

```
1 ssh://sangsq@10.50.221.195:22/home/sangsq/anaconda3/bin/
  python -u /home/sangsq/flower/PSEP/model/main.py
2 loading data
3 remove 0 isolated drugs: []
4 remove finished
5 963 polypharmacy side effects
6 data has been loaded
7 cuda
8 model training ...
9   0    loss:1.3868    auprc:0.5004    auroc:0.5006    ap@50:0.
  5010
10   0    loss:1.3868    auprc:0.5042    auroc:0.5032    ap@50:0.
  5081    time:110.7
11
12   1    loss:1.3864    auprc:0.4997    auroc:0.5013    ap@50:0.
  5003
13   1    loss:1.3864    auprc:0.5026    auroc:0.5028    ap@50:0.
  5065    time:111.8
14
15   2    loss:1.3863    auprc:0.4979    auroc:0.5027    ap@50:0.
  4985
16   2    loss:1.3863    auprc:0.5004    auroc:0.5034    ap@50:0.
  5043    time:110.3
17
18   3    loss:1.3861    auprc:0.5024    auroc:0.5083    ap@50:0.
  5029
19   3    loss:1.3861    auprc:0.5058    auroc:0.5104    ap@50:0.
  5096    time:109.8
20
21   4    loss:1.3854    auprc:0.5161    auroc:0.5206    ap@50:0.
  5166
22   4    loss:1.3854    auprc:0.5214    auroc:0.5253    ap@50:0.
  5251    time:109.6
23
24   5    loss:1.3841    auprc:0.5377    auroc:0.5386    ap@50:0.
  5382
25   5    loss:1.3841    auprc:0.5445    auroc:0.5453    ap@50:0.
  5478    time:109.4
26
27   6    loss:1.3815    auprc:0.5617    auroc:0.5592    ap@50:0.
  5621
28   6    loss:1.3815    auprc:0.5705    auroc:0.5685    ap@50:0.
  5735    time:109.5
29
30   7    loss:1.3768    auprc:0.5879    auroc:0.5834    ap@50:0.
  5882
31   7    loss:1.3768    auprc:0.5986    auroc:0.5951    ap@50:0.
  6013    time:110.5
32
33   8    loss:1.3682    auprc:0.6154    auroc:0.6108    ap@50:0.
  6157
```

34	8	loss:1.3682 6305	auprc:0.6280 time:110.0	auroc:0.6249	ap@50:0.
35					
36	9	loss:1.3539 6418	auprc:0.6415	auroc:0.6392	ap@50:0.
37	9	loss:1.3539 6583	auprc:0.6560 time:111.1	auroc:0.6556	ap@50:0.
38					
39	10	loss:1.3314 6663	auprc:0.6660	auroc:0.6682	ap@50:0.
40	10	loss:1.3314 6828	auprc:0.6806 time:109.9	auroc:0.6852	ap@50:0.
41					
42	11	loss:1.2994 6871	auprc:0.6868	auroc:0.6954	ap@50:0.
43	11	loss:1.2994 7036	auprc:0.7015 time:109.5	auroc:0.7126	ap@50:0.
44					
45	12	loss:1.2586 7043	auprc:0.7040	auroc:0.7204	ap@50:0.
46	12	loss:1.2586 7212	auprc:0.7191 time:109.7	auroc:0.7376	ap@50:0.
47					
48	13	loss:1.2139 7192	auprc:0.7189	auroc:0.7431	ap@50:0.
49	13	loss:1.2139 7357	auprc:0.7336 time:109.7	auroc:0.7600	ap@50:0.
50					
51	14	loss:1.1683 7323	auprc:0.7320	auroc:0.7649	ap@50:0.
52	14	loss:1.1683 7489	auprc:0.7467 time:111.4	auroc:0.7815	ap@50:0.
53					
54	15	loss:1.1192 7537	auprc:0.7534	auroc:0.7916	ap@50:0.
55	15	loss:1.1192 7707	auprc:0.7685 time:111.1	auroc:0.8077	ap@50:0.
56					
57	16	loss:1.0674 7692	auprc:0.7689	auroc:0.8112	ap@50:0.
58	16	loss:1.0674 7856	auprc:0.7835 time:110.5	auroc:0.8260	ap@50:0.
59					
60	17	loss:1.0117 7982	auprc:0.7979	auroc:0.8380	ap@50:0.
61	17	loss:1.0117 8143	auprc:0.8123 time:109.9	auroc:0.8518	ap@50:0.
62					
63	18	loss:0.9572 8210	auprc:0.8207	auroc:0.8580	ap@50:0.
64	18	loss:0.9572	auprc:0.8343	auroc:0.8708	ap@50:0.

64	8360	time:110.5			
65					
66	19	loss:0.9087	auprc:0.8427	auroc:0.8770	ap@50:0.
	8430				
67	19	loss:0.9087	auprc:0.8556	auroc:0.8888	ap@50:0.
	8571	time:108.5			
68					
69	20	loss:0.8692	auprc:0.8656	auroc:0.8961	ap@50:0.
	8658				
70	20	loss:0.8692	auprc:0.8771	auroc:0.9056	ap@50:0.
	8784	time:109.6			
71					
72	21	loss:0.8384	auprc:0.8716	auroc:0.9012	ap@50:0.
	8718				
73	21	loss:0.8384	auprc:0.8817	auroc:0.9095	ap@50:0.
	8829	time:109.3			
74					
75	22	loss:0.8077	auprc:0.8909	auroc:0.9169	ap@50:0.
	8910				
76	22	loss:0.8077	auprc:0.8994	auroc:0.9235	ap@50:0.
	9005	time:110.2			
77					
78	23	loss:0.7751	auprc:0.8961	auroc:0.9216	ap@50:0.
	8962				
79	23	loss:0.7751	auprc:0.9032	auroc:0.9268	ap@50:0.
	9042	time:110.0			
80					
81	24	loss:0.7553	auprc:0.8995	auroc:0.9243	ap@50:0.
	8996				
82	24	loss:0.7553	auprc:0.9060	auroc:0.9291	ap@50:0.
	9070	time:109.3			
83					
84	25	loss:0.7295	auprc:0.9100	auroc:0.9325	ap@50:0.
	9102				
85	25	loss:0.7295	auprc:0.9158	auroc:0.9360	ap@50:0.
	9166	time:109.1			
86					
87	26	loss:0.7114	auprc:0.9151	auroc:0.9363	ap@50:0.
	9152				
88	26	loss:0.7114	auprc:0.9203	auroc:0.9394	ap@50:0.
	9211	time:109.5			
89					
90	27	loss:0.6962	auprc:0.9160	auroc:0.9371	ap@50:0.
	9161				
91	27	loss:0.6962	auprc:0.9212	auroc:0.9404	ap@50:0.
	9219	time:108.7			
92					
93	28	loss:0.6773	auprc:0.9213	auroc:0.9411	ap@50:0.
	9214				
94	28	loss:0.6773	auprc:0.9259	auroc:0.9436	ap@50:0.
	9266	time:109.0			

95					
96	29	loss:0.6671	auprc:0.9263	auroc:0.9444	ap@50:0.
	9264				
97	29	loss:0.6671	auprc:0.9299	auroc:0.9462	ap@50:0.
	9306	time:109.5			
98					
99	30	loss:0.6527	auprc:0.9277	auroc:0.9453	ap@50:0.
	9277				
100	30	loss:0.6527	auprc:0.9310	auroc:0.9470	ap@50:0.
	9316	time:109.6			
101					
102	31	loss:0.6444	auprc:0.9296	auroc:0.9466	ap@50:0.
	9297				
103	31	loss:0.6444	auprc:0.9329	auroc:0.9483	ap@50:0.
	9335	time:109.4			
104					
105	32	loss:0.6338	auprc:0.9334	auroc:0.9491	ap@50:0.
	9335				
106	32	loss:0.6338	auprc:0.9361	auroc:0.9503	ap@50:0.
	9367	time:110.5			
107					
108	33	loss:0.6266	auprc:0.9355	auroc:0.9503	ap@50:0.
	9356				
109	33	loss:0.6266	auprc:0.9380	auroc:0.9514	ap@50:0.
	9384	time:108.9			
110					
111	34	loss:0.6212	auprc:0.9362	auroc:0.9508	ap@50:0.
	9363				
112	34	loss:0.6212	auprc:0.9387	auroc:0.9519	ap@50:0.
	9392	time:109.4			
113					
114	35	loss:0.6142	auprc:0.9377	auroc:0.9518	ap@50:0.
	9378				
115	35	loss:0.6142	auprc:0.9399	auroc:0.9527	ap@50:0.
	9404	time:109.6			
116					
117	36	loss:0.6109	auprc:0.9392	auroc:0.9527	ap@50:0.
	9393				
118	36	loss:0.6109	auprc:0.9412	auroc:0.9535	ap@50:0.
	9416	time:109.0			
119					
120	37	loss:0.6052	auprc:0.9394	auroc:0.9530	ap@50:0.
	9395				
121	37	loss:0.6052	auprc:0.9415	auroc:0.9537	ap@50:0.
	9419	time:109.0			
122					
123	38	loss:0.6028	auprc:0.9399	auroc:0.9533	ap@50:0.
	9400				
124	38	loss:0.6028	auprc:0.9418	auroc:0.9540	ap@50:0.
	9422	time:109.3			
125					

126	39	loss:0.5986	auprc:0.9410	auroc:0.9539	ap@50:0.
	9411				
127	39	loss:0.5986	auprc:0.9426	auroc:0.9545	ap@50:0.
	9430	time:108.6			
128					
129	40	loss:0.5970	auprc:0.9414	auroc:0.9543	ap@50:0.
	9415				
130	40	loss:0.5970	auprc:0.9431	auroc:0.9548	ap@50:0.
	9435	time:109.3			
131					
132	41	loss:0.5944	auprc:0.9416	auroc:0.9544	ap@50:0.
	9416				
133	41	loss:0.5944	auprc:0.9431	auroc:0.9549	ap@50:0.
	9435	time:109.8			
134					
135	42	loss:0.5923	auprc:0.9417	auroc:0.9545	ap@50:0.
	9418				
136	42	loss:0.5923	auprc:0.9435	auroc:0.9552	ap@50:0.
	9439	time:109.1			
137					
138	43	loss:0.5906	auprc:0.9422	auroc:0.9549	ap@50:0.
	9423				
139	43	loss:0.5906	auprc:0.9439	auroc:0.9555	ap@50:0.
	9443	time:108.4			
140					
141	44	loss:0.5884	auprc:0.9425	auroc:0.9550	ap@50:0.
	9425				
142	44	loss:0.5884	auprc:0.9439	auroc:0.9555	ap@50:0.
	9443	time:109.3			
143					
144	45	loss:0.5876	auprc:0.9426	auroc:0.9551	ap@50:0.
	9426				
145	45	loss:0.5876	auprc:0.9441	auroc:0.9557	ap@50:0.
	9445	time:109.8			
146					
147	46	loss:0.5864	auprc:0.9428	auroc:0.9553	ap@50:0.
	9429				
148	46	loss:0.5864	auprc:0.9445	auroc:0.9559	ap@50:0.
	9449	time:110.3			
149					
150	47	loss:0.5844	auprc:0.9431	auroc:0.9554	ap@50:0.
	9431				
151	47	loss:0.5844	auprc:0.9446	auroc:0.9560	ap@50:0.
	9449	time:108.5			
152					
153	48	loss:0.5839	auprc:0.9430	auroc:0.9554	ap@50:0.
	9430				
154	48	loss:0.5839	auprc:0.9446	auroc:0.9561	ap@50:0.
	9450	time:109.3			
155					
156	49	loss:0.5827	auprc:0.9436	auroc:0.9558	ap@50:0.

156	9437				
157	49	loss:0.5827	auprc:0.9449	auroc:0.9563	ap@50:0.
	9453	time:108.9			
158					
159	50	loss:0.5819	auprc:0.9431	auroc:0.9555	ap@50:0.
	9431				
160	50	loss:0.5819	auprc:0.9448	auroc:0.9562	ap@50:0.
	9452	time:109.2			
161					
162	51	loss:0.5810	auprc:0.9433	auroc:0.9556	ap@50:0.
	9434				
163	51	loss:0.5810	auprc:0.9448	auroc:0.9562	ap@50:0.
	9452	time:109.4			
164					
165	52	loss:0.5808	auprc:0.9435	auroc:0.9558	ap@50:0.
	9435				
166	52	loss:0.5808	auprc:0.9451	auroc:0.9564	ap@50:0.
	9454	time:108.7			
167					
168	53	loss:0.5791	auprc:0.9436	auroc:0.9558	ap@50:0.
	9437				
169	53	loss:0.5791	auprc:0.9450	auroc:0.9564	ap@50:0.
	9454	time:108.8			
170					
171	54	loss:0.5786	auprc:0.9436	auroc:0.9558	ap@50:0.
	9437				
172	54	loss:0.5786	auprc:0.9451	auroc:0.9564	ap@50:0.
	9454	time:108.6			
173					
174	55	loss:0.5785	auprc:0.9438	auroc:0.9559	ap@50:0.
	9438				
175	55	loss:0.5785	auprc:0.9453	auroc:0.9565	ap@50:0.
	9456	time:108.9			
176					
177	56	loss:0.5779	auprc:0.9437	auroc:0.9558	ap@50:0.
	9437				
178	56	loss:0.5779	auprc:0.9452	auroc:0.9565	ap@50:0.
	9455	time:109.8			
179					
180	57	loss:0.5772	auprc:0.9436	auroc:0.9559	ap@50:0.
	9437				
181	57	loss:0.5772	auprc:0.9453	auroc:0.9566	ap@50:0.
	9456	time:109.7			
182					
183	58	loss:0.5769	auprc:0.9440	auroc:0.9561	ap@50:0.
	9440				
184	58	loss:0.5769	auprc:0.9454	auroc:0.9566	ap@50:0.
	9458	time:109.6			
185					
186	59	loss:0.5769	auprc:0.9438	auroc:0.9560	ap@50:0.
	9439				

187	59	loss:0.5769 9457	auprc:0.9453 time:111.6	auroc:0.9566	ap@50:0.
188	60	loss:0.5758 9442	auprc:0.9441	auroc:0.9561	ap@50:0.
190	60	loss:0.5758 9459	auprc:0.9456 time:109.4	auroc:0.9567	ap@50:0.
191	61	loss:0.5754 9441	auprc:0.9441	auroc:0.9561	ap@50:0.
193	61	loss:0.5754 9459	auprc:0.9456 time:108.9	auroc:0.9567	ap@50:0.
194	62	loss:0.5755 9440	auprc:0.9439	auroc:0.9560	ap@50:0.
196	62	loss:0.5755 9459	auprc:0.9456 time:110.0	auroc:0.9567	ap@50:0.
197	63	loss:0.5753 9443	auprc:0.9443	auroc:0.9562	ap@50:0.
199	63	loss:0.5753 9461	auprc:0.9457 time:109.5	auroc:0.9568	ap@50:0.
200	64	loss:0.5750 9440	auprc:0.9440	auroc:0.9561	ap@50:0.
202	64	loss:0.5750 9460	auprc:0.9456 time:109.7	auroc:0.9568	ap@50:0.
203	65	loss:0.5742 9443	auprc:0.9443	auroc:0.9563	ap@50:0.
205	65	loss:0.5742 9461	auprc:0.9458 time:110.2	auroc:0.9569	ap@50:0.
206	66	loss:0.5742 9443	auprc:0.9442	auroc:0.9563	ap@50:0.
208	66	loss:0.5742 9461	auprc:0.9457 time:110.5	auroc:0.9569	ap@50:0.
209	67	loss:0.5734 9443	auprc:0.9442	auroc:0.9563	ap@50:0.
211	67	loss:0.5734 9462	auprc:0.9458 time:110.2	auroc:0.9569	ap@50:0.
212	68	loss:0.5726 9445	auprc:0.9445	auroc:0.9564	ap@50:0.
214	68	loss:0.5726 9462	auprc:0.9459 time:108.5	auroc:0.9570	ap@50:0.
215	69	loss:0.5727 9442	auprc:0.9442	auroc:0.9563	ap@50:0.
217	69	loss:0.5727 9442	auprc:0.9459	auroc:0.9570	ap@50:0.

217	9462	time:109.1			
218					
219	70	loss:0.5723	auprc:0.9445	auroc:0.9564	ap@50:0.
	9446				
220	70	loss:0.5723	auprc:0.9460	auroc:0.9570	ap@50:0.
	9463	time:110.5			
221					
222	71	loss:0.5723	auprc:0.9443	auroc:0.9564	ap@50:0.
	9444				
223	71	loss:0.5723	auprc:0.9459	auroc:0.9570	ap@50:0.
	9463	time:109.9			
224					
225	72	loss:0.5723	auprc:0.9448	auroc:0.9567	ap@50:0.
	9448				
226	72	loss:0.5723	auprc:0.9461	auroc:0.9572	ap@50:0.
	9465	time:109.7			
227					
228	73	loss:0.5730	auprc:0.9443	auroc:0.9563	ap@50:0.
	9443				
229	73	loss:0.5730	auprc:0.9459	auroc:0.9570	ap@50:0.
	9463	time:110.0			
230					
231	74	loss:0.5748	auprc:0.9446	auroc:0.9566	ap@50:0.
	9446				
232	74	loss:0.5748	auprc:0.9464	auroc:0.9573	ap@50:0.
	9467	time:110.0			
233					
234	75	loss:0.5772	auprc:0.9442	auroc:0.9564	ap@50:0.
	9443				
235	75	loss:0.5772	auprc:0.9457	auroc:0.9569	ap@50:0.
	9460	time:109.8			
236					
237	76	loss:0.5785	auprc:0.9448	auroc:0.9567	ap@50:0.
	9449				
238	76	loss:0.5785	auprc:0.9465	auroc:0.9574	ap@50:0.
	9469	time:109.2			
239					
240	77	loss:0.5740	auprc:0.9441	auroc:0.9564	ap@50:0.
	9442				
241	77	loss:0.5740	auprc:0.9459	auroc:0.9571	ap@50:0.
	9462	time:109.7			
242					
243	78	loss:0.5703	auprc:0.9448	auroc:0.9567	ap@50:0.
	9448				
244	78	loss:0.5703	auprc:0.9462	auroc:0.9573	ap@50:0.
	9466	time:109.1			
245					
246	79	loss:0.5734	auprc:0.9449	auroc:0.9569	ap@50:0.
	9450				
247	79	loss:0.5734	auprc:0.9466	auroc:0.9575	ap@50:0.
	9469	time:109.5			

248					
249	80	loss:0.5740	auprc:0.9444	auroc:0.9566	ap@50:0.
	9444				
250	80	loss:0.5740	auprc:0.9460	auroc:0.9572	ap@50:0.
	9463	time:109.5			
251					
252	81	loss:0.5701	auprc:0.9447	auroc:0.9568	ap@50:0.
	9448				
253	81	loss:0.5701	auprc:0.9465	auroc:0.9575	ap@50:0.
	9468	time:110.0			
254					
255	82	loss:0.5705	auprc:0.9448	auroc:0.9569	ap@50:0.
	9449				
256	82	loss:0.5705	auprc:0.9465	auroc:0.9576	ap@50:0.
	9469	time:109.5			
257					
258	83	loss:0.5718	auprc:0.9445	auroc:0.9567	ap@50:0.
	9446				
259	83	loss:0.5718	auprc:0.9461	auroc:0.9573	ap@50:0.
	9464	time:108.8			
260					
261	84	loss:0.5692	auprc:0.9447	auroc:0.9568	ap@50:0.
	9448				
262	84	loss:0.5692	auprc:0.9465	auroc:0.9576	ap@50:0.
	9469	time:110.2			
263					
264	85	loss:0.5697	auprc:0.9450	auroc:0.9570	ap@50:0.
	9451				
265	85	loss:0.5697	auprc:0.9467	auroc:0.9577	ap@50:0.
	9470	time:110.0			
266					
267	86	loss:0.5701	auprc:0.9447	auroc:0.9569	ap@50:0.
	9448				
268	86	loss:0.5701	auprc:0.9463	auroc:0.9575	ap@50:0.
	9466	time:108.9			
269					
270	87	loss:0.5676	auprc:0.9452	auroc:0.9572	ap@50:0.
	9452				
271	87	loss:0.5676	auprc:0.9467	auroc:0.9577	ap@50:0.
	9470	time:109.1			
272					
273	88	loss:0.5685	auprc:0.9450	auroc:0.9571	ap@50:0.
	9451				
274	88	loss:0.5685	auprc:0.9468	auroc:0.9578	ap@50:0.
	9472	time:109.9			
275					
276	89	loss:0.5686	auprc:0.9447	auroc:0.9569	ap@50:0.
	9447				
277	89	loss:0.5686	auprc:0.9465	auroc:0.9577	ap@50:0.
	9468	time:109.8			
278					

279	90	loss:0.5672 9449	auprc:0.9448	auroc:0.9571	ap@50:0.
280	90	loss:0.5672 9472	auprc:0.9469 time:108.9	auroc:0.9579	ap@50:0.
281					
282	91	loss:0.5672 9452	auprc:0.9451	auroc:0.9572	ap@50:0.
283	91	loss:0.5672 9474	auprc:0.9470 time:109.4	auroc:0.9580	ap@50:0.
284					
285	92	loss:0.5673 9451	auprc:0.9450	auroc:0.9572	ap@50:0.
286	92	loss:0.5673 9471	auprc:0.9468 time:109.6	auroc:0.9579	ap@50:0.
287					
288	93	loss:0.5654 9454	auprc:0.9453	auroc:0.9574	ap@50:0.
289	93	loss:0.5654 9474	auprc:0.9471 time:109.0	auroc:0.9581	ap@50:0.
290					
291	94	loss:0.5653 9455	auprc:0.9455	auroc:0.9575	ap@50:0.
292	94	loss:0.5653 9476	auprc:0.9472 time:109.4	auroc:0.9582	ap@50:0.
293					
294	95	loss:0.5650 9453	auprc:0.9452	auroc:0.9574	ap@50:0.
295	95	loss:0.5650 9473	auprc:0.9470 time:109.9	auroc:0.9581	ap@50:0.
296					
297	96	loss:0.5643 9455	auprc:0.9454	auroc:0.9576	ap@50:0.
298	96	loss:0.5643 9476	auprc:0.9473 time:109.7	auroc:0.9583	ap@50:0.
299					
300	97	loss:0.5638 9457	auprc:0.9456	auroc:0.9577	ap@50:0.
301	97	loss:0.5638 9478	auprc:0.9474 time:108.5	auroc:0.9584	ap@50:0.
302					
303	98	loss:0.5636 9455	auprc:0.9455	auroc:0.9577	ap@50:0.
304	98	loss:0.5636 9476	auprc:0.9473 time:110.2	auroc:0.9583	ap@50:0.
305					
306	99	loss:0.5627 9458	auprc:0.9458	auroc:0.9578	ap@50:0.
307	99	loss:0.5627 9479	auprc:0.9476 time:109.6	auroc:0.9585	ap@50:0.
308					
309	Traceback (most recent call last):				

File - main

```
310     File "/home/sangsq/flower/PSEP/model/main.py", line 316
, in <module>
311         plt.plot(x, tr_out[0, :], label='train_prc')
312     File "/home/sangsq/anaconda3/lib/python3.7/site-packages
/matplotlib/pyplot.py", line 2811, in plot
313         is not None else {}), **kwargs)
314     File "/home/sangsq/anaconda3/lib/python3.7/site-packages
/matplotlib/__init__.py", line 1810, in inner
315         return func(ax, *args, **kwargs)
316     File "/home/sangsq/anaconda3/lib/python3.7/site-packages
/matplotlib/axes/_axes.py", line 1611, in plot
317         for line in self._get_lines(*args, **kwargs):
318     File "/home/sangsq/anaconda3/lib/python3.7/site-packages
/matplotlib/axes/_base.py", line 393, in _grab_next_args
319         yield from self._plot_args(this, kwargs)
320     File "/home/sangsq/anaconda3/lib/python3.7/site-packages
/matplotlib/axes/_base.py", line 370, in _plot_args
321         x, y = self._xy_from_xy(x, y)
322     File "/home/sangsq/anaconda3/lib/python3.7/site-packages
/matplotlib/axes/_base.py", line 231, in _xy_from_xy
323         "have shapes {} and {}".format(x.shape, y.shape))
324 ValueError: x and y must have same first dimension, but
have shapes (20,) and (100,)
325 File: /home/sangsq/flower/PSEP/model/main.py
326 Function: train at line 186
327
328 Line # Max usage Peak usage diff max diff peak Line
Contents
329 =====
=====
330     186                                     @profile
331     187                                     def train
332     ():

333     189
334     190     344.77M      364.00M    59.33M    62.00M      model
335     .train()
336     189
337     190     344.77M      364.00M    0.00B      0.00B
338     optimizer.zero_grad()
339     191     1.33G       4.80G 1012.99M    4.45G      z =
340     model.encoder(data.d_feat, data.dd_train_idx, data.
341     dd_train_et, data.dd_train_range, data.d_norm, data.p_feat
, data.pp_train_indices, data.dp_edge_index, data.
342     dp_range_list)
343     192
344     193     1.33G       1.34G    0.00B     -3.46G
345     pos_index = data.dd_train_idx
346     194     1.45G       1.59G 126.00M   254.00M
347     neg_index = negative_sampling(data.dd_train_idx, data.
348     n_drug).to(device)
349     195
350     196     1.48G       2.94G 31.42M    1.35G
```

```

340 pos_score = checkpoint(model.decoder, z, pos_index, data.
    dd_train_et)
341     197      1.51G      3.43G  31.42M  504.00M
    neg_score = checkpoint(model.decoder, z, neg_index, data.
    dd_train_et)
342     198
343     199
    pos_loss = F.binary_cross_entropy(pos_score, torch.ones(
        pos_score.shape[0]).cuda())
344     200
    neg_loss = F.binary_cross_entropy(neg_score, torch.ones(
        neg_score.shape[0]).cuda())
345     201      1.54G      1.95G  31.42M  -1.48G
    pos_loss = -torch.log(pos_score + EPS).mean()
346     202      1.57G      1.95G  31.42M  0.00B
    neg_loss = -torch.log(1 - neg_score + EPS).mean()
347     203      1.57G      1.95G  512.00B  0.00B    loss
    = pos_loss + neg_loss
348     204
    loss = pos_loss
349     205
350     206  533.66M      7.86G  -1.05G  5.90G    loss.
    backward()
351     207  533.66M  994.00M  0.00B  -6.88G
    optimizer.step()
352     208
353     209  533.66M  994.00M  0.00B  0.00B
    record = np.zeros((3, data.n_dd_et)) # auprc, auroc, ap
354     210  534.05M  996.00M  401.50K  2.00M    for i
    in range(data.dd_train_range.shape[0]):
355     211  534.05M  996.00M  0.00B  0.00B    [
    start, end] = data.dd_train_range[i]
356     212  534.05M  996.00M  0.00B  0.00B
    p_s = pos_score[start: end]
357     213  534.05M  996.00M  0.00B  0.00B
    n_s = neg_score[start: end]
358     214
359     215  534.05M  996.00M  0.00B  0.00B
    pos_target = torch.ones(p_s.shape[0])
360     216  534.05M  996.00M  0.00B  0.00B
    neg_target = torch.zeros(n_s.shape[0])
361     217
362     218  534.05M  996.00M  0.00B  0.00B
    score = torch.cat([p_s, n_s])
363     219  534.05M  996.00M  0.00B  0.00B
    target = torch.cat([pos_target, neg_target])
364     220
365     221  534.05M  996.00M  0.00B  0.00B
    record[0, i], record[1, i], record[2, i] = auprc_auroc_ap(
        target,
366     222  534.05M  996.00M  0.00B  0.00B

```

```
366
        score)
367    223
368    224    533.67M      994.00M -394.00K    -2.00M
    train_record[epoch] = record
369    225    533.67M      994.00M      0.00B      0.00B      [
    auprc, auroc, ap] = record.sum(axis=1) / data.n_dd_et
370    226    533.67M      994.00M      0.00B      0.00B
    train_out[epoch] = [auprc, auroc, ap]
371    227
372    228    533.67M      994.00M      0.00B      0.00B      print
    ('{:3d}    loss:{:0.4f}    auprc:{:0.4f}    auroc:{:0.4f}
    ap@50:{:0.4f}')
373    229    533.67M      994.00M      0.00B      0.00B
    .format(epoch, loss.tolist(), auprc, auroc, ap
    ))
374    230    344.77M      994.00M -188.90M      0.00B
375    231    533.67M      994.00M      0.00B      0.00B
    return z, loss
376
377
378 Process finished with exit code 1
379
```