

```
1 ssh://sangsq@10.50.221.195:22/home/sangsq/anaconda3/bin/
2   python -u /home/sangsq/.pycharm_helpers/pydev/pydevconsole.py --mode=server
3
4 import sys; print('Python %s on %s' % (sys.version, sys.
5   platform))
6 sys.path.extend(['/home/sangsq/flower/PSEP', '/home/sangsq/
7   flower/PSEP'])
8
9 Python 3.7.3 (default, Mar 27 2019, 22:11:17)
10 Type 'copyright', 'credits' or 'license' for more
11 information
12 IPython 7.4.0 -- An enhanced Interactive Python. Type '?' for help.
13 PyDev console: using IPython 7.4.0
14
15 Python 3.7.3 (default, Mar 27 2019, 22:11:17)
16 [GCC 7.3.0] on linux
17 In[2]: runfile('/home/sangsq/flower/PSEP/model/
18   dd_rgcn_distmult.py', wdir='/home/sangsq/flower/PSEP/model
19 ')
20 loading data
21 remove 0 isolated drugs: []
22 remove finished
23 963 polypharmacy side effects
24 data has been loaded
25 cuda
26 model training ...
27   0 loss:1.3882 auprc:0.5018 auroc:0.4996 ap@50:0.
28     5028
29   0 loss:1.3882 auprc:0.5041 auroc:0.4997 ap@50:0.
30     5079      time:65.5
31
32   1 loss:1.3871 auprc:0.5017 auroc:0.5004 ap@50:0.
33     5024
34   1 loss:1.3871 auprc:0.5037 auroc:0.5004 ap@50:0.
35     5074      time:61.1
36
37   2 loss:1.3866 auprc:0.5011 auroc:0.5012 ap@50:0.
38     5022
39   2 loss:1.3866 auprc:0.5026 auroc:0.5009 ap@50:0.
40     5068      time:61.7
41
42   3 loss:1.3864 auprc:0.5017 auroc:0.5022 ap@50:0.
43     5021
44   3 loss:1.3864 auprc:0.5031 auroc:0.5021 ap@50:0.
45     5067      time:61.1
46
47   4 loss:1.3863 auprc:0.5014 auroc:0.5024 ap@50:0.
48     5009
49   4 loss:1.3863 auprc:0.5037 auroc:0.5030 ap@50:0.
```

34	5056	time:62.1			
35					
36	5	loss:1.3862	auprc:0.5023	auroc:0.5042	ap@50:0.
	5021				
37	5	loss:1.3862	auprc:0.5030	auroc:0.5037	ap@50:0.
	5060	time:60.8			
38					
39	6	loss:1.3862	auprc:0.5022	auroc:0.5049	ap@50:0.
	5039				
40	6	loss:1.3862	auprc:0.5039	auroc:0.5053	ap@50:0.
	5081	time:60.2			
41					
42	7	loss:1.3862	auprc:0.5023	auroc:0.5064	ap@50:0.
	5063				
43	7	loss:1.3862	auprc:0.5045	auroc:0.5074	ap@50:0.
	5106	time:59.3			
44					
45	8	loss:1.3861	auprc:0.5033	auroc:0.5083	ap@50:0.
	5098				
46	8	loss:1.3861	auprc:0.5050	auroc:0.5092	ap@50:0.
	5137	time:60.2			
47					
48	9	loss:1.3860	auprc:0.5056	auroc:0.5099	ap@50:0.
	5134				
49	9	loss:1.3860	auprc:0.5064	auroc:0.5108	ap@50:0.
	5171	time:59.3			
50					
51	10	loss:1.3859	auprc:0.5086	auroc:0.5123	ap@50:0.
	5150				
52	10	loss:1.3859	auprc:0.5097	auroc:0.5128	ap@50:0.
	5186	time:59.9			
53					
54	11	loss:1.3857	auprc:0.5128	auroc:0.5164	ap@50:0.
	5219				
55	11	loss:1.3857	auprc:0.5145	auroc:0.5177	ap@50:0.
	5258	time:61.4			
56					
57	12	loss:1.3852	auprc:0.5177	auroc:0.5199	ap@50:0.
	5245				
58	12	loss:1.3852	auprc:0.5188	auroc:0.5211	ap@50:0.
	5283	time:61.5			
59					
60	13	loss:1.3846	auprc:0.5233	auroc:0.5246	ap@50:0.
	5290				
61	13	loss:1.3846	auprc:0.5262	auroc:0.5257	ap@50:0.
	5330	time:61.9			
62					
63	14	loss:1.3835	auprc:0.5271	auroc:0.5288	ap@50:0.
	5291				
64	14	loss:1.3835	auprc:0.5299	auroc:0.5311	ap@50:0.
	5339	time:61.7			

65					
66	15	loss:1.3820	auprc:0.5333	auroc:0.5350	ap@50:0.
	5327				
67	15	loss:1.3820	auprc:0.5388	auroc:0.5386	ap@50:0.
	5388	time:62.2			
68					
69	16	loss:1.3797	auprc:0.5417	auroc:0.5440	ap@50:0.
	5422				
70	16	loss:1.3797	auprc:0.5465	auroc:0.5475	ap@50:0.
	5479	time:61.9			
71					
72	17	loss:1.3767	auprc:0.5511	auroc:0.5530	ap@50:0.
	5503				
73	17	loss:1.3767	auprc:0.5562	auroc:0.5571	ap@50:0.
	5566	time:62.2			
74					
75	18	loss:1.3727	auprc:0.5613	auroc:0.5639	ap@50:0.
	5603				
76	18	loss:1.3727	auprc:0.5662	auroc:0.5684	ap@50:0.
	5668	time:62.9			
77					
78	19	loss:1.3676	auprc:0.5741	auroc:0.5757	ap@50:0.
	5735				
79	19	loss:1.3676	auprc:0.5798	auroc:0.5812	ap@50:0.
	5806	time:62.5			
80					
81	20	loss:1.3611	auprc:0.5887	auroc:0.5894	ap@50:0.
	5883				
82	20	loss:1.3611	auprc:0.5944	auroc:0.5954	ap@50:0.
	5957	time:63.5			
83					
84	21	loss:1.3525	auprc:0.6046	auroc:0.6040	ap@50:0.
	6045				
85	21	loss:1.3525	auprc:0.6107	auroc:0.6107	ap@50:0.
	6123	time:61.9			
86					
87	22	loss:1.3411	auprc:0.6225	auroc:0.6204	ap@50:0.
	6224				
88	22	loss:1.3411	auprc:0.6289	auroc:0.6274	ap@50:0.
	6304	time:62.7			
89					
90	23	loss:1.3275	auprc:0.6409	auroc:0.6373	ap@50:0.
	6406				
91	23	loss:1.3275	auprc:0.6479	auroc:0.6453	ap@50:0.
	6493	time:62.5			
92					
93	24	loss:1.3111	auprc:0.6588	auroc:0.6565	ap@50:0.
	6586				
94	24	loss:1.3111	auprc:0.6660	auroc:0.6646	ap@50:0.
	6674	time:62.7			
95					

96	25	loss:1.2916	auprc:0.6771	auroc:0.6768	ap@50:0.
	6769				
97	25	loss:1.2916	auprc:0.6854	auroc:0.6857	ap@50:0.
	6868	time:63.5			
98					
99	26	loss:1.2689	auprc:0.6966	auroc:0.6981	ap@50:0.
	6966				
100	26	loss:1.2689	auprc:0.7054	auroc:0.7078	ap@50:0.
	7068	time:62.9			
101					
102	27	loss:1.2439	auprc:0.7166	auroc:0.7195	ap@50:0.
	7166				
103	27	loss:1.2439	auprc:0.7256	auroc:0.7290	ap@50:0.
	7269	time:63.0			
104					
105	28	loss:1.2166	auprc:0.7365	auroc:0.7397	ap@50:0.
	7365				
106	28	loss:1.2166	auprc:0.7454	auroc:0.7491	ap@50:0.
	7467	time:62.7			
107					
108	29	loss:1.1871	auprc:0.7541	auroc:0.7576	ap@50:0.
	7541				
109	29	loss:1.1871	auprc:0.7633	auroc:0.7671	ap@50:0.
	7644	time:63.4			
110					
111	30	loss:1.1555	auprc:0.7700	auroc:0.7739	ap@50:0.
	7700				
112	30	loss:1.1555	auprc:0.7794	auroc:0.7834	ap@50:0.
	7806	time:62.7			
113					
114	31	loss:1.1233	auprc:0.7851	auroc:0.7892	ap@50:0.
	7851				
115	31	loss:1.1233	auprc:0.7945	auroc:0.7985	ap@50:0.
	7955	time:61.6			
116					
117	32	loss:1.0909	auprc:0.7995	auroc:0.8041	ap@50:0.
	7995				
118	32	loss:1.0909	auprc:0.8091	auroc:0.8136	ap@50:0.
	8100	time:62.0			
119					
120	33	loss:1.0593	auprc:0.8139	auroc:0.8191	ap@50:0.
	8139				
121	33	loss:1.0593	auprc:0.8233	auroc:0.8287	ap@50:0.
	8242	time:61.9			
122					
123	34	loss:1.0288	auprc:0.8272	auroc:0.8334	ap@50:0.
	8272				
124	34	loss:1.0288	auprc:0.8366	auroc:0.8427	ap@50:0.
	8374	time:63.3			
125					
126	35	loss:0.9987	auprc:0.8393	auroc:0.8460	ap@50:0.

126	8392				
127	35	loss:0.9987	auprc:0.8488	auroc:0.8552	ap@50:0.
	8495	time:61.6			
128					
129	36	loss:0.9694	auprc:0.8503	auroc:0.8576	ap@50:0.
	8501				
130	36	loss:0.9694	auprc:0.8596	auroc:0.8663	ap@50:0.
	8602	time:61.5			
131					
132	37	loss:0.9417	auprc:0.8606	auroc:0.8683	ap@50:0.
	8604				
133	37	loss:0.9417	auprc:0.8692	auroc:0.8766	ap@50:0.
	8697	time:62.8			
134					
135	38	loss:0.9136	auprc:0.8705	auroc:0.8788	ap@50:0.
	8703				
136	38	loss:0.9136	auprc:0.8780	auroc:0.8862	ap@50:0.
	8785	time:62.1			
137					
138	39	loss:0.8880	auprc:0.8791	auroc:0.8884	ap@50:0.
	8791				
139	39	loss:0.8880	auprc:0.8868	auroc:0.8958	ap@50:0.
	8874	time:62.6			
140					
141	40	loss:0.8647	auprc:0.8875	auroc:0.8977	ap@50:0.
	8875				
142	40	loss:0.8647	auprc:0.8950	auroc:0.9048	ap@50:0.
	8957	time:63.2			
143					
144	41	loss:0.8423	auprc:0.8955	auroc:0.9063	ap@50:0.
	8955				
145	41	loss:0.8423	auprc:0.9021	auroc:0.9122	ap@50:0.
	9028	time:63.2			
146					
147	42	loss:0.8225	auprc:0.9018	auroc:0.9130	ap@50:0.
	9019				
148	42	loss:0.8225	auprc:0.9081	auroc:0.9183	ap@50:0.
	9087	time:62.7			
149					
150	43	loss:0.8027	auprc:0.9077	auroc:0.9189	ap@50:0.
	9078				
151	43	loss:0.8027	auprc:0.9134	auroc:0.9237	ap@50:0.
	9139	time:63.1			
152					
153	44	loss:0.7842	auprc:0.9127	auroc:0.9242	ap@50:0.
	9127				
154	44	loss:0.7842	auprc:0.9183	auroc:0.9286	ap@50:0.
	9189	time:63.1			
155					
156	45	loss:0.7676	auprc:0.9171	auroc:0.9285	ap@50:0.
	9171				

157	45	loss:0.7676 9222	auprc:0.9217 time:63.9	auroc:0.9320	ap@50:0.
158					
159	46	loss:0.7516 9202	auprc:0.9202	auroc:0.9318	ap@50:0.
160	46	loss:0.7516 9247	auprc:0.9242 time:61.7	auroc:0.9345	ap@50:0.
161					
162	47	loss:0.7363 9229	auprc:0.9229	auroc:0.9344	ap@50:0.
163	47	loss:0.7363 9269	auprc:0.9265 time:62.6	auroc:0.9368	ap@50:0.
164					
165	48	loss:0.7230 9248	auprc:0.9248	auroc:0.9364	ap@50:0.
166	48	loss:0.7230 9288	auprc:0.9284 time:63.2	auroc:0.9387	ap@50:0.
167					
168	49	loss:0.7101 9270	auprc:0.9270	auroc:0.9385	ap@50:0.
169	49	loss:0.7101 9306	auprc:0.9302 time:62.6	auroc:0.9406	ap@50:0.
170					
171	50	loss:0.6990 9288	auprc:0.9288	auroc:0.9403	ap@50:0.
172	50	loss:0.6990 9323	auprc:0.9319 time:62.9	auroc:0.9425	ap@50:0.
173					
174	51	loss:0.6882 9303	auprc:0.9302	auroc:0.9419	ap@50:0.
175	51	loss:0.6882 9341	auprc:0.9336 time:62.0	auroc:0.9441	ap@50:0.
176					
177	52	loss:0.6790 9319	auprc:0.9319	auroc:0.9437	ap@50:0.
178	52	loss:0.6790 9358	auprc:0.9354 time:61.8	auroc:0.9459	ap@50:0.
179					
180	53	loss:0.6699 9341	auprc:0.9341	auroc:0.9456	ap@50:0.
181	53	loss:0.6699 9372	auprc:0.9368 time:62.6	auroc:0.9472	ap@50:0.
182					
183	54	loss:0.6618 9356	auprc:0.9355	auroc:0.9471	ap@50:0.
184	54	loss:0.6618 9383	auprc:0.9379 time:63.2	auroc:0.9484	ap@50:0.
185					
186	55	loss:0.6545 9365	auprc:0.9365	auroc:0.9481	ap@50:0.
187	55	loss:0.6545	auprc:0.9389	auroc:0.9493	ap@50:0.

187	9392	time:63.2			
188					
189	56	loss:0.6486	auprc:0.9374	auroc:0.9489	ap@50:0.
	9375				
190	56	loss:0.6486	auprc:0.9396	auroc:0.9501	ap@50:0.
	9400	time:62.3			
191					
192	57	loss:0.6424	auprc:0.9381	auroc:0.9496	ap@50:0.
	9382				
193	57	loss:0.6424	auprc:0.9403	auroc:0.9507	ap@50:0.
	9406	time:62.7			
194					
195	58	loss:0.6370	auprc:0.9387	auroc:0.9502	ap@50:0.
	9387				
196	58	loss:0.6370	auprc:0.9408	auroc:0.9513	ap@50:0.
	9412	time:63.1			
197					
198	59	loss:0.6326	auprc:0.9392	auroc:0.9508	ap@50:0.
	9393				
199	59	loss:0.6326	auprc:0.9414	auroc:0.9518	ap@50:0.
	9417	time:63.7			
200					
201	60	loss:0.6278	auprc:0.9400	auroc:0.9513	ap@50:0.
	9400				
202	60	loss:0.6278	auprc:0.9419	auroc:0.9522	ap@50:0.
	9422	time:62.2			
203					
204	61	loss:0.6240	auprc:0.9403	auroc:0.9518	ap@50:0.
	9403				
205	61	loss:0.6240	auprc:0.9423	auroc:0.9527	ap@50:0.
	9427	time:62.7			
206					
207	62	loss:0.6205	auprc:0.9407	auroc:0.9520	ap@50:0.
	9407				
208	62	loss:0.6205	auprc:0.9428	auroc:0.9531	ap@50:0.
	9431	time:63.0			
209					
210	63	loss:0.6169	auprc:0.9409	auroc:0.9524	ap@50:0.
	9410				
211	63	loss:0.6169	auprc:0.9432	auroc:0.9535	ap@50:0.
	9435	time:62.2			
212					
213	64	loss:0.6137	auprc:0.9412	auroc:0.9527	ap@50:0.
	9413				
214	64	loss:0.6137	auprc:0.9434	auroc:0.9538	ap@50:0.
	9438	time:63.3			
215					
216	65	loss:0.6105	auprc:0.9417	auroc:0.9531	ap@50:0.
	9418				
217	65	loss:0.6105	auprc:0.9437	auroc:0.9540	ap@50:0.
	9440	time:62.0			

218					
219	66	loss:0.6089	auprc:0.9418	auroc:0.9532	ap@50:0.
	9418				
220	66	loss:0.6089	auprc:0.9439	auroc:0.9543	ap@50:0.
	9442	time:62.5			
221					
222	67	loss:0.6062	auprc:0.9421	auroc:0.9535	ap@50:0.
	9421				
223	67	loss:0.6062	auprc:0.9440	auroc:0.9545	ap@50:0.
	9444	time:63.2			
224					
225	68	loss:0.6031	auprc:0.9422	auroc:0.9537	ap@50:0.
	9423				
226	68	loss:0.6031	auprc:0.9442	auroc:0.9547	ap@50:0.
	9445	time:62.6			
227					
228	69	loss:0.6005	auprc:0.9425	auroc:0.9540	ap@50:0.
	9425				
229	69	loss:0.6005	auprc:0.9444	auroc:0.9549	ap@50:0.
	9447	time:63.7			
230					
231	70	loss:0.5988	auprc:0.9425	auroc:0.9541	ap@50:0.
	9426				
232	70	loss:0.5988	auprc:0.9446	auroc:0.9551	ap@50:0.
	9449	time:61.3			
233					
234	71	loss:0.5973	auprc:0.9427	auroc:0.9543	ap@50:0.
	9428				
235	71	loss:0.5973	auprc:0.9447	auroc:0.9553	ap@50:0.
	9451	time:63.2			
236					
237	72	loss:0.5961	auprc:0.9430	auroc:0.9545	ap@50:0.
	9430				
238	72	loss:0.5961	auprc:0.9450	auroc:0.9555	ap@50:0.
	9453	time:62.7			
239					
240	73	loss:0.5950	auprc:0.9431	auroc:0.9547	ap@50:0.
	9432				
241	73	loss:0.5950	auprc:0.9451	auroc:0.9557	ap@50:0.
	9454	time:62.8			
242					
243	74	loss:0.5934	auprc:0.9435	auroc:0.9549	ap@50:0.
	9435				
244	74	loss:0.5934	auprc:0.9454	auroc:0.9559	ap@50:0.
	9457	time:62.0			
245					
246	75	loss:0.5913	auprc:0.9434	auroc:0.9550	ap@50:0.
	9434				
247	75	loss:0.5913	auprc:0.9454	auroc:0.9560	ap@50:0.
	9457	time:63.1			
248					

249	76	loss:0.5903 9438	auprc:0.9438	auroc:0.9552	ap@50:0.
250	76	loss:0.5903 9459	auprc:0.9456 time:63.2	auroc:0.9561	ap@50:0.
251					
252	77	loss:0.5895 9439	auprc:0.9439	auroc:0.9554	ap@50:0.
253	77	loss:0.5895 9460	auprc:0.9457 time:61.8	auroc:0.9562	ap@50:0.
254					
255	78	loss:0.5889 9439	auprc:0.9438	auroc:0.9553	ap@50:0.
256	78	loss:0.5889 9460	auprc:0.9457 time:61.9	auroc:0.9562	ap@50:0.
257					
258	79	loss:0.5883 9441	auprc:0.9440	auroc:0.9555	ap@50:0.
259	79	loss:0.5883 9461	auprc:0.9458 time:63.9	auroc:0.9564	ap@50:0.
260					
261	80	loss:0.5869 9439	auprc:0.9438	auroc:0.9554	ap@50:0.
262	80	loss:0.5869 9461	auprc:0.9458 time:62.3	auroc:0.9563	ap@50:0.
263					
264	81	loss:0.5859 9439	auprc:0.9439	auroc:0.9554	ap@50:0.
265	81	loss:0.5859 9461	auprc:0.9458 time:63.8	auroc:0.9564	ap@50:0.
266					
267	82	loss:0.5852 9442	auprc:0.9441	auroc:0.9556	ap@50:0.
268	82	loss:0.5852 9462	auprc:0.9459 time:63.7	auroc:0.9565	ap@50:0.
269					
270	83	loss:0.5847 9441	auprc:0.9441	auroc:0.9556	ap@50:0.
271	83	loss:0.5847 9462	auprc:0.9458 time:63.7	auroc:0.9564	ap@50:0.
272					
273	84	loss:0.5850 9441	auprc:0.9441	auroc:0.9556	ap@50:0.
274	84	loss:0.5850 9463	auprc:0.9459 time:63.2	auroc:0.9566	ap@50:0.
275					
276	85	loss:0.5844 9440	auprc:0.9440	auroc:0.9556	ap@50:0.
277	85	loss:0.5844 9462	auprc:0.9459 time:63.3	auroc:0.9565	ap@50:0.
278					
279	86	loss:0.5833	auprc:0.9441	auroc:0.9557	ap@50:0.

279	9442				
280	86	loss:0.5833	auprc:0.9460	auroc:0.9566	ap@50:0.
	9463	time:63.1			
281					
282	87	loss:0.5821	auprc:0.9441	auroc:0.9557	ap@50:0.
	9442				
283	87	loss:0.5821	auprc:0.9460	auroc:0.9566	ap@50:0.
	9463	time:63.4			
284					
285	88	loss:0.5826	auprc:0.9441	auroc:0.9556	ap@50:0.
	9441				
286	88	loss:0.5826	auprc:0.9460	auroc:0.9566	ap@50:0.
	9463	time:62.7			
287					
288	89	loss:0.5826	auprc:0.9440	auroc:0.9556	ap@50:0.
	9441				
289	89	loss:0.5826	auprc:0.9461	auroc:0.9567	ap@50:0.
	9464	time:62.5			
290					
291	90	loss:0.5825	auprc:0.9439	auroc:0.9556	ap@50:0.
	9439				
292	90	loss:0.5825	auprc:0.9460	auroc:0.9566	ap@50:0.
	9463	time:62.9			
293					
294	91	loss:0.5821	auprc:0.9441	auroc:0.9558	ap@50:0.
	9442				
295	91	loss:0.5821	auprc:0.9461	auroc:0.9567	ap@50:0.
	9464	time:62.9			
296					
297	92	loss:0.5814	auprc:0.9441	auroc:0.9557	ap@50:0.
	9442				
298	92	loss:0.5814	auprc:0.9461	auroc:0.9567	ap@50:0.
	9464	time:62.7			
299					
300	93	loss:0.5802	auprc:0.9444	auroc:0.9559	ap@50:0.
	9445				
301	93	loss:0.5802	auprc:0.9461	auroc:0.9568	ap@50:0.
	9464	time:63.1			
302					
303	94	loss:0.5800	auprc:0.9442	auroc:0.9558	ap@50:0.
	9442				
304	94	loss:0.5800	auprc:0.9461	auroc:0.9568	ap@50:0.
	9465	time:61.9			
305					
306	95	loss:0.5799	auprc:0.9444	auroc:0.9559	ap@50:0.
	9444				
307	95	loss:0.5799	auprc:0.9461	auroc:0.9567	ap@50:0.
	9464	time:62.5			
308					
309	96	loss:0.5804	auprc:0.9443	auroc:0.9559	ap@50:0.
	9443				

310	96	loss:0.5804	auprc:0.9462	auroc:0.9568	ap@50:0.
	9465	time:61.7			
311					
312	97	loss:0.5796	auprc:0.9443	auroc:0.9558	ap@50:0.
	9443				
313	97	loss:0.5796	auprc:0.9461	auroc:0.9568	ap@50:0.
	9464	time:61.9			
314					
315	98	loss:0.5792	auprc:0.9444	auroc:0.9560	ap@50:0.
	9445				
316	98	loss:0.5792	auprc:0.9462	auroc:0.9568	ap@50:0.
	9465	time:62.1			
317					
318	99	loss:0.5791	auprc:0.9443	auroc:0.9559	ap@50:0.
	9443				
319	99	loss:0.5791	auprc:0.9462	auroc:0.9568	ap@50:0.
	9465	time:62.3			
320					
321					