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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:1.3870 auprc:0.4959 auroc:0.4999 ap@50:0.4965
10 0 loss:1.3870 auprc:0.4987 auroc:0.5013 ap@50:0.5025 time:116.9
11
12 1 loss:1.3864 auprc:0.4947 auroc:0.5010 ap@50:0.4953
13 1 loss:1.3864 auprc:0.4965 auroc:0.5011 ap@50:0.5004 time:116.2
14
15 2 loss:1.3862 auprc:0.4938 auroc:0.5032 ap@50:0.4943
16 2 loss:1.3862 auprc:0.4961 auroc:0.5040 ap@50:0.5000 time:116.2
17
18 3 loss:1.3857 auprc:0.5016 auroc:0.5116 ap@50:0.5022
19 3 loss:1.3857 auprc:0.5044 auroc:0.5136 ap@50:0.5081 time:116.1
20
21 4 loss:1.3846 auprc:0.5186 auroc:0.5242 ap@50:0.5191
22 4 loss:1.3846 auprc:0.5221 auroc:0.5283 ap@50:0.5256 time:116.2
23
24 5 loss:1.3826 auprc:0.5400 auroc:0.5395 ap@50:0.5404
25 5 loss:1.3826 auprc:0.5443 auroc:0.5454 ap@50:0.5475 time:116.2
26
27 6 loss:1.3789 auprc:0.5621 auroc:0.5578 ap@50:0.5625
28 6 loss:1.3789 auprc:0.5671 auroc:0.5651 ap@50:0.5700 time:116.2
29
30 7 loss:1.3723 auprc:0.5836 auroc:0.5790 ap@50:0.5840
31 7 loss:1.3723 auprc:0.5901 auroc:0.5881 ap@50:0.5927 time:116.2
32
33 8 loss:1.3612 auprc:0.6055 auroc:0.6035 ap@50:0.6059
34 8 loss:1.3612 auprc:0.6131 auroc:0.6143 ap@50:0.6156 time:116.2
35
36 9 loss:1.3437 auprc:0.6280 auroc:0.6309 ap@50:0.6284
37 9 loss:1.3437 auprc:0.6358 auroc:0.6429 ap@50:0.6383 time:116.1
38
39 10 loss:1.3177 auprc:0.6498 auroc:0.6607 ap@50:0.6501
40 10 loss:1.3177 auprc:0.6585 auroc:0.6735 ap@50:0.6609 time:116.2
41
42 11 loss:1.2818 auprc:0.6727 auroc:0.6915 ap@50:0.6730
43 11 loss:1.2818 auprc:0.6822 auroc:0.7051 ap@50:0.6845 time:116.2
44
45 12 loss:1.2388 auprc:0.6977 auroc:0.7220 ap@50:0.6980
46 12 loss:1.2388 auprc:0.7067 auroc:0.7352 ap@50:0.7090 time:116.2
47
48 13 loss:1.1939 auprc:0.7258 auroc:0.7523 ap@50:0.7261
49 13 loss:1.1939 auprc:0.7331 auroc:0.7636 ap@50:0.7351 time:116.1
50
51 14 loss:1.1439 auprc:0.7499 auroc:0.7781 ap@50:0.7502
52 14 loss:1.1439 auprc:0.7566 auroc:0.7886 ap@50:0.7585 time:116.1
53
54 15 loss:1.0952 auprc:0.7707 auroc:0.8001 ap@50:0.7710
55 15 loss:1.0952 auprc:0.7759 auroc:0.8088 ap@50:0.7776 time:116.1
56
57 16 loss:1.0486 auprc:0.7941 auroc:0.8225 ap@50:0.7943
58 16 loss:1.0486 auprc:0.7980 auroc:0.8301 ap@50:0.7995 time:116.1
59
60 17 loss:1.0049 auprc:0.8164 auroc:0.8437 ap@50:0.8166
61 17 loss:1.0049 auprc:0.8184 auroc:0.8496 ap@50:0.8198 time:116.1

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|     |    |             |              |              |              |            |
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| 62  |    |             |              |              |              |            |
| 63  | 18 | loss:0.9653 | auprc:0.8340 | euroc:0.8611 | ap@50:0.8342 |            |
| 64  | 18 | loss:0.9653 | auprc:0.8349 | euroc:0.8654 | ap@50:0.8362 | time:116.1 |
| 65  |    |             |              |              |              |            |
| 66  | 19 | loss:0.9293 | auprc:0.8473 | euroc:0.8743 | ap@50:0.8474 |            |
| 67  | 19 | loss:0.9293 | auprc:0.8466 | euroc:0.8765 | ap@50:0.8478 | time:116.0 |
| 68  |    |             |              |              |              |            |
| 69  | 20 | loss:0.9019 | auprc:0.8579 | euroc:0.8844 | ap@50:0.8581 |            |
| 70  | 20 | loss:0.9019 | auprc:0.8559 | euroc:0.8847 | ap@50:0.8570 | time:116.0 |
| 71  |    |             |              |              |              |            |
| 72  | 21 | loss:0.8837 | auprc:0.8644 | euroc:0.8911 | ap@50:0.8645 |            |
| 73  | 21 | loss:0.8837 | auprc:0.8605 | euroc:0.8896 | ap@50:0.8616 | time:116.0 |
| 74  |    |             |              |              |              |            |
| 75  | 22 | loss:0.8624 | auprc:0.8733 | euroc:0.8980 | ap@50:0.8734 |            |
| 76  | 22 | loss:0.8624 | auprc:0.8673 | euroc:0.8948 | ap@50:0.8683 | time:116.0 |
| 77  |    |             |              |              |              |            |
| 78  | 23 | loss:0.8382 | auprc:0.8772 | euroc:0.9019 | ap@50:0.8773 |            |
| 79  | 23 | loss:0.8382 | auprc:0.8703 | euroc:0.8977 | ap@50:0.8713 | time:116.0 |
| 80  |    |             |              |              |              |            |
| 81  | 24 | loss:0.8315 | auprc:0.8802 | euroc:0.9045 | ap@50:0.8803 |            |
| 82  | 24 | loss:0.8315 | auprc:0.8720 | euroc:0.8993 | ap@50:0.8729 | time:116.2 |
| 83  |    |             |              |              |              |            |
| 84  | 25 | loss:0.8135 | auprc:0.8844 | euroc:0.9073 | ap@50:0.8845 |            |
| 85  | 25 | loss:0.8135 | auprc:0.8753 | euroc:0.9014 | ap@50:0.8762 | time:116.0 |
| 86  |    |             |              |              |              |            |
| 87  | 26 | loss:0.8057 | auprc:0.8869 | euroc:0.9091 | ap@50:0.8871 |            |
| 88  | 26 | loss:0.8057 | auprc:0.8772 | euroc:0.9028 | ap@50:0.8781 | time:116.0 |
| 89  |    |             |              |              |              |            |
| 90  | 27 | loss:0.7960 | auprc:0.8879 | euroc:0.9100 | ap@50:0.8880 |            |
| 91  | 27 | loss:0.7960 | auprc:0.8779 | euroc:0.9035 | ap@50:0.8787 | time:116.0 |
| 92  |    |             |              |              |              |            |
| 93  | 28 | loss:0.7901 | auprc:0.8892 | euroc:0.9109 | ap@50:0.8893 |            |
| 94  | 28 | loss:0.7901 | auprc:0.8790 | euroc:0.9043 | ap@50:0.8798 | time:116.0 |
| 95  |    |             |              |              |              |            |
| 96  | 29 | loss:0.7848 | auprc:0.8912 | euroc:0.9121 | ap@50:0.8913 |            |
| 97  | 29 | loss:0.7848 | auprc:0.8804 | euroc:0.9054 | ap@50:0.8812 | time:116.0 |
| 98  |    |             |              |              |              |            |
| 99  | 30 | loss:0.7802 | auprc:0.8917 | euroc:0.9126 | ap@50:0.8918 |            |
| 100 | 30 | loss:0.7802 | auprc:0.8810 | euroc:0.9059 | ap@50:0.8818 | time:116.0 |
| 101 |    |             |              |              |              |            |
| 102 | 31 | loss:0.7773 | auprc:0.8922 | euroc:0.9129 | ap@50:0.8923 |            |
| 103 | 31 | loss:0.7773 | auprc:0.8811 | euroc:0.9060 | ap@50:0.8819 | time:116.0 |
| 104 |    |             |              |              |              |            |
| 105 | 32 | loss:0.7738 | auprc:0.8925 | euroc:0.9133 | ap@50:0.8926 |            |
| 106 | 32 | loss:0.7738 | auprc:0.8814 | euroc:0.9064 | ap@50:0.8823 | time:116.0 |
| 107 |    |             |              |              |              |            |
| 108 | 33 | loss:0.7721 | auprc:0.8931 | euroc:0.9139 | ap@50:0.8932 |            |
| 109 | 33 | loss:0.7721 | auprc:0.8820 | euroc:0.9068 | ap@50:0.8828 | time:116.0 |
| 110 |    |             |              |              |              |            |
| 111 | 34 | loss:0.7692 | auprc:0.8930 | euroc:0.9139 | ap@50:0.8931 |            |
| 112 | 34 | loss:0.7692 | auprc:0.8820 | euroc:0.9069 | ap@50:0.8828 | time:116.1 |
| 113 |    |             |              |              |              |            |
| 114 | 35 | loss:0.7676 | auprc:0.8930 | euroc:0.9139 | ap@50:0.8931 |            |
| 115 | 35 | loss:0.7676 | auprc:0.8816 | euroc:0.9068 | ap@50:0.8824 | time:116.1 |
| 116 |    |             |              |              |              |            |
| 117 | 36 | loss:0.7657 | auprc:0.8929 | euroc:0.9140 | ap@50:0.8930 |            |
| 118 | 36 | loss:0.7657 | auprc:0.8818 | euroc:0.9069 | ap@50:0.8826 | time:116.1 |
| 119 |    |             |              |              |              |            |
| 120 | 37 | loss:0.7648 | auprc:0.8934 | euroc:0.9143 | ap@50:0.8935 |            |
| 121 | 37 | loss:0.7648 | auprc:0.8822 | euroc:0.9073 | ap@50:0.8830 | time:116.1 |
| 122 |    |             |              |              |              |            |
| 123 | 38 | loss:0.7626 | auprc:0.8936 | euroc:0.9145 | ap@50:0.8937 |            |

|     |    |             |              |              |              |            |
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| 124 | 38 | loss:0.7626 | auprc:0.8823 | euroc:0.9075 | ap@50:0.8831 | time:116.1 |
| 125 |    |             |              |              |              |            |
| 126 | 39 | loss:0.7620 | auprc:0.8932 | euroc:0.9144 | ap@50:0.8933 |            |
| 127 | 39 | loss:0.7620 | auprc:0.8821 | euroc:0.9074 | ap@50:0.8829 | time:116.1 |
| 128 |    |             |              |              |              |            |
| 129 | 40 | loss:0.7597 | auprc:0.8938 | euroc:0.9148 | ap@50:0.8939 |            |
| 130 | 40 | loss:0.7597 | auprc:0.8824 | euroc:0.9076 | ap@50:0.8832 | time:116.1 |
| 131 |    |             |              |              |              |            |
| 132 | 41 | loss:0.7591 | auprc:0.8944 | euroc:0.9152 | ap@50:0.8945 |            |
| 133 | 41 | loss:0.7591 | auprc:0.8828 | euroc:0.9080 | ap@50:0.8836 | time:116.1 |
| 134 |    |             |              |              |              |            |
| 135 | 42 | loss:0.7575 | auprc:0.8939 | euroc:0.9149 | ap@50:0.8940 |            |
| 136 | 42 | loss:0.7575 | auprc:0.8827 | euroc:0.9080 | ap@50:0.8835 | time:116.2 |
| 137 |    |             |              |              |              |            |
| 138 | 43 | loss:0.7575 | auprc:0.8940 | euroc:0.9150 | ap@50:0.8941 |            |
| 139 | 43 | loss:0.7575 | auprc:0.8825 | euroc:0.9079 | ap@50:0.8833 | time:116.1 |
| 140 |    |             |              |              |              |            |
| 141 | 44 | loss:0.7558 | auprc:0.8940 | euroc:0.9151 | ap@50:0.8941 |            |
| 142 | 44 | loss:0.7558 | auprc:0.8829 | euroc:0.9082 | ap@50:0.8837 | time:116.1 |
| 143 |    |             |              |              |              |            |
| 144 | 45 | loss:0.7555 | auprc:0.8942 | euroc:0.9153 | ap@50:0.8944 |            |
| 145 | 45 | loss:0.7555 | auprc:0.8830 | euroc:0.9083 | ap@50:0.8839 | time:116.1 |
| 146 |    |             |              |              |              |            |
| 147 | 46 | loss:0.7547 | auprc:0.8945 | euroc:0.9154 | ap@50:0.8946 |            |
| 148 | 46 | loss:0.7547 | auprc:0.8828 | euroc:0.9081 | ap@50:0.8836 | time:116.3 |
| 149 |    |             |              |              |              |            |
| 150 | 47 | loss:0.7539 | auprc:0.8943 | euroc:0.9153 | ap@50:0.8944 |            |
| 151 | 47 | loss:0.7539 | auprc:0.8829 | euroc:0.9082 | ap@50:0.8837 | time:116.1 |
| 152 |    |             |              |              |              |            |
| 153 | 48 | loss:0.7540 | auprc:0.8948 | euroc:0.9156 | ap@50:0.8949 |            |
| 154 | 48 | loss:0.7540 | auprc:0.8832 | euroc:0.9084 | ap@50:0.8840 | time:116.1 |
| 155 |    |             |              |              |              |            |
| 156 | 49 | loss:0.7524 | auprc:0.8948 | euroc:0.9156 | ap@50:0.8949 |            |
| 157 | 49 | loss:0.7524 | auprc:0.8831 | euroc:0.9083 | ap@50:0.8839 | time:116.1 |
| 158 |    |             |              |              |              |            |
| 159 | 50 | loss:0.7525 | auprc:0.8946 | euroc:0.9155 | ap@50:0.8947 |            |
| 160 | 50 | loss:0.7525 | auprc:0.8831 | euroc:0.9084 | ap@50:0.8839 | time:116.1 |
| 161 |    |             |              |              |              |            |
| 162 | 51 | loss:0.7526 | auprc:0.8947 | euroc:0.9156 | ap@50:0.8948 |            |
| 163 | 51 | loss:0.7526 | auprc:0.8835 | euroc:0.9086 | ap@50:0.8843 | time:116.1 |
| 164 |    |             |              |              |              |            |
| 165 | 52 | loss:0.7508 | auprc:0.8949 | euroc:0.9156 | ap@50:0.8950 |            |
| 166 | 52 | loss:0.7508 | auprc:0.8834 | euroc:0.9086 | ap@50:0.8842 | time:116.0 |
| 167 |    |             |              |              |              |            |
| 168 | 53 | loss:0.7504 | auprc:0.8953 | euroc:0.9159 | ap@50:0.8954 |            |
| 169 | 53 | loss:0.7504 | auprc:0.8834 | euroc:0.9086 | ap@50:0.8842 | time:116.2 |
| 170 |    |             |              |              |              |            |
| 171 | 54 | loss:0.7504 | auprc:0.8952 | euroc:0.9159 | ap@50:0.8953 |            |
| 172 | 54 | loss:0.7504 | auprc:0.8837 | euroc:0.9087 | ap@50:0.8845 | time:116.1 |
| 173 |    |             |              |              |              |            |
| 174 | 55 | loss:0.7496 | auprc:0.8953 | euroc:0.9159 | ap@50:0.8954 |            |
| 175 | 55 | loss:0.7496 | auprc:0.8836 | euroc:0.9087 | ap@50:0.8844 | time:116.2 |
| 176 |    |             |              |              |              |            |
| 177 | 56 | loss:0.7494 | auprc:0.8951 | euroc:0.9158 | ap@50:0.8952 |            |
| 178 | 56 | loss:0.7494 | auprc:0.8836 | euroc:0.9087 | ap@50:0.8844 | time:116.1 |
| 179 |    |             |              |              |              |            |
| 180 | 57 | loss:0.7490 | auprc:0.8953 | euroc:0.9160 | ap@50:0.8954 |            |
| 181 | 57 | loss:0.7490 | auprc:0.8839 | euroc:0.9089 | ap@50:0.8847 | time:116.1 |
| 182 |    |             |              |              |              |            |
| 183 | 58 | loss:0.7488 | auprc:0.8951 | euroc:0.9159 | ap@50:0.8952 |            |
| 184 | 58 | loss:0.7488 | auprc:0.8837 | euroc:0.9088 | ap@50:0.8845 | time:116.2 |
| 185 |    |             |              |              |              |            |

|     |    |             |              |              |              |            |
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| 186 | 59 | loss:0.7482 | auprc:0.8955 | euroc:0.9161 | ap@50:0.8956 |            |
| 187 | 59 | loss:0.7482 | auprc:0.8839 | euroc:0.9089 | ap@50:0.8847 | time:116.0 |
| 188 |    |             |              |              |              |            |
| 189 | 60 | loss:0.7475 | auprc:0.8956 | euroc:0.9162 | ap@50:0.8957 |            |
| 190 | 60 | loss:0.7475 | auprc:0.8839 | euroc:0.9090 | ap@50:0.8847 | time:116.1 |
| 191 |    |             |              |              |              |            |
| 192 | 61 | loss:0.7476 | auprc:0.8954 | euroc:0.9161 | ap@50:0.8955 |            |
| 193 | 61 | loss:0.7476 | auprc:0.8838 | euroc:0.9089 | ap@50:0.8846 | time:116.1 |
| 194 |    |             |              |              |              |            |
| 195 | 62 | loss:0.7476 | auprc:0.8957 | euroc:0.9163 | ap@50:0.8958 |            |
| 196 | 62 | loss:0.7476 | auprc:0.8841 | euroc:0.9091 | ap@50:0.8849 | time:116.1 |
| 197 |    |             |              |              |              |            |
| 198 | 63 | loss:0.7475 | auprc:0.8953 | euroc:0.9161 | ap@50:0.8954 |            |
| 199 | 63 | loss:0.7475 | auprc:0.8840 | euroc:0.9090 | ap@50:0.8848 | time:116.1 |
| 200 |    |             |              |              |              |            |
| 201 | 64 | loss:0.7465 | auprc:0.8960 | euroc:0.9164 | ap@50:0.8960 |            |
| 202 | 64 | loss:0.7465 | auprc:0.8842 | euroc:0.9092 | ap@50:0.8850 | time:116.0 |
| 203 |    |             |              |              |              |            |
| 204 | 65 | loss:0.7459 | auprc:0.8959 | euroc:0.9165 | ap@50:0.8960 |            |
| 205 | 65 | loss:0.7459 | auprc:0.8842 | euroc:0.9092 | ap@50:0.8850 | time:116.0 |
| 206 |    |             |              |              |              |            |
| 207 | 66 | loss:0.7458 | auprc:0.8958 | euroc:0.9164 | ap@50:0.8959 |            |
| 208 | 66 | loss:0.7458 | auprc:0.8843 | euroc:0.9093 | ap@50:0.8851 | time:116.3 |
| 209 |    |             |              |              |              |            |
| 210 | 67 | loss:0.7455 | auprc:0.8960 | euroc:0.9165 | ap@50:0.8961 |            |
| 211 | 67 | loss:0.7455 | auprc:0.8844 | euroc:0.9094 | ap@50:0.8852 | time:116.1 |
| 212 |    |             |              |              |              |            |
| 213 | 68 | loss:0.7453 | auprc:0.8958 | euroc:0.9164 | ap@50:0.8959 |            |
| 214 | 68 | loss:0.7453 | auprc:0.8844 | euroc:0.9093 | ap@50:0.8852 | time:116.0 |
| 215 |    |             |              |              |              |            |
| 216 | 69 | loss:0.7456 | auprc:0.8961 | euroc:0.9166 | ap@50:0.8962 |            |
| 217 | 69 | loss:0.7456 | auprc:0.8847 | euroc:0.9095 | ap@50:0.8855 | time:116.1 |
| 218 |    |             |              |              |              |            |
| 219 | 70 | loss:0.7457 | auprc:0.8958 | euroc:0.9165 | ap@50:0.8959 |            |
| 220 | 70 | loss:0.7457 | auprc:0.8844 | euroc:0.9094 | ap@50:0.8851 | time:116.0 |
| 221 |    |             |              |              |              |            |
| 222 | 71 | loss:0.7471 | auprc:0.8967 | euroc:0.9170 | ap@50:0.8968 |            |
| 223 | 71 | loss:0.7471 | auprc:0.8850 | euroc:0.9097 | ap@50:0.8857 | time:116.1 |
| 224 |    |             |              |              |              |            |
| 225 | 72 | loss:0.7507 | auprc:0.8955 | euroc:0.9163 | ap@50:0.8957 |            |
| 226 | 72 | loss:0.7507 | auprc:0.8841 | euroc:0.9092 | ap@50:0.8849 | time:116.1 |
| 227 |    |             |              |              |              |            |
| 228 | 73 | loss:0.7531 | auprc:0.8968 | euroc:0.9171 | ap@50:0.8969 |            |
| 229 | 73 | loss:0.7531 | auprc:0.8852 | euroc:0.9099 | ap@50:0.8860 | time:116.2 |
| 230 |    |             |              |              |              |            |
| 231 | 74 | loss:0.7492 | auprc:0.8957 | euroc:0.9165 | ap@50:0.8958 |            |
| 232 | 74 | loss:0.7492 | auprc:0.8841 | euroc:0.9093 | ap@50:0.8849 | time:116.2 |
| 233 |    |             |              |              |              |            |
| 234 | 75 | loss:0.7431 | auprc:0.8964 | euroc:0.9169 | ap@50:0.8965 |            |
| 235 | 75 | loss:0.7431 | auprc:0.8849 | euroc:0.9098 | ap@50:0.8857 | time:116.1 |
| 236 |    |             |              |              |              |            |
| 237 | 76 | loss:0.7457 | auprc:0.8970 | euroc:0.9173 | ap@50:0.8971 |            |
| 238 | 76 | loss:0.7457 | auprc:0.8853 | euroc:0.9100 | ap@50:0.8861 | time:116.1 |
| 239 |    |             |              |              |              |            |
| 240 | 77 | loss:0.7484 | auprc:0.8961 | euroc:0.9167 | ap@50:0.8962 |            |
| 241 | 77 | loss:0.7484 | auprc:0.8844 | euroc:0.9096 | ap@50:0.8852 | time:116.1 |
| 242 |    |             |              |              |              |            |
| 243 | 78 | loss:0.7431 | auprc:0.8971 | euroc:0.9173 | ap@50:0.8972 |            |
| 244 | 78 | loss:0.7431 | auprc:0.8853 | euroc:0.9101 | ap@50:0.8861 | time:116.1 |
| 245 |    |             |              |              |              |            |
| 246 | 79 | loss:0.7431 | auprc:0.8969 | euroc:0.9174 | ap@50:0.8970 |            |
| 247 | 79 | loss:0.7431 | auprc:0.8854 | euroc:0.9102 | ap@50:0.8862 | time:116.1 |

|     |                                    |             |              |              |              |            |
|-----|------------------------------------|-------------|--------------|--------------|--------------|------------|
| 248 |                                    |             |              |              |              |            |
| 249 | 80                                 | loss:0.7455 | auprc:0.8963 | euroc:0.9170 | ap@50:0.8964 |            |
| 250 | 80                                 | loss:0.7455 | auprc:0.8848 | euroc:0.9099 | ap@50:0.8856 | time:116.1 |
| 251 |                                    |             |              |              |              |            |
| 252 | 81                                 | loss:0.7417 | auprc:0.8972 | euroc:0.9175 | ap@50:0.8973 |            |
| 253 | 81                                 | loss:0.7417 | auprc:0.8855 | euroc:0.9104 | ap@50:0.8863 | time:116.2 |
| 254 |                                    |             |              |              |              |            |
| 255 | 82                                 | loss:0.7417 | auprc:0.8974 | euroc:0.9177 | ap@50:0.8975 |            |
| 256 | 82                                 | loss:0.7417 | auprc:0.8857 | euroc:0.9105 | ap@50:0.8865 | time:116.2 |
| 257 |                                    |             |              |              |              |            |
| 258 | 83                                 | loss:0.7432 | auprc:0.8969 | euroc:0.9174 | ap@50:0.8970 |            |
| 259 | 83                                 | loss:0.7432 | auprc:0.8852 | euroc:0.9102 | ap@50:0.8860 | time:116.2 |
| 260 |                                    |             |              |              |              |            |
| 261 | 84                                 | loss:0.7398 | auprc:0.8975 | euroc:0.9177 | ap@50:0.8976 |            |
| 262 | 84                                 | loss:0.7398 | auprc:0.8858 | euroc:0.9106 | ap@50:0.8866 | time:116.2 |
| 263 |                                    |             |              |              |              |            |
| 264 | 85                                 | loss:0.7403 | auprc:0.8977 | euroc:0.9179 | ap@50:0.8978 |            |
| 265 | 85                                 | loss:0.7403 | auprc:0.8861 | euroc:0.9108 | ap@50:0.8869 | time:116.3 |
| 266 |                                    |             |              |              |              |            |
| 267 | 86                                 | loss:0.7412 | auprc:0.8972 | euroc:0.9176 | ap@50:0.8973 |            |
| 268 | 86                                 | loss:0.7412 | auprc:0.8856 | euroc:0.9106 | ap@50:0.8864 | time:116.1 |
| 269 |                                    |             |              |              |              |            |
| 270 | 87                                 | loss:0.7385 | auprc:0.8978 | euroc:0.9181 | ap@50:0.8979 |            |
| 271 | 87                                 | loss:0.7385 | auprc:0.8861 | euroc:0.9109 | ap@50:0.8869 | time:116.1 |
| 272 |                                    |             |              |              |              |            |
| 273 | 88                                 | loss:0.7389 | auprc:0.8983 | euroc:0.9184 | ap@50:0.8984 |            |
| 274 | 88                                 | loss:0.7389 | auprc:0.8865 | euroc:0.9111 | ap@50:0.8872 | time:116.1 |
| 275 |                                    |             |              |              |              |            |
| 276 | 89                                 | loss:0.7384 | auprc:0.8980 | euroc:0.9183 | ap@50:0.8981 |            |
| 277 | 89                                 | loss:0.7384 | auprc:0.8861 | euroc:0.9110 | ap@50:0.8869 | time:116.1 |
| 278 |                                    |             |              |              |              |            |
| 279 | 90                                 | loss:0.7363 | auprc:0.8983 | euroc:0.9185 | ap@50:0.8984 |            |
| 280 | 90                                 | loss:0.7363 | auprc:0.8866 | euroc:0.9113 | ap@50:0.8874 | time:116.2 |
| 281 |                                    |             |              |              |              |            |
| 282 | 91                                 | loss:0.7374 | auprc:0.8984 | euroc:0.9186 | ap@50:0.8985 |            |
| 283 | 91                                 | loss:0.7374 | auprc:0.8870 | euroc:0.9116 | ap@50:0.8878 | time:116.1 |
| 284 |                                    |             |              |              |              |            |
| 285 | 92                                 | loss:0.7363 | auprc:0.8984 | euroc:0.9186 | ap@50:0.8985 |            |
| 286 | 92                                 | loss:0.7363 | auprc:0.8867 | euroc:0.9115 | ap@50:0.8875 | time:116.0 |
| 287 |                                    |             |              |              |              |            |
| 288 | 93                                 | loss:0.7347 | auprc:0.8988 | euroc:0.9189 | ap@50:0.8989 |            |
| 289 | 93                                 | loss:0.7347 | auprc:0.8872 | euroc:0.9118 | ap@50:0.8879 | time:116.0 |
| 290 |                                    |             |              |              |              |            |
| 291 | 94                                 | loss:0.7347 | auprc:0.8993 | euroc:0.9193 | ap@50:0.8994 |            |
| 292 | 94                                 | loss:0.7347 | auprc:0.8875 | euroc:0.9121 | ap@50:0.8883 | time:116.0 |
| 293 |                                    |             |              |              |              |            |
| 294 | 95                                 | loss:0.7344 | auprc:0.8991 | euroc:0.9192 | ap@50:0.8992 |            |
| 295 | 95                                 | loss:0.7344 | auprc:0.8873 | euroc:0.9120 | ap@50:0.8881 | time:116.2 |
| 296 |                                    |             |              |              |              |            |
| 297 | 96                                 | loss:0.7323 | auprc:0.8995 | euroc:0.9196 | ap@50:0.8996 |            |
| 298 | 96                                 | loss:0.7323 | auprc:0.8877 | euroc:0.9123 | ap@50:0.8885 | time:116.1 |
| 299 |                                    |             |              |              |              |            |
| 300 | 97                                 | loss:0.7323 | auprc:0.8999 | euroc:0.9198 | ap@50:0.9000 |            |
| 301 | 97                                 | loss:0.7323 | auprc:0.8881 | euroc:0.9126 | ap@50:0.8888 | time:116.2 |
| 302 |                                    |             |              |              |              |            |
| 303 | 98                                 | loss:0.7318 | auprc:0.8998 | euroc:0.9198 | ap@50:0.8999 |            |
| 304 | 98                                 | loss:0.7318 | auprc:0.8879 | euroc:0.9125 | ap@50:0.8887 | time:116.1 |
| 305 |                                    |             |              |              |              |            |
| 306 | 99                                 | loss:0.7311 | auprc:0.9000 | euroc:0.9199 | ap@50:0.9001 |            |
| 307 | 99                                 | loss:0.7311 | auprc:0.8884 | euroc:0.9129 | ap@50:0.8892 | time:116.1 |
| 308 |                                    |             |              |              |              |            |
| 309 | Traceback (most recent call last): |             |              |              |              |            |

## File - main

```

310   File "/home/sangsq/flower/PSEP/model/main.py", line 283, in <module>
311       with open(out_dir + 'train_out.pkl', 'wb') as f:
312     FileNotFoundError: [Errno 2] No such file or directory: '../out_new/tip-cat(32-16)-(16-16-48-32-16)/train_out.pkl'
313 File: /home/sangsq/flower/PSEP/model/main.py
314 Function: train at line 188
315
316 Line # Max usage Peak usage diff max diff peak Line Contents
317 =====
318   188                                     @profile
319   189                                     def train():
320   190   345.04M    518.00M  59.49M  208.00M      model.train()
321   191
322   192   345.04M    518.00M  0.00B   0.00B      optimizer.zero_grad()
323   193   1.33G     5.29G  1013.39M  4.78G      z = model.encoder(data.d_feat,
324   data.dd_train_idx, data.dd_train_et, data.dd_train_range, data.d_norm, data.p_feat,
325   data.pp_train_indices, data.dp_edge_index, data.dp_range_list)
326   194
327   195   1.33G     1.49G  0.00B   -3.80G      pos_index = data.dd_train_idx
328   196   1.45G     1.74G  126.00M  252.00M      neg_index =
329   typed_negative_sampling(data.dd_train_idx, data.n_drug, data.dd_train_range).to(
330   device)
331   197
332   198   1.48G     3.09G  31.42M  1.35G      pos_score = checkpoint(model.
333   decoder, z, pos_index, data.dd_train_et)
334   199   1.51G     3.09G  31.42M  0.00B      neg_score = checkpoint(model.
335   decoder, z, neg_index, data.dd_train_et)
336   200
337   201                                     # pos_loss = F.
338   202                                     binary_cross_entropy(pos_score, torch.ones(pos_score.shape[0]).cuda())
339   203                                     # neg_loss = F.
340   204                                     binary_cross_entropy(neg_score, torch.ones(neg_score.shape[0]).cuda())
341   205   1.54G     1.64G  31.42M  -1.45G      pos_loss = -torch.log(pos_score
342   + EPS).mean()
343   206   1.57G     1.68G  32.00M  32.00M      neg_loss = -torch.log(1 -
344   neg_score + EPS).mean()
345   207   1.57G     1.64G  512.00B  -32.00M      loss = pos_loss + neg_loss
346   208   533.93M    9.47G  -1.05G  7.83G      loss.backward()
347   209   533.93M    644.00M  0.00B   -8.85G      optimizer.step()
348   210
349   211   533.93M    644.00M  0.00B   0.00B      record = np.zeros((3, data.
350   n_dd_et)) # auprc, auroc, ap
351   212   534.32M    646.00M  401.50K  2.00M      for i in range(data.
352   dd_train_range.shape[0]):
353   213   534.32M    646.00M  0.00B   0.00B      [start, end] = data.
354   dd_train_range[i]
355   214   534.32M    646.00M  0.00B   0.00B      p_s = pos_score[start: end]
356   215   534.32M    646.00M  0.00B   0.00B      n_s = neg_score[start: end]
357   216
358   217   534.32M    646.00M  0.00B   0.00B      pos_target = torch.ones(p_s
359   .shape[0])
360   218   534.32M    646.00M  0.00B   0.00B      neg_target = torch.zeros(
361   n_s.shape[0])
362   219
363   220   534.32M    646.00M  0.00B   0.00B      score = torch.cat([p_s, n_s
364   ])
365   221   534.32M    646.00M  0.00B   0.00B      target = torch.cat([
366   pos_target, neg_target])
367   222
368   223   534.32M    646.00M  0.00B   0.00B      record[0, i], record[1, i]

```

## File - main

```
353 ], record[2, i] = auprc_auroc_ap(target,
354    224  534.32M   646.00M  0.00B  0.00B
355    225
356    226  533.94M   644.00M -394.00K -2.00M  train_record[epoch] = record
357    227  533.94M   644.00M  0.00B  0.00B  [auprc, auroc, ap] = record.sum
358    228  533.94M   644.00M  0.00B  0.00B  train_out[epoch] = [auprc,
359    229
360    230  533.94M   644.00M  0.00B  0.00B  auprc:{:0.4f}  auroc:{:0.4f}  ap@50:{:0.4f}' .format(epoch, loss.
361    231  533.94M   644.00M  0.00B  0.00B  tolist(), auprc, auroc, ap))
362    232  345.04M   924.00M -188.90M  280.00M
363    233  533.94M   644.00M  0.00B  0.00B
364
365
366 Process finished with exit code 1
367
```