	-5.75	-8.19	-2.14	0.23	-7.20	-8.84
SpConvM	H_v	**12.78**	**15.81**	**8.31**	**11.11**	**7.29**	**15.03**	**10.52**
	H_l	11.71	9.88	5.45	8.12	6.20	12.09	7.72
	H_i	10.18	8.09	7.40	9.58	6.65	10.38	8.09
	MS	5.25	3.68	2.96	4.81	4.49	13.54	6.87
MHCflurry	H_v	11.20	11.53	7.09	7.44	6.32	10.38	8.31
	H_l	1.87	0.36	0.09	1.16	3.22	13.76	9.80
	H_i	7.64	8.25	5.83	6.28	5.36	8.66	7.74
	MS	0.00	0.00	0.00	0.00	0.00	0.00	0.00

The values in the table are percentage improvement compared with the baseline `MHCflurry` with MS. Models are trained using `BLOSUM+Onehot+Deep` encoding methods, and selected with respect to `ROC_5` and evaluated using the 7 evaluation metrics. The best improvement with respect to each metric is **bold**.

Table A5. Encoding Performance Comparison on `SpConvM` with H_v (AR_{100})

encoding	AR_{100}	HR_{100}	AR_{500}	HR_{500}	AUC	ROC_5	ROC_{10}
BLOSUM	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Onehot	-6.04	-4.09	-6.00	-1.75	-1.13	-5.38	-5.34
Deep	-4.74	-0.98	-2.55	-0.09	-0.13	0.26	-1.17
BLOSUM +Onehot	-0.62	-0.06	-0.62	1.68	0.27	3.17	1.22
BLOSUM +Deep	**1.43**	**3.33**	**0.66**	2.62	**0.57**	4.88	2.73
Onehot +Deep	-4.10	-3.16	-2.64	-0.37	0.01	-1.83	-2.29
BLOSUM +Onehot +Deep	0.15	-0.15	-0.47	**3.53**	0.53	**6.29**	**3.53**

The values in the table are percentage improvement compared with the `BLOSUM` encoding method. Models are selected with respect to `AR_100` and evaluated using the 7 evaluation metrics. The best improvement with respect to each metric is **bold**.

Table A6. Encoding Performance Comparison on SpConvM with H_v (HR_{100})

encoding	AR_{100}	HR_{100}	AR_{500}	HR_{500}	AUC	ROC_5	ROC_{10}
BLOSUM	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Onehot	-6.20	-3.31	-5.71	-3.85	-0.69	-7.10	-5.47
Deep	-3.81	-0.44	-2.64	-0.21	0.26	-0.36	0.09
BLOSUM +Onehot	-1.47	0.98	-0.70	-0.04	0.11	1.61	0.85
BLOSUM +Deep	-0.40	**2.45**	-0.30	0.57	0.28	3.39	1.97
Onehot +Deep	-6.45	-2.48	-4.34	-1.71	-0.55	-3.08	-3.13
BLOSUM +Onehot +Deep	**0.58**	0.07	**0.98**	**2.16**	**0.75**	**4.56**	**3.50**

The values in the table are percentage improvement compared with the BLOSUM encoding method. Models are selected with respect to HR_{100} and evaluated using the 7 evaluation metrics. The best improvement with respect to each metric is **bold**.

Table A7. Encoding Performance Comparison on SpConvM with H_v (AUC)

encoding	AR_{100}	HR_{100}	AR_{500}	HR_{500}	AUC	ROC_5	ROC_{10}
BLOSUM	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Onehot	-6.75	-4.84	-4.37	-2.55	-0.91	-6.85	-5.34
Deep	-3.31	-0.59	-2.09	-0.71	-0.19	-1.06	-1.49
BLOSUM +Onehot	-0.45	**0.97**	0.22	0.52	0.09	1.41	1.02
BLOSUM +Deep	**0.95**	-0.84	1.09	**1.58**	0.55	3.25	2.00
Onehot +Deep	-2.90	-3.40	-2.68	-1.56	-0.39	-4.13	-3.26
BLOSUM +Onehot +Deep	0.77	-0.67	**1.43**	1.05	**0.62**	**5.90**	**3.95**

The values in the table are percentage improvement compared with the BLOSUM encoding method. Models are selected with respect to AUC and evaluated using the 7 evaluation metrics. The best improvement with respect to each metric is **bold**.

Table A8. Encoding Performance Comparison on SpConvM with H_v (ROC_5)

encoding	AR_{100}	HR_{100}	AR_{500}	HR_{500}	AUC	ROC_5	ROC_{10}
BLOSUM	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Onehot	-7.96	-7.56	-5.22	-2.32	-1.05	-5.61	-4.81
Deep	-2.29	-0.84	-2.76	-0.78	-0.54	-0.69	-1.28
BLOSUM +Onehot	1.24	-0.16	0.18	0.40	0.00	1.38	1.12
BLOSUM +Deep	**2.84**	0.15	1.41	**1.90**	0.60	3.20	3.14
Onehot +Deep	-4.76	-2.90	-3.31	-1.28	-0.61	-2.58	-2.30
BLOSUM +Onehot +Deep	2.57	**0.20**	**2.08**	1.46	**0.82**	**3.83**	**3.47**

The values in the table are percentage improvement compared with the BLOSUM encoding method. Models are selected with respect to ROC_5 and evaluated using the 7 evaluation metrics. The best improvement with respect to each metric is **bold**.