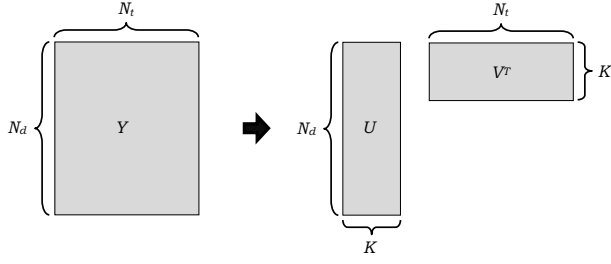# 1 Figures

Figure 1: Schematic figure of matrix factorization.
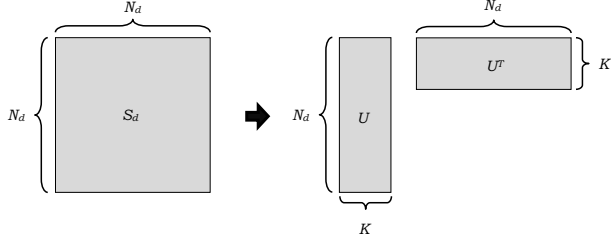

Figure 2: Schematic figure of drug similarity approximation.
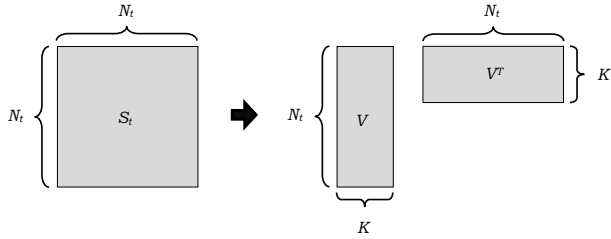

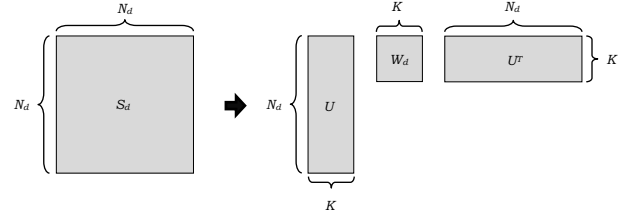Figure 3: Schematic figure of target similarity approximation.

Figure 4: Schematic figure of drug similarity approximation.
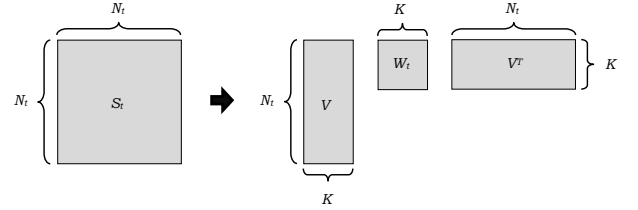
Figure 5: Schematic figure of target similarity approximation.

2 Why only pair prediction

I think my supervisor has answered this question in the email.

3 T test

See table1. We computed the p value for each method with the best method.

4 Table of weights

This is one case of similarity weights under pair prediction of MSTMF-weight. We can see that it is quite different from MSCMF compare to Table3 in the KDD2013 paper. Because the weights are sensitive to the choosing of λ_α and λ_β, so different cases may have quite different weights.

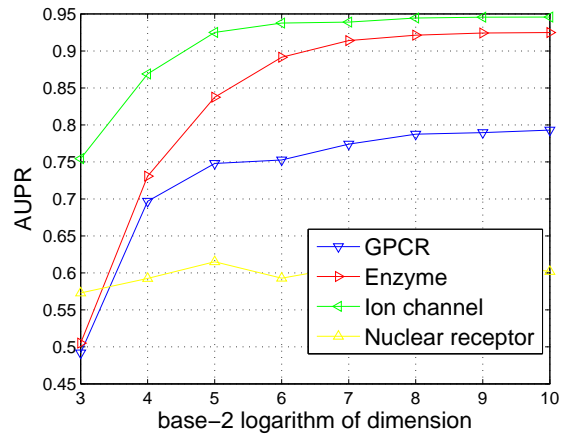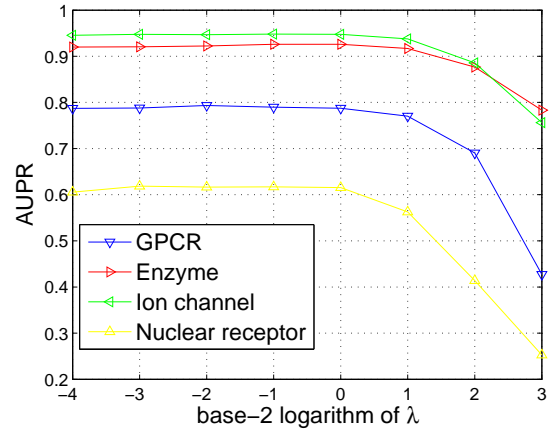

Figure 6: effect of lambda and dim.

Table 1: AUPR values obtained by 5×10-fold cross validation. The highest AUPR value for each column is highlighted in boldface.

Pair prediction

Methods	GPCR	Enzyme	IC	NR
BLM	0.666(1.20e-28)	0.830(5.54e-41)	0.847(4.74e-38)	0.509(7.26e-08)
PKM	0.401(2.14e-22)	0.633(1.27e-47)	0.617(1.11e-47)	0.499(9.14e-12)
LapRLS	0.639(3.35e-31)	0.826(4.50e-45)	0.804(1.28e-37)	0.539(3.08e-08)
NetLapRLS	0.660(7.22e-30)	0.840(5.41e-44)	0.848(3.55e-32)	0.545(2.18e-08)
GIP	0.710(7.08e-25)	0.869(5.68e-35)	0.889(9.37e-30)	0.596(3.47e-04)
KBMF2K	0.686(9.83e-25)	0.796(4.01e-43)	0.876(3.29e-28)	0.508(9.13e-10)
CMF	0.739(5.90e-20)	0.896(1.28e-32)	0.938(4.21e-14)	0.568(3.80e-05)
TMF	**0.794**(2.11e-01)	**0.913**(1.67e-19)	**0.945**(5.53e-09)	**0.611**(3.02e-03)
MSCMF	0.743(7.16e-18)	0.913(4.16e-21)	0.938(8.43e-13)	0.562(1.71e-05)
MSTMF	0.787(3.16e-05)	**0.927**	0.949(5.00e-03)	**0.658**
MSTMF-weight	**0.796**	0.925(1.75e-06)	**0.951**	0.645(1.63e-01)

Table 2: A typical case of resultant similarity weights under pair prediction.

(a)similarities over drugs

	GPCR	*Enzyme*	*IC*	*NR*
CS	0.5477	0.5367	0.6231	0.6077
ATC	0.4523	0.4633	0.3769	0.3923

(b)similarities over targets

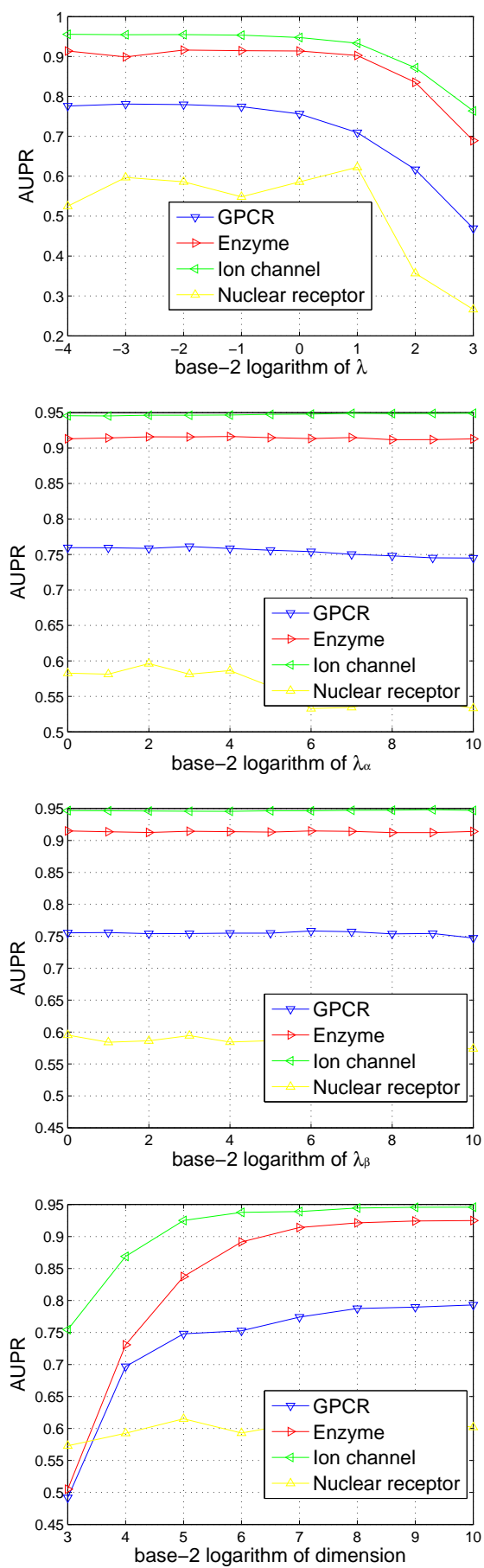|	*GPCR*	*Enzyme*	*IC*	*NR*
GS	0.8350	0.8436	0.6220	0.9589
GO(MF)	0.1650	0.1564	0.3780	0.0411

Figure 7: effect of lambda and dim.