

Supplementary Materials

EPI-Trans: An Effective Transformer-based Deep Learning Model for Enhancer Promoter Interaction Prediction

Table S 1: The performance of EPI-Trans-specific model due to using different optimizers in terms of AUROC on six different cell lines

Optimizer/ cell lines	GM12878	HeLa-S3	HUVEC	IMR90	K562	NHEK	AVG
Adam	0.928	0.959	0.933	0.902	0.920	0.979	0.937
SGD	0.912	0.957	0.925	0.885	0.932	0.981	0.932
RMSprop	0.922	0.960	0.922	0.894	0.927	0.975	0.933
Adamax	0.501	0.500	0.500	0.500	0.500	0.500	0.500
Nadam	0.927	0.952	0.934	0.909	0.935	0.975	0.939

Note: The best performance in each cell line, the best average, and the final optimizer that is used in our experiments are given in boldface

Table S 2: The performance of EPI-Trans-specific model due to using different optimizers in terms of AUPR on six different cell lines

Optimizer/ cell lines	GM12878	HeLa-S3	HUVEC	IMR90	K562	NHEK	AVG
Adam	0.743	0.848	0.705	0.713	0.764	0.896	0.778
SGD	0.692	0.768	0.629	0.636	0.712	0.869	0.718
RMSprop	0.777	0.838	0.689	0.716	0.735	0.892	0.774
Adamax	0.048	0.048	0.048	0.048	0.048	0.048	0.048
Nadam	0.788	0.855	0.718	0.721	0.755	0.902	0.790

Note: The best performance in each cell line, the best average, and the final optimizer that is used in our experiments are given in boldface

Table S 3: The performance of EPI-Trans-specific model due to using different learning rates of Nadam optimizer in terms of AUROC on six different cell lines

Learning Rate/ cell lines	GM12878	HeLa-S3	HUVEC	IMR90	K562	NHEK	AVG
0.01	0.892	0.932	0.893	0.872	0.908	0.960	0.910
0.001	0.927	0.952	0.934	0.909	0.935	0.975	0.939
0.0001	0.901	0.954	0.915	0.885	0.920	0.977	0.925

Note: The best performance in each cell line, the best average, and the final value of the learning rate that is used in our experiments are given in boldface

Table S 4: The performance of EPI-Trans-specific model due to using different learning rates of Nadam optimizer in terms of AUPR on six different cell lines

Learning Rate/ cell lines	GM12878	HeLa-S3	HUVEC	IMR90	K562	NHEK	AVG
0.01	0.432	0.518	0.445	0.512	0.354	0.727	0.498
0.001	0.788	0.855	0.718	0.721	0.755	0.902	0.790
0.0001	0.700	0.791	0.586	0.645	0.727	0.849	0.716

Note: The best performance in each cell line, the best average, and the final value of the learning rate that is used in our experiments are given in boldface

Table S 5: The performance of EPI-Trans-specific model due to using different batch sizes, and using Nadam optimizer with learning rate 0.001 in terms of AUROC on six different cell lines

Batch Size/ cell lines	GM12878	HeLa-S3	HUVEC	IMR90	K562	NHEK	AVG
16	0.921	0.964	0.931	0.878	0.930	0.980	0.934
32	0.921	0.956	0.919	0.911	0.931	0.977	0.936
64	0.928	0.960	0.943	0.888	0.943	0.982	0.941
128	0.930	0.964	0.926	0.898	0.928	0.976	0.937
256	0.910	0.958	0.927	0.898	0.945	0.982	0.937

Note: The best performance in each cell line, the best average, and the final value of the batch size that is used in our experiments are given in boldface

Table S 6: The performance of EPI-Trans-specific model due to using different batch sizes, and using Nadam optimizer with learning rate 0.001 in terms of AUPR on six different cell lines

Batch Size/ cell lines	GM12878	HeLa-S3	HUVEC	IMR90	K562	NHEK	AVG
16	0.726	0.712	0.643	0.670	0.759	0.882	0.732
32	0.770	0.859	0.669	0.730	0.771	0.889	0.781
64	0.779	0.849	0.713	0.742	0.783	0.919	0.797
128	0.790	0.859	0.691	0.720	0.753	0.914	0.788
256	0.707	0.865	0.650	0.683	0.743	0.908	0.759

Note: The best performance in each cell line, the best average, and the final value of the batch size that is used in our experiments are given in boldface

Table S 7: The performance of EPI-Trans-specific model due to using different values for epochs, using Nadam optimizer with learning rate 0.001, and batch size 64 in terms of AUROC on six different cell lines

Epochs/cell lines	GM12878	HeLa-S3	HUVEC	IMR90	K562	NHEK	AVG
15	0.928	0.960	0.943	0.888	0.943	0.982	0.941
20	0.933	0.963	0.939	0.898	0.931	0.984	0.941
25	0.929	0.963	0.926	0.893	0.934	0.980	0.938
30	0.929	0.963	0.923	0.911	0.935	0.981	0.940

Note: The best performance in each cell line, the best average, and the final value of the number of epochs that is used in our experiments are given in boldface

Table S 8: The performance of EPI-Trans-specific model due to using different values for epochs, using Nadam optimizer with learning rate 0.001, and batch size 64 in terms of AUPR on six different cell lines

Epochs/cell lines	GM12878	HeLa-S3	HUVEC	IMR90	K562	NHEK	AVG
15	0.779	0.849	0.713	0.742	0.783	0.919	0.797
20	0.795	0.854	0.736	0.733	0.783	0.922	0.804
25	0.788	0.852	0.730	0.746	0.774	0.918	0.801
30	0.800	0.861	0.711	0.747	0.782	0.919	0.803

Note: The best performance in each cell line, the best average, and the final value of the number of epochs that is used in our experiments are given in boldface

Table S 9: The performance of EPI-Trans-general model due to using different values for epochs, using Nadam optimizer with learning rate 0.001, and batch size 64 in terms of AUROC on six different cell lines

Epochs/cell lines	GM12878	HeLa-S3	HUVEC	IMR90	K562	NHEK	AVG
20	0.938	0.955	0.941	0.932	0.940	0.967	0.946
25	0.944	0.963	0.944	0.933	0.942	0.975	0.950
30	0.940	0.958	0.938	0.929	0.943	0.971	0.947

Note: The best performance in each cell line, the best average, and the final value of the number of epochs that is used in our experiments are given in boldface

Table S 10: The performance of EPI-Trans-general model due to using different values for epochs, using Nadam optimizer with learning rate 0.001, and batch size 64 in terms of AUPR on six different cell lines

Epochs/cell lines	GM12878	HeLa-S3	HUVEC	IMR90	K562	NHEK	AVG
20	0.668	0.715	0.564	0.607	0.666	0.716	0.656
25	0.643	0.749	0.584	0.611	0.658	0.723	0.661
30	0.629	0.728	0.585	0.606	0.645	0.731	0.654

Note: The best performance in each cell line, the best average, and the final value of the number of epochs that is used in our experiments are given in boldface

Table S 11: The performance of EPI-Trans-best model due to using different values for epochs, using Nadam optimizer with learning rate 0.001, and batch size 64 in terms of AUROC on six different cell lines

Epochs/cell lines	GM12878	HeLa-S3	HUVEC	IMR90	K562	NHEK	AVG
20	0.945	0.963	0.954	0.934	0.952	0.985	0.956
25	0.947	0.969	0.942	0.931	0.941	0.980	0.952
30	0.946	0.964	0.952	0.941	0.956	0.983	0.957

Note: The best performance in each cell line, the best average, and the final value of the number of epochs that is used in our experiments are given in boldface

Table S 12: The performance of EPI-Trans-best model due to using different values for epochs, using Nadam optimizer with learning rate 0.001, and batch size 64 in terms of AUPR on six different cell lines

Epochs/cell lines	GM12878	HeLa-S3	HUVEC	IMR90	K562	NHEK	AVG
20	0.763	0.838	0.732	0.758	0.770	0.894	0.793
25	0.742	0.846	0.727	0.760	0.731	0.876	0.780
30	0.778	0.857	0.724	0.758	0.758	0.901	0.796

Note: The best performance in each cell line, the best average, and the final value of the number of epochs that is used in our experiments are given in boldface

Table S 13: The training time for all samples in minutes of the EPI-Trans models for the six cell lines

Model/Cell line	GM12878	HeLa-S3	HUVEC	IMR90	K562	NHEK	AVG
EPI-Trans-spec	49.621	54.620	53.646	42.424	59.760	45.525	50.932
EPI-Trans-gen	-	-	-	-	-	-	318.220
EPI-Trans-best	75.397	65.100	56.247	45.364	73.012	46.254	60.229

Table S 14: The test time per a sample in milliseconds of the EPI-Trans models for the six cell lines

Model/Cell line	GM12878	HeLa-S3	HUVEC	IMR90	K562	NHEK	AVG
EPI-Trans-spec	0.868	0.427	0.453	0.424	0.436	0.415	0.504
EPI-Trans-gen	0.878	0.425	0.472	0.417	0.445	0.409	0.508
EPI-Trans-best	0.842	0.436	0.471	0.431	0.446	0.422	0.508