Table 1. Comparison of DeepDDG with Other Nonintegrated Methods

methods	training set		test set		test set (5% of outliers removed)	
	R	MAE (kcal/mol)	*R*	MAE (kcal/mol)	*R*	MAE (kcal/mol)
SCooP[41]	NA[a]	NA[a]	0.078	6.44	0.180	4.35
MUpro1.1[3]	0.551	1.10	0.190	1.06	0.310	0.93
EASE-MM[42]	0.607	1.16	0.402	0.91	0.591	0.76
PopMusic[6]	NA[a]	NA[a]	0.443	0.91	0.619	0.77
STRUM[43]	0.715	1.02	0.447	0.88	0.518	0.77
I-Mutant3.0[11]	0.565	1.17	0.453	0.91	0.538	0.79
mCSM[9]	0.630	1.14	0.467	0.90	0.572	0.78
SDM[2]	0.491	1.41	0.483	1.02	0.604	0.89
DeepDDG	0.681 ± 0.019	1.04 ± 0.02	0.557 ± 0.015	0.86 ± 0.04	0.658 ± 0.014	0.74 ± 0.04

Conv2D (feature118)	CrossValid(train->test)	0.6548	1.0964	0.3514	1.049	10折实验平均结果AVG(10)
		0.607	1.1511	0.3716	1.0064	10折实验最好测试结果Best(10)
Conv1D (feature118)	CrossValid(train->test)	0.6698	1.0436	0.3485	1.0185	10折实验平均结果AVG(10)
		0.4791	1.293	0.4151	1.0951	10折实验最好测试结果Best(10)
SimpleConv1D (feature118)	CrossValid(train->test)	0.6272	1.1276	0.4471	0.897	10折实验平均结果AVG(10)
		0.6496	1.1213	0.4885	0.8551	10折实验最好测试结果Best(10)
	EpochBest=15(train+valid->test)	0.6808	1.069	0.4348	0.9429	10次实验平均结果AVG(10)
		0.6194	1.1364	0.4877	0.9531	10次实验最好测试结果Best(10)
	Test EpochValid(train+valid->test)	0.6459	1.1081	0.4288	0.9149	10次实验平均结果AVG(10)
		0.6243	1.1317	0.4708	0.8664	10次实验最好测试结果Best(10)
SimpleConv1D (feature158)	CrossValid(train->test)	0.6586	1.0863	0.4599	0.9058	10折实验平均结果AVG(10)
		0.6186	1.1406	0.5129	0.8272	10折实验最好测试结果Best(10)
	EpochBest=11(train+valid->test)	0.6242	1.1448	0.4671	0.9353	10次实验平均结果AVG(10)
		0.5957	1.1769	0.4987	0.9157	10次实验最好测试结果Best(10)
	Test EpochValid(train+valid->test)	0.683	1.0594	0.4386	0.9447	10次实验平均结果AVG(10)
		0.6777	1.0693	0.4955	0.8335	10次实验最好测试结果Best(10) val_pcc
		0.6485	1.1025	0.4533	0.8955	10次实验平均结果AVG(10)
		0.7028	1.0413	0.4913	0.8939	10次实验最好测试结果Best(10) val_loss
	ensemble	0.7311 (0.7711)	1.0702 (0.9696)	0.5272 (0.5195)	0.9144 (0.8099)	
		0.7599	1.0069	0.5279	0.8440	

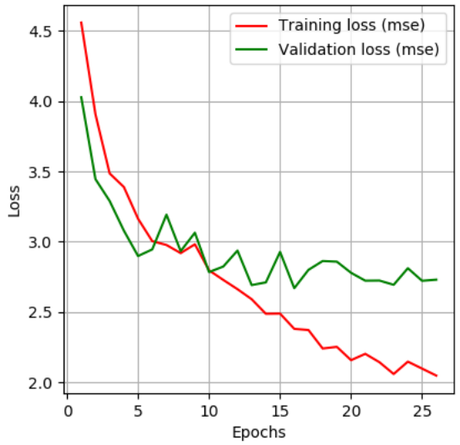
10折交叉验证，每一折都有一个最好的Epoch,
EpochBest是10个最好的Epoch中能够产生最好结果的那一个

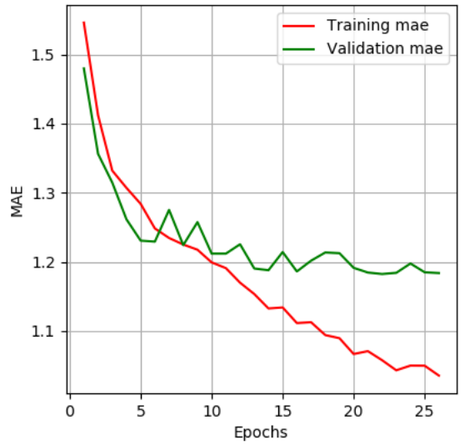
EpochValid是每折选择自己最好的Epoch

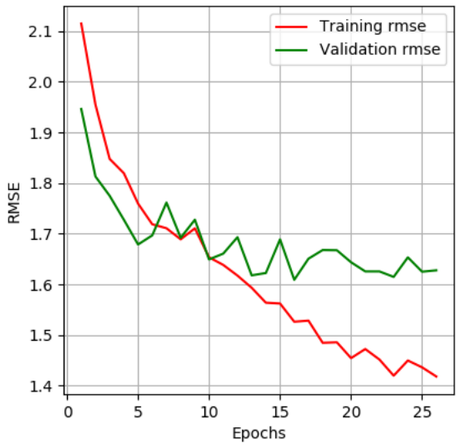
EpochValid v.s. EpochBest矛盾

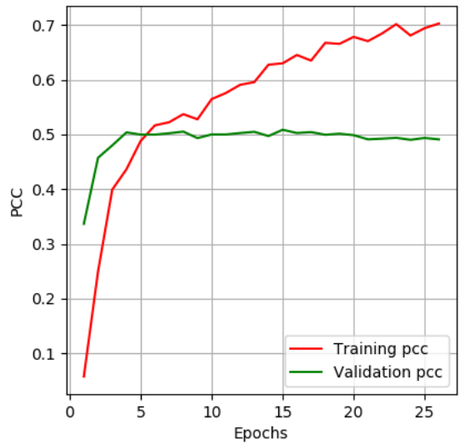
hse,depth, orientation,vector

depth by win-msms

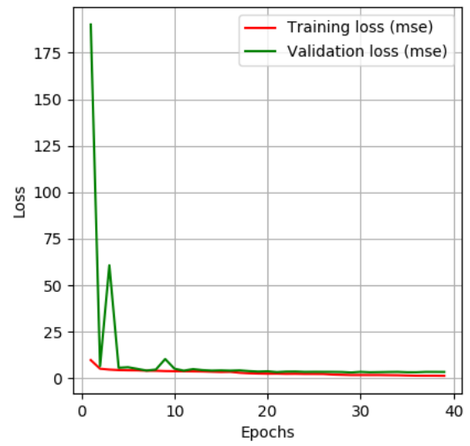


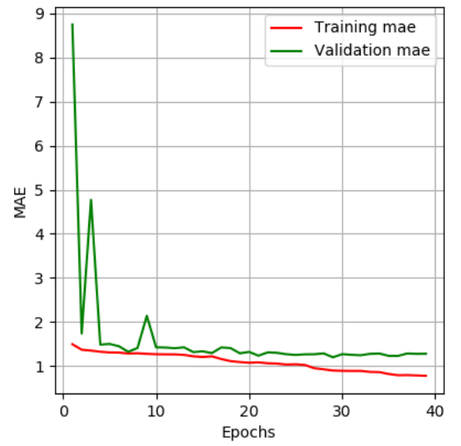




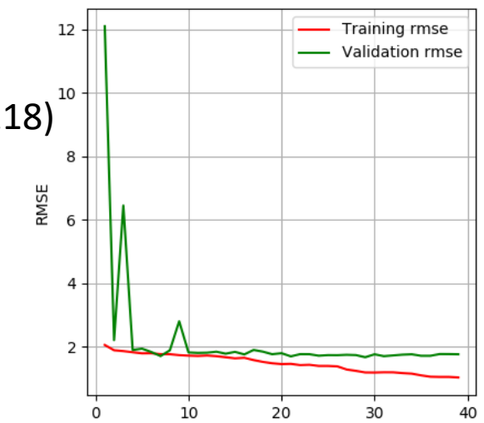


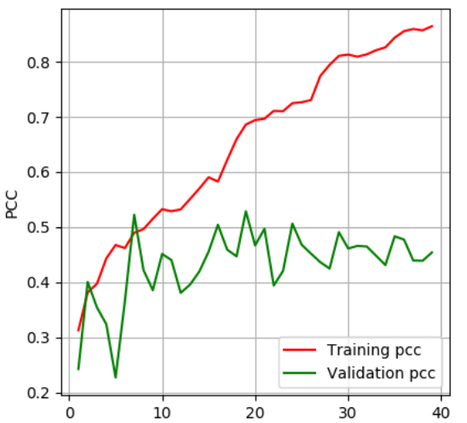
SimpleConv1D(118)





Conv1D(118)





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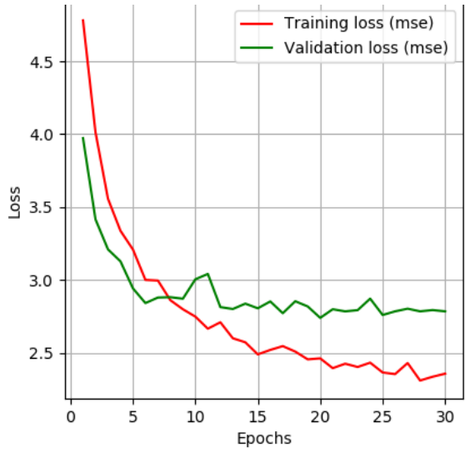

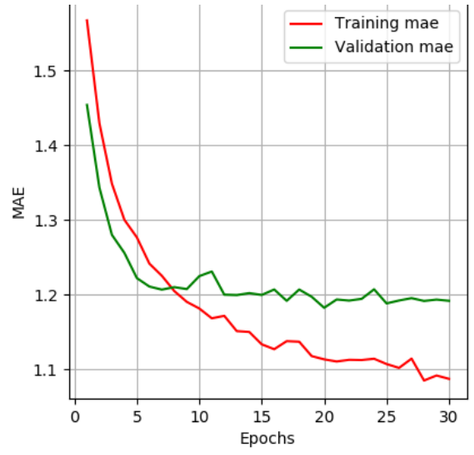

Conv2D(118)