

We conducted new simulations in the same setting but with a different benchmark. We compare our PMI score with the following benchmark to avoid ties between candidate datasets: we first train a classifier on the evaluated candidate dataset using logistic regression, and then use its cross entropy on the small test set  $T$  as its score. We tried three different Gaussian priors with covariance matrices  $\sigma^2 \cdot \mathbf{I}$  with  $\sigma^2 = 1, 9, 25$ . The generalization accuracies of the two methods are shown in the tables and the win rates of the two methods are shown in the figures.

The results for different  $\sigma$  are similar. In addition, our PMI score still achieves a higher generalization accuracy consistently, although with a smaller margin. Furthermore, our PMI score wins the test cross entropy roughly 60% of the time. Finally, we again observe similar patterns in the disparity between the two methods, which again might indicate that the PMI score is more robust to overfitting: (1) the gap increases and the number of candidate datasets  $M$  increases; (2) the gap decreases as the size of the small test set  $N_T$  increases.

$K, N_T, M$	PMI score	Cross entropy	Difference
1, 20, 200	0.7699	0.7677	0.0022
1, 20, 400	0.7696	0.7670	0.0026
1, 20, 600	0.7677	0.7647	0.0030
1, 30, 200	0.7757	0.7738	0.0019
1, 30, 400	0.7761	0.7743	0.0018
1, 30, 600	0.7737	0.7713	0.0024
1, 40, 200	0.7784	0.7773	0.0011
1, 40, 400	0.7753	0.7740	0.0014
1, 40, 600	0.7773	0.7758	0.0015
3, 20, 200	0.7735	0.7712	0.0022
3, 20, 400	0.7747	0.7714	0.0033
3, 20, 600	0.7719	0.7682	0.0038
3, 30, 200	0.7781	0.7761	0.0020
3, 30, 400	0.7791	0.7763	0.0028
3, 30, 600	0.7758	0.7727	0.0032
3, 40, 200	0.7793	0.7774	0.0018
3, 40, 400	0.7794	0.7771	0.0023
3, 40, 600	0.7790	0.7762	0.0028
5, 20, 200	0.7749	0.7733	0.0016
5, 20, 400	0.7750	0.7724	0.0027
5, 20, 600	0.7721	0.7690	0.0031
5, 30, 200	0.7764	0.7745	0.0019
5, 30, 400	0.7782	0.7756	0.0026
5, 30, 600	0.7786	0.7755	0.0031
5, 40, 200	0.7804	0.7785	0.0018
5, 40, 400	0.7826	0.7804	0.0022
5, 40, 600	0.7782	0.7752	0.0030

Table 1: Generalization accuracies of the two methods when  $\sigma^2 = 1$ . Our method consistently outperforms the benchmark.

$K, N_T, M$	PMI score	Cross entropy	Difference
1, 20, 200	0.7686	0.7671	0.0015
1, 20, 400	0.7685	0.7661	0.0024
1, 20, 600	0.7669	0.7642	0.0027
1, 30, 200	0.7766	0.7754	0.0012
1, 30, 400	0.7747	0.7729	0.0018
1, 30, 600	0.7740	0.7719	0.0022
1, 40, 200	0.7754	0.7747	0.0007
1, 40, 400	0.7763	0.7752	0.0011
1, 40, 600	0.7766	0.7752	0.0014
3, 20, 200	0.7732	0.7713	0.0019
3, 20, 400	0.7739	0.7713	0.0026
3, 20, 600	0.7715	0.7678	0.0037
3, 30, 200	0.7783	0.7763	0.0020
3, 30, 400	0.7797	0.7773	0.0024
3, 30, 600	0.7777	0.7745	0.0032
3, 40, 200	0.7807	0.7792	0.0015
3, 40, 400	0.7795	0.7771	0.0024
3, 40, 600	0.7797	0.7769	0.0028
5, 20, 200	0.7738	0.7724	0.0014
5, 20, 400	0.7730	0.7704	0.0026
5, 20, 600	0.7735	0.7703	0.0031
5, 30, 200	0.7780	0.7764	0.0016
5, 30, 400	0.7777	0.7753	0.0023
5, 30, 600	0.7771	0.7743	0.0028
5, 40, 200	0.7826	0.7810	0.0016
5, 40, 400	0.7794	0.7773	0.0022
5, 40, 600	0.7812	0.7785	0.0027

Table 2: Generalization accuracies of the two methods when  $\sigma^2 = 9$ . Our method consistently outperforms the benchmark.

$K, N_T, M$	PMI score	Cross entropy	Difference
1, 20, 200	0.7684	0.7671	0.0013
1, 20, 400	0.7691	0.7671	0.0020
1, 20, 600	0.7703	0.7677	0.0025
1, 30, 200	0.7726	0.7713	0.0013
1, 30, 400	0.7741	0.7722	0.0019
1, 30, 600	0.7764	0.7745	0.0019
1, 40, 200	0.7785	0.7775	0.0010
1, 40, 400	0.7748	0.7738	0.0010
1, 40, 600	0.7754	0.7741	0.0013
3, 20, 200	0.7721	0.7704	0.0017
3, 20, 400	0.7731	0.7706	0.0024
3, 20, 600	0.7713	0.7685	0.0028
3, 30, 200	0.7765	0.7750	0.0015
3, 30, 400	0.7773	0.7746	0.0027
3, 30, 600	0.7773	0.7739	0.0034
3, 40, 200	0.7806	0.7788	0.0018
3, 40, 400	0.7801	0.7777	0.0024
3, 40, 600	0.7793	0.7767	0.0026
5, 20, 200	0.7727	0.7715	0.0013
5, 20, 400	0.7726	0.7704	0.0022
5, 20, 600	0.7731	0.7704	0.0027
5, 30, 200	0.7775	0.7760	0.0014
5, 30, 400	0.7776	0.7749	0.0026
5, 30, 600	0.7799	0.7770	0.0030
5, 40, 200	0.7804	0.7788	0.0015
5, 40, 400	0.7796	0.7773	0.0024
5, 40, 600	0.7798	0.7769	0.0028

Table 3: Generalization accuracies of the two methods when  $\sigma^2 = 25$ . Our method consistently outperforms the benchmark.

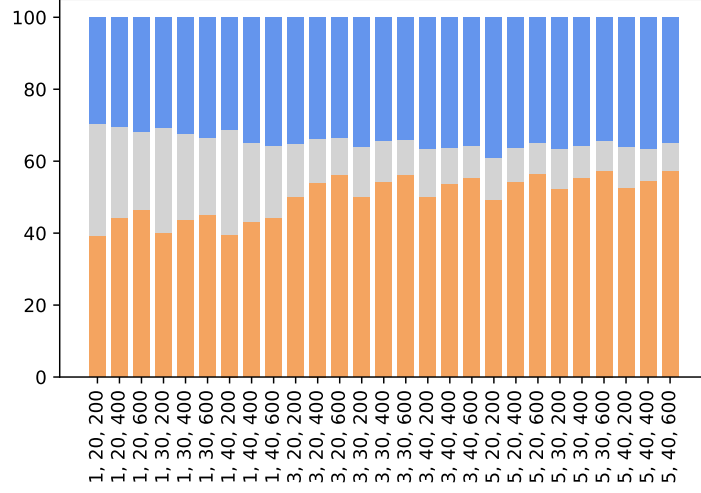


Figure 1: The win rates of the two methods when  $\sigma^2 = 1$ . The orange bars represent the win rates of our PMI score, the blue bars represent the win rates of the cross entropy benchmark, and the gray bars represent the rates of ties. The label under the bar indicates  $K, N_T, M$ .

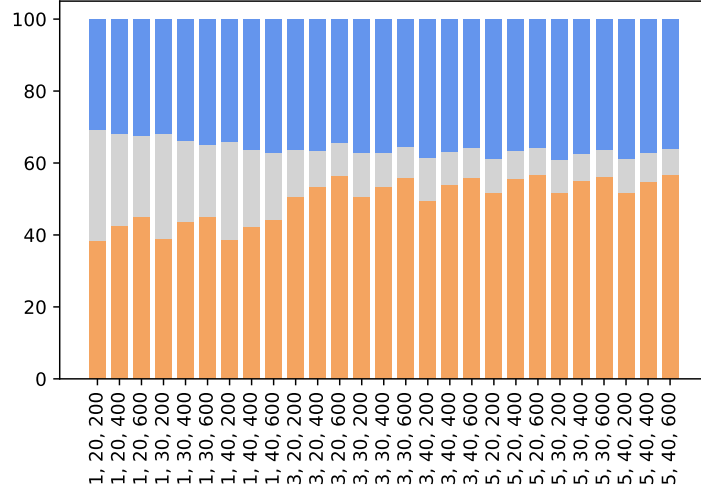


Figure 2: The win rates of the two methods when  $\sigma^2 = 9$ . The orange bars represent the win rates of our PMI score, the blue bars represent the win rates of the cross entropy benchmark, and the gray bars represent the rates of ties. The label under the bar indicates  $K, N_T, M$ .

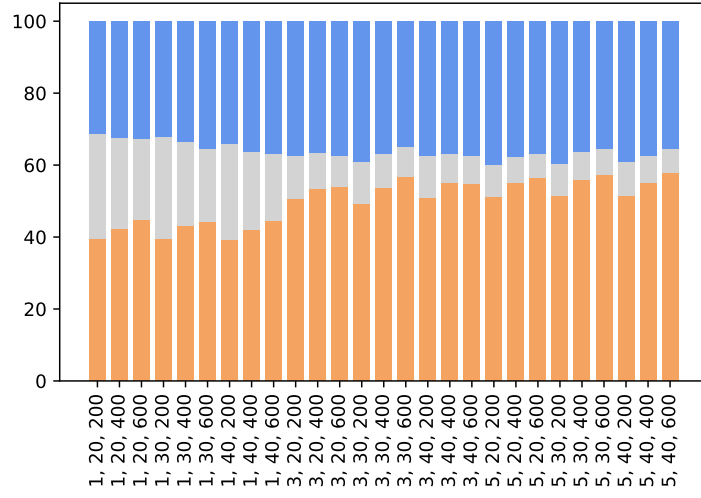


Figure 3: The win rates of the two methods when  $\sigma^2 = 25$ . The orange bars represent the win rates of our PMI score, the blue bars represent the win rates of the cross entropy benchmark, and the gray bars represent the rates of ties. The label under the bar indicates  $K, N_T, M$ .