

```
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:1.3868 auprc:0.4913 auroc:0.5004 ap@50:0.
28     4918
29   0 loss:1.3868 auprc:0.4942 auroc:0.5024 ap@50:0.
30     4981      time:112.3
31
32   1 loss:1.3862 auprc:0.4994 auroc:0.5052 ap@50:0.
33     5000
34   1 loss:1.3862 auprc:0.5025 auroc:0.5067 ap@50:0.
35     5064      time:108.9
36
37   2 loss:1.3860 auprc:0.5247 auroc:0.5113 ap@50:0.
38     5264
39   2 loss:1.3860 auprc:0.5283 auroc:0.5136 ap@50:0.
40     5327      time:108.8
41
42   3 loss:1.3854 auprc:0.5450 auroc:0.5158 ap@50:0.
43     5463
44   3 loss:1.3854 auprc:0.5482 auroc:0.5182 ap@50:0.
45     5520      time:108.7
46
47   4 loss:1.3841 auprc:0.5567 auroc:0.5270 ap@50:0.
48     5572
49   4 loss:1.3841 auprc:0.5614 auroc:0.5310 ap@50:0.
```

34	5642	time:110.5			
35					
36	5	loss:1.3814	auprc:0.5745	auroc:0.5430	ap@50:0.
	5748				
37	5	loss:1.3814	auprc:0.5807	auroc:0.5491	ap@50:0.
	5831	time:109.2			
38					
39	6	loss:1.3766	auprc:0.5962	auroc:0.5631	ap@50:0.
	5965				
40	6	loss:1.3766	auprc:0.6048	auroc:0.5722	ap@50:0.
	6069	time:109.1			
41					
42	7	loss:1.3686	auprc:0.6189	auroc:0.5860	ap@50:0.
	6191				
43	7	loss:1.3686	auprc:0.6290	auroc:0.5975	ap@50:0.
	6310	time:109.2			
44					
45	8	loss:1.3561	auprc:0.6432	auroc:0.6116	ap@50:0.
	6435				
46	8	loss:1.3561	auprc:0.6544	auroc:0.6245	ap@50:0.
	6563	time:109.7			
47					
48	9	loss:1.3375	auprc:0.6682	auroc:0.6391	ap@50:0.
	6684				
49	9	loss:1.3375	auprc:0.6807	auroc:0.6538	ap@50:0.
	6825	time:108.7			
50					
51	10	loss:1.3112	auprc:0.6936	auroc:0.6694	ap@50:0.
	6938				
52	10	loss:1.3112	auprc:0.7069	auroc:0.6855	ap@50:0.
	7085	time:109.1			
53					
54	11	loss:1.2765	auprc:0.7179	auroc:0.7014	ap@50:0.
	7181				
55	11	loss:1.2765	auprc:0.7328	auroc:0.7190	ap@50:0.
	7343	time:109.6			
56					
57	12	loss:1.2354	auprc:0.7415	auroc:0.7326	ap@50:0.
	7417				
58	12	loss:1.2354	auprc:0.7571	auroc:0.7506	ap@50:0.
	7586	time:109.0			
59					
60	13	loss:1.1911	auprc:0.7623	auroc:0.7604	ap@50:0.
	7625				
61	13	loss:1.1911	auprc:0.7783	auroc:0.7784	ap@50:0.
	7797	time:109.6			
62					
63	14	loss:1.1460	auprc:0.7807	auroc:0.7854	ap@50:0.
	7809				
64	14	loss:1.1460	auprc:0.7965	auroc:0.8030	ap@50:0.
	7978	time:109.3			

65					
66	15	loss:1.1019	auprc:0.7977	auroc:0.8080	ap@50:0.
	7979				
67	15	loss:1.1019	auprc:0.8132	auroc:0.8242	ap@50:0.
	8144	time:109.0			
68					
69	16	loss:1.0594	auprc:0.8138	auroc:0.8283	ap@50:0.
	8140				
70	16	loss:1.0594	auprc:0.8283	auroc:0.8432	ap@50:0.
	8295	time:108.8			
71					
72	17	loss:1.0169	auprc:0.8291	auroc:0.8471	ap@50:0.
	8293				
73	17	loss:1.0169	auprc:0.8434	auroc:0.8611	ap@50:0.
	8444	time:109.0			
74					
75	18	loss:0.9759	auprc:0.8446	auroc:0.8651	ap@50:0.
	8447				
76	18	loss:0.9759	auprc:0.8576	auroc:0.8775	ap@50:0.
	8586	time:109.9			
77					
78	19	loss:0.9364	auprc:0.8592	auroc:0.8806	ap@50:0.
	8593				
79	19	loss:0.9364	auprc:0.8704	auroc:0.8911	ap@50:0.
	8713	time:110.2			
80					
81	20	loss:0.9066	auprc:0.8731	auroc:0.8951	ap@50:0.
	8732				
82	20	loss:0.9066	auprc:0.8829	auroc:0.9040	ap@50:0.
	8838	time:110.5			
83					
84	21	loss:0.8747	auprc:0.8795	auroc:0.9010	ap@50:0.
	8796				
85	21	loss:0.8747	auprc:0.8882	auroc:0.9087	ap@50:0.
	8890	time:109.9			
86					
87	22	loss:0.8365	auprc:0.8902	auroc:0.9118	ap@50:0.
	8903				
88	22	loss:0.8365	auprc:0.8980	auroc:0.9180	ap@50:0.
	8987	time:110.8			
89					
90	23	loss:0.8165	auprc:0.8995	auroc:0.9202	ap@50:0.
	8995				
91	23	loss:0.8165	auprc:0.9062	auroc:0.9254	ap@50:0.
	9068	time:109.7			
92					
93	24	loss:0.7838	auprc:0.9042	auroc:0.9249	ap@50:0.
	9042				
94	24	loss:0.7838	auprc:0.9112	auroc:0.9299	ap@50:0.
	9117	time:110.3			
95					

96	25	loss:0.7656 9100	auprc:0.9100	auroc:0.9296	ap@50:0.
97	25	loss:0.7656 9169	auprc:0.9164 time:110.7	auroc:0.9338	ap@50:0.
98					
99	26	loss:0.7431 9166	auprc:0.9165	auroc:0.9349	ap@50:0.
100	26	loss:0.7431 9227	auprc:0.9222 time:110.7	auroc:0.9384	ap@50:0.
101					
102	27	loss:0.7251 9213	auprc:0.9213	auroc:0.9384	ap@50:0.
103	27	loss:0.7251 9269	auprc:0.9264 time:110.8	auroc:0.9416	ap@50:0.
104					
105	28	loss:0.7105 9248	auprc:0.9249	auroc:0.9411	ap@50:0.
106	28	loss:0.7105 9301	auprc:0.9297 time:110.1	auroc:0.9438	ap@50:0.
107					
108	29	loss:0.6937 9288	auprc:0.9289	auroc:0.9441	ap@50:0.
109	29	loss:0.6937 9331	auprc:0.9327 time:110.7	auroc:0.9460	ap@50:0.
110					
111	30	loss:0.6846 9315	auprc:0.9316	auroc:0.9458	ap@50:0.
112	30	loss:0.6846 9352	auprc:0.9348 time:108.8	auroc:0.9474	ap@50:0.
113					
114	31	loss:0.6694 9335	auprc:0.9335	auroc:0.9474	ap@50:0.
115	31	loss:0.6694 9373	auprc:0.9370 time:108.9	auroc:0.9490	ap@50:0.
116					
117	32	loss:0.6624 9356	auprc:0.9356	auroc:0.9488	ap@50:0.
118	32	loss:0.6624 9390	auprc:0.9387 time:108.5	auroc:0.9503	ap@50:0.
119					
120	33	loss:0.6524 9371	auprc:0.9370	auroc:0.9496	ap@50:0.
121	33	loss:0.6524 9398	auprc:0.9395 time:109.2	auroc:0.9508	ap@50:0.
122					
123	34	loss:0.6438 9382	auprc:0.9381	auroc:0.9504	ap@50:0.
124	34	loss:0.6438 9408	auprc:0.9405 time:110.0	auroc:0.9515	ap@50:0.
125					
126	35	loss:0.6400	auprc:0.9391	auroc:0.9513	ap@50:0.

126	9391				
127	35	loss:0.6400	auprc:0.9414	auroc:0.9524	ap@50:0.
	9417	time:109.0			
128					
129	36	loss:0.6314	auprc:0.9394	auroc:0.9515	ap@50:0.
	9395				
130	36	loss:0.6314	auprc:0.9418	auroc:0.9527	ap@50:0.
	9421	time:108.4			
131					
132	37	loss:0.6267	auprc:0.9402	auroc:0.9520	ap@50:0.
	9403				
133	37	loss:0.6267	auprc:0.9422	auroc:0.9531	ap@50:0.
	9426	time:109.5			
134					
135	38	loss:0.6225	auprc:0.9410	auroc:0.9528	ap@50:0.
	9410				
136	38	loss:0.6225	auprc:0.9429	auroc:0.9538	ap@50:0.
	9432	time:108.6			
137					
138	39	loss:0.6154	auprc:0.9414	auroc:0.9532	ap@50:0.
	9415				
139	39	loss:0.6154	auprc:0.9434	auroc:0.9541	ap@50:0.
	9437	time:109.0			
140					
141	40	loss:0.6124	auprc:0.9416	auroc:0.9534	ap@50:0.
	9417				
142	40	loss:0.6124	auprc:0.9438	auroc:0.9544	ap@50:0.
	9441	time:109.6			
143					
144	41	loss:0.6094	auprc:0.9423	auroc:0.9539	ap@50:0.
	9423				
145	41	loss:0.6094	auprc:0.9441	auroc:0.9548	ap@50:0.
	9445	time:109.6			
146					
147	42	loss:0.6049	auprc:0.9424	auroc:0.9541	ap@50:0.
	9425				
148	42	loss:0.6049	auprc:0.9444	auroc:0.9551	ap@50:0.
	9447	time:109.1			
149					
150	43	loss:0.6006	auprc:0.9429	auroc:0.9545	ap@50:0.
	9430				
151	43	loss:0.6006	auprc:0.9447	auroc:0.9553	ap@50:0.
	9450	time:109.5			
152					
153	44	loss:0.5992	auprc:0.9431	auroc:0.9547	ap@50:0.
	9432				
154	44	loss:0.5992	auprc:0.9448	auroc:0.9555	ap@50:0.
	9452	time:109.4			
155					
156	45	loss:0.5983	auprc:0.9431	auroc:0.9548	ap@50:0.
	9432				

157	45	loss:0.5983 9454	auprc:0.9451 time:110.1	auroc:0.9558	ap@50:0.
158					
159	46	loss:0.5957 9432	auprc:0.9432	auroc:0.9549	ap@50:0.
160	46	loss:0.5957 9455	auprc:0.9452 time:108.5	auroc:0.9559	ap@50:0.
161					
162	47	loss:0.5917 9436	auprc:0.9436	auroc:0.9552	ap@50:0.
163	47	loss:0.5917 9457	auprc:0.9454 time:109.6	auroc:0.9561	ap@50:0.
164					
165	48	loss:0.5901 9436	auprc:0.9435	auroc:0.9552	ap@50:0.
166	48	loss:0.5901 9458	auprc:0.9455 time:109.4	auroc:0.9562	ap@50:0.
167					
168	49	loss:0.5891 9438	auprc:0.9437	auroc:0.9554	ap@50:0.
169	49	loss:0.5891 9458	auprc:0.9455 time:109.8	auroc:0.9562	ap@50:0.
170					
171	50	loss:0.5893 9439	auprc:0.9438	auroc:0.9555	ap@50:0.
172	50	loss:0.5893 9460	auprc:0.9457 time:110.1	auroc:0.9564	ap@50:0.
173					
174	51	loss:0.5889 9437	auprc:0.9437	auroc:0.9554	ap@50:0.
175	51	loss:0.5889 9459	auprc:0.9456 time:108.8	auroc:0.9563	ap@50:0.
176					
177	52	loss:0.5881 9439	auprc:0.9438	auroc:0.9556	ap@50:0.
178	52	loss:0.5881 9462	auprc:0.9459 time:108.5	auroc:0.9566	ap@50:0.
179					
180	53	loss:0.5858 9438	auprc:0.9437	auroc:0.9556	ap@50:0.
181	53	loss:0.5858 9461	auprc:0.9458 time:108.9	auroc:0.9565	ap@50:0.
182					
183	54	loss:0.5835 9442	auprc:0.9442	auroc:0.9559	ap@50:0.
184	54	loss:0.5835 9463	auprc:0.9460 time:109.4	auroc:0.9567	ap@50:0.
185					
186	55	loss:0.5820 9440	auprc:0.9440	auroc:0.9557	ap@50:0.
187	55	loss:0.5820	auprc:0.9460	auroc:0.9567	ap@50:0.

187	9463	time:109.5			
188					
189	56	loss:0.5818	auprc:0.9440	auroc:0.9558	ap@50:0.
	9441				
190	56	loss:0.5818	auprc:0.9460	auroc:0.9567	ap@50:0.
	9463	time:108.8			
191					
192	57	loss:0.5818	auprc:0.9441	auroc:0.9559	ap@50:0.
	9441				
193	57	loss:0.5818	auprc:0.9462	auroc:0.9568	ap@50:0.
	9465	time:109.2			
194					
195	58	loss:0.5825	auprc:0.9440	auroc:0.9558	ap@50:0.
	9440				
196	58	loss:0.5825	auprc:0.9461	auroc:0.9567	ap@50:0.
	9464	time:110.2			
197					
198	59	loss:0.5843	auprc:0.9443	auroc:0.9561	ap@50:0.
	9443				
199	59	loss:0.5843	auprc:0.9463	auroc:0.9570	ap@50:0.
	9466	time:109.9			
200					
201	60	loss:0.5857	auprc:0.9441	auroc:0.9558	ap@50:0.
	9441				
202	60	loss:0.5857	auprc:0.9460	auroc:0.9567	ap@50:0.
	9463	time:109.0			
203					
204	61	loss:0.5844	auprc:0.9445	auroc:0.9563	ap@50:0.
	9445				
205	61	loss:0.5844	auprc:0.9465	auroc:0.9571	ap@50:0.
	9467	time:109.1			
206					
207	62	loss:0.5805	auprc:0.9441	auroc:0.9560	ap@50:0.
	9442				
208	62	loss:0.5805	auprc:0.9462	auroc:0.9569	ap@50:0.
	9465	time:109.5			
209					
210	63	loss:0.5784	auprc:0.9443	auroc:0.9561	ap@50:0.
	9443				
211	63	loss:0.5784	auprc:0.9463	auroc:0.9570	ap@50:0.
	9466	time:109.0			
212					
213	64	loss:0.5803	auprc:0.9444	auroc:0.9563	ap@50:0.
	9444				
214	64	loss:0.5803	auprc:0.9465	auroc:0.9572	ap@50:0.
	9468	time:109.9			
215					
216	65	loss:0.5814	auprc:0.9443	auroc:0.9561	ap@50:0.
	9444				
217	65	loss:0.5814	auprc:0.9462	auroc:0.9569	ap@50:0.
	9465	time:108.5			

218					
219	66	loss:0.5794	auprc:0.9446	auroc:0.9563	ap@50:0.
	9446				
220	66	loss:0.5794	auprc:0.9466	auroc:0.9572	ap@50:0.
	9469	time:109.1			
221					
222	67	loss:0.5767	auprc:0.9444	auroc:0.9562	ap@50:0.
	9445				
223	67	loss:0.5767	auprc:0.9465	auroc:0.9571	ap@50:0.
	9468	time:109.5			
224					
225	68	loss:0.5774	auprc:0.9444	auroc:0.9562	ap@50:0.
	9444				
226	68	loss:0.5774	auprc:0.9464	auroc:0.9571	ap@50:0.
	9467	time:109.0			
227					
228	69	loss:0.5783	auprc:0.9447	auroc:0.9565	ap@50:0.
	9448				
229	69	loss:0.5783	auprc:0.9467	auroc:0.9573	ap@50:0.
	9470	time:110.2			
230					
231	70	loss:0.5770	auprc:0.9444	auroc:0.9562	ap@50:0.
	9445				
232	70	loss:0.5770	auprc:0.9464	auroc:0.9571	ap@50:0.
	9467	time:108.3			
233					
234	71	loss:0.5751	auprc:0.9446	auroc:0.9564	ap@50:0.
	9447				
235	71	loss:0.5751	auprc:0.9466	auroc:0.9573	ap@50:0.
	9469	time:109.8			
236					
237	72	loss:0.5759	auprc:0.9448	auroc:0.9565	ap@50:0.
	9448				
238	72	loss:0.5759	auprc:0.9467	auroc:0.9573	ap@50:0.
	9470	time:110.1			
239					
240	73	loss:0.5769	auprc:0.9445	auroc:0.9563	ap@50:0.
	9445				
241	73	loss:0.5769	auprc:0.9465	auroc:0.9572	ap@50:0.
	9468	time:109.4			
242					
243	74	loss:0.5759	auprc:0.9450	auroc:0.9566	ap@50:0.
	9450				
244	74	loss:0.5759	auprc:0.9468	auroc:0.9574	ap@50:0.
	9471	time:108.9			
245					
246	75	loss:0.5740	auprc:0.9447	auroc:0.9564	ap@50:0.
	9448				
247	75	loss:0.5740	auprc:0.9467	auroc:0.9574	ap@50:0.
	9470	time:109.6			
248					

249	76	loss:0.5741 9449	auprc:0.9449	auroc:0.9565	ap@50:0.
250	76	loss:0.5741 9470	auprc:0.9467 time:109.4	auroc:0.9574	ap@50:0.
251					
252	77	loss:0.5748 9452	auprc:0.9451	auroc:0.9567	ap@50:0.
253	77	loss:0.5748 9472	auprc:0.9469 time:108.6	auroc:0.9575	ap@50:0.
254					
255	78	loss:0.5746 9448	auprc:0.9448	auroc:0.9565	ap@50:0.
256	78	loss:0.5746 9470	auprc:0.9467 time:108.5	auroc:0.9574	ap@50:0.
257					
258	79	loss:0.5735 9452	auprc:0.9451	auroc:0.9568	ap@50:0.
259	79	loss:0.5735 9473	auprc:0.9470 time:110.7	auroc:0.9576	ap@50:0.
260					
261	80	loss:0.5723 9450	auprc:0.9450	auroc:0.9567	ap@50:0.
262	80	loss:0.5723 9473	auprc:0.9470 time:108.7	auroc:0.9576	ap@50:0.
263					
264	81	loss:0.5724 9450	auprc:0.9449	auroc:0.9566	ap@50:0.
265	81	loss:0.5724 9473	auprc:0.9470 time:110.5	auroc:0.9576	ap@50:0.
266					
267	82	loss:0.5726 9454	auprc:0.9453	auroc:0.9570	ap@50:0.
268	82	loss:0.5726 9475	auprc:0.9472 time:110.1	auroc:0.9578	ap@50:0.
269					
270	83	loss:0.5723 9452	auprc:0.9452	auroc:0.9568	ap@50:0.
271	83	loss:0.5723 9473	auprc:0.9470 time:109.9	auroc:0.9577	ap@50:0.
272					
273	84	loss:0.5724 9454	auprc:0.9454	auroc:0.9570	ap@50:0.
274	84	loss:0.5724 9476	auprc:0.9473 time:109.5	auroc:0.9579	ap@50:0.
275					
276	85	loss:0.5716 9452	auprc:0.9451	auroc:0.9569	ap@50:0.
277	85	loss:0.5716 9475	auprc:0.9472 time:109.9	auroc:0.9578	ap@50:0.
278					
279	86	loss:0.5705	auprc:0.9455	auroc:0.9571	ap@50:0.

279	9455				
280	86	loss:0.5705	auprc:0.9474	auroc:0.9580	ap@50:0.
	9477	time:109.4			
281					
282	87	loss:0.5695	auprc:0.9455	auroc:0.9572	ap@50:0.
	9455				
283	87	loss:0.5695	auprc:0.9474	auroc:0.9580	ap@50:0.
	9477	time:109.4			
284					
285	88	loss:0.5699	auprc:0.9455	auroc:0.9571	ap@50:0.
	9455				
286	88	loss:0.5699	auprc:0.9474	auroc:0.9581	ap@50:0.
	9477	time:109.0			
287					
288	89	loss:0.5701	auprc:0.9454	auroc:0.9572	ap@50:0.
	9454				
289	89	loss:0.5701	auprc:0.9476	auroc:0.9582	ap@50:0.
	9479	time:108.9			
290					
291	90	loss:0.5704	auprc:0.9452	auroc:0.9571	ap@50:0.
	9453				
292	90	loss:0.5704	auprc:0.9475	auroc:0.9581	ap@50:0.
	9478	time:109.5			
293					
294	91	loss:0.5712	auprc:0.9458	auroc:0.9574	ap@50:0.
	9459				
295	91	loss:0.5712	auprc:0.9478	auroc:0.9584	ap@50:0.
	9481	time:109.5			
296					
297	92	loss:0.5730	auprc:0.9454	auroc:0.9572	ap@50:0.
	9454				
298	92	loss:0.5730	auprc:0.9475	auroc:0.9582	ap@50:0.
	9478	time:109.0			
299					
300	93	loss:0.5746	auprc:0.9462	auroc:0.9577	ap@50:0.
	9462				
301	93	loss:0.5746	auprc:0.9481	auroc:0.9586	ap@50:0.
	9483	time:109.5			
302					
303	94	loss:0.5758	auprc:0.9453	auroc:0.9572	ap@50:0.
	9454				
304	94	loss:0.5758	auprc:0.9474	auroc:0.9582	ap@50:0.
	9478	time:108.4			
305					
306	95	loss:0.5721	auprc:0.9463	auroc:0.9578	ap@50:0.
	9463				
307	95	loss:0.5721	auprc:0.9481	auroc:0.9586	ap@50:0.
	9484	time:109.2			
308					
309	96	loss:0.5677	auprc:0.9458	auroc:0.9576	ap@50:0.
	9458				

310	96	loss:0.5677	auprc:0.9478	auroc:0.9585	ap@50:0.
	9481	time:108.6			
311					
312	97	loss:0.5664	auprc:0.9460	auroc:0.9577	ap@50:0.
	9461				
313	97	loss:0.5664	auprc:0.9479	auroc:0.9586	ap@50:0.
	9482	time:108.6			
314					
315	98	loss:0.5690	auprc:0.9464	auroc:0.9579	ap@50:0.
	9465				
316	98	loss:0.5690	auprc:0.9483	auroc:0.9588	ap@50:0.
	9486	time:109.0			
317					
318	99	loss:0.5696	auprc:0.9461	auroc:0.9578	ap@50:0.
	9461				
319	99	loss:0.5696	auprc:0.9479	auroc:0.9586	ap@50:0.
	9482	time:109.1			
320					
321					