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1  #!/usr/bin/env python3 -B
2  """
3  xai.py: explainable multi-objective optimization
4  (c) 2025 Tim Menzies, MIT license
5
6  Input is CSV. Header (row 1) defines column roles as follows:
7  [A-Z]*: Numeric (e.g. "Age"). [a-z]*: Symbolic (e.g. "job").
8  *+ : Mximize (e.g. "Pay+"). *- : Minimize (e.g. "Cost-").
9  *X : Ignored (e.g. "idX"). ? : Missing value (not in header)
10
11 To download example data:
12 mkdir -p $HOME/gits
13 git clone http://github.com/timm/moot $HOME/gits/moot
14
15 To download code, install it, then test it, download this file then:
16 chmod +x xai.py
17 ./xai.py --xai ~/gits/moot/optimize/misc/auto93.csv
18
19 For help on command line options:
20 ./xai.py -h """
21 import ast,sys,random,re
22 from math import sqrt,exp,floor
23 from types import SimpleNamespace as obj
24 from pathlib import Path
25
26 # ATOM = str | int | float
27 # ROW = list[ATOM]
28 # ROWS = list[ROW]
29 # NUM, SYM, DATA = obj,obj,obj
30 # COL = NUM | SYM
31 # THING = COL | DATA
32 BIG=1e32
33 the=obj(bins=7, budget=50, seed=1, data="data.csv")
34
35 ### Constructors -----
36 def Sym(): return obj(it=Sym, n=0, has={})
37 def Num(): return obj(it=Num, n=0, mu=0, m2=0)
38
39 def Col(at=0, txt=" "):
40     col = (Num if txt[0].isupper() else Sym)()
41     col.at, col.txt, col.best = at, txt, 0 if txt[-1]=="-" else 1
42     return col
43
44 def Cols(names): # (list[str]) -> Cols
45     cols = [Col(n,s) for n,s in enumerate(names)]
46     return obj(it=Cols, names=names, all=cols,
47               x=[col for col in cols if col.txt[-1] not in "+-X"],
48               y=[col for col in cols if col.txt[-1] in "+-"])
49
50 def Data(rows=None):
51     return adds(rows, obj(it=Data, rows=[], n=0, cols=None, _centroid=None))
52
53 def clone(data, rows=None): return adds(rows, Data([data.cols.names]))
54
55 ### Functions -----
56 def adds(src, i=None): # (src:Iterable, ?i) -> i
57     i = i or Num(); [add(i,v) for v in src or []]; return i
58
59 def add(i, v, inc=1):
60     if v!="?":
61         if Data is i.it and not i.cols: i.cols = Cols(v) # init, not adding
62         else:
63             i.n += inc # adding
64             if Sym is i.it: i.has[v] = inc + i.has.get(v,0)
65             elif Num is i.it:
66                 if inc < 0 and i.n < 2:
67                     i.mu = i.m2 = i.n=0
68                 else:
69                     d = v-i.mu; i.mu += inc*d/i.n; i.m2 += inc*d*(v-i.mu)
70             else:
71                 i._centroid = None # old centroid now out of date
72                 [add(col, v[col.at], inc) for col in i.cols.all] # recursive add
73                 (i.rows.append if inc>0 else i.rows.remove)(v) # row storage
74     return v # convention: always return the thing being added
75
76 def norm(num,n):
77     z = (n - num.mu) / sd(num)
78     z = max(-3, min(3, z))
79     return 1 / (1 + exp(-1.7 * z))
80
81 def sd(num): return 1/BIG + (0 if num.n<2 else sqrt(max(0,num.m2)/(num.n-1)))
82
83 def mid(col): return col.mu if Num is col.it else max(col.has,key=col.has.get)
84
85 def mids(data):
86     data._centroid = data._centroid or [mid(col) for col in data.cols.all]
87     return data._centroid
88
89 def disty(data,row):
90     ys = data.cols.y
91     return sqrt(sum(abs(norm(y,row[y.at]) - y.best)**2 for y in ys) / len(ys))
92
93 def distx(data,row1,row2):
94     xs = data.cols.x
95     return sqrt(sum(_aha(x, row1[x.at], row2[x.at])**2 for x in xs) / len(xs))
96
97 def _aha(col,u,v):
98     if u==v=="?": return 1
99     if Sym is col.it: return u != v
100     u,v = norm(col,u), norm(col,v)
101     u = u if u != "?" else (0 if v>0.5 else 1)
102     v = v if v != "?" else (0 if u>0.5 else 1)
103     return abs(u - v)
104
105 ## Cutting -----
106 def score(num): return num.mu + sd(num) / (sqrt(num.n) + 1/BIG)
107
108 def select(rule, row):
109     if (x:=row[rule.at]) == "?" or rule.xlo == rule.xhi == x: return True
110     return rule.xlo <= x < rule.xhi
111
112 def cut(data, rows):
113     all_bins = (b for col in data.cols.x for b in cuts(col, rows, data))
114     return min(all_bins, key=lambda b: score(b.y), default=None)
115
116 def cuts(col, rows, data):
117     d, xys = {}, [(r[col.at], disty(data, r)) for r in rows if r[col.at]!="?"]
118     for x, y in sorted(xys):
119         k = x if Sym is col.it else floor(the.bins * norm(col, x))
120         if k not in d: d[k] = obj(at=col.at, txt=col.txt, xlo=x, xhi=x, y=Num())
121         add(d[k].y, y)
122         d[k].xhi = x
123     return _complete(col, sorted(d.values(), key=lambda b: b.xlo))
124
125 def _complete(col, lst):
126     if Num is col.it:
127         for n, b in enumerate(lst):
128             b.xlo = lst[n-1].xhi if n > 0 else -BIG
129             b.xhi = lst[n+1].xlo if n < len(lst)-1 else BIG
130     return lst

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131 ## Lib -----
132 def gauss(mid,div):
133     return mid + 2 * div * (sum(random.random() for _ in range(3)) - 1.5)
134
135 def o(v=None, DEC=3,**D):
136     if D: return o(D,DEC=DEC)
137     isa = isinstance
138     if isa(v, (int, float)): return f"round(v.DEC):_"
139     if isa(v, list): return f"[{','.join(o(k,DEC) for k in v)}]"
140     if isa(v, tuple): return f"({','.join(o(k,DEC) for k in v)})"
141     if callable(v): return v.__name__
142     if hasattr(v, "__dict__"): v = vars(v)
143     if isa(v, dict): return f"{{'+ '.join(f'{o(v[k],DEC)}' for k in v) + '}}'"
144     return str(v)
145
146 def coerce(s):
147     try: return int(s)
148     except Exception as _:
149         try: return float(s)
150         except Exception as _:
151             s=s.strip()
152             return {"true":True, "false":False}.get(s,s)
153
154 def csv(fileName):
155     with open(fileName,encoding="utf-8") as f:
156         for l in f:
157             if (l:=l.split("%")[0].strip()):
158                 yield [coerce(x) for x in l.split(",")]
159
160 def shuffle(lst): random.shuffle(lst); return lst
161
162
163

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163 #
164 def go_h(_=None):
165     ".:show help"
166     print(_doc_, "\n\nOptions:\n")
167     for k,f in globals().items():
168         if k.startswith("go_") and f.__doc__:
169             left, right = f.__doc__.split(":")
170             left = k[2:].replace("_", "-") + " " + left.strip()
171             d = f.__defaults__
172             default = f"(default: {d[0]})" if d else ""
173             print(f" {left:15} {right.strip():15} {default}")
174
175 def go_s(n=the.seed):
176     "INT: set random SEED"
177     the.seed = n; random.seed(the.seed)
178
179 def go_b(n=the.bins):
180     "INT: set number of BINS used on discretization"
181     the.bins = n
182
183 def go_B(n=the.budget):
184     "INT: set BUDGET for rows labelled each round"
185     the.budget = n
186
187 def go_all(file=the.file):
188     "FILE: run all actions that use a FILE"
189     for k,fun in globals().items():
190         if k.startswith("go_") and k != "go_all":
191             print("\n# ", k, " "); fun(file)
192
193 def go_num(_=None):
194     ".:test Nums"
195     num = adds(gauss(10, 2) for _ in range(1000))
196     print(o(mu=num.mu, sd=sd(num)))
197     assert 9.9 <= num.mu <= 10.1 and 1.9 <= sd(num) <= 2.1
198
199 def go_sym(_=None):
200     ".:test Syms"
201     sym = adds('Previously, we have defined an iterative data mining', Sym())
202     print(sym.has)
203     assert sym.has["a"]==5
204
205 def go_csv(file=the.file):
206     "FILE: test csv loading"
207     total=0
208     for n,row in enumerate(csv(file)):
209         if n > 0: total += len(row)
210         if n > 0: assert isinstance(row[1], (float,int))
211         if n % 40==0: print(row)
212     assert 3184 == total
213
214 def go_data(file=the.file):
215     "FILE: test adding columns from file"
216     data = Data(csv(file))
217     total = sum(len(row) for row in data.rows)
218     print(*data.cols.names)
219     assert Num in data.cols.all[0].it
220     assert 3184 == total
221     for col in data.cols.x: print(o(col))
222
223 def go_clone(file=the.file):
224     "FILE: test echoing structure of a table to a new table"
225     data1 = Data(csv(file))
226     data2 = clone(data1, data1.rows)
227     assert data1.cols.x[1].mu == data2.cols.x[1].mu
228
229 def go_distx(file=the.file):
230     "FILE: can we sort rows by their distance to one row?"
231     data=Data(csv(file))
232     print(*data.cols.names, "distx", sep=",")
233     r1 = data.rows[0]
234     data.rows.sort(key=lambda r2: distx(data, r1, r2))
235     for n,r2 in enumerate(data.rows[1:]):
236         assert 0 <= distx(data, r1, r2) <= 1
237         if n%40==0: print(*r2, o(distx(data, r1, r2)), sep=",")
238
239 def go_disty(file=the.file):
240     "FILE: can we sort rows by their distance to heaven?"
241     data=Data(csv(file))
242     print(*data.cols.names, "disty", sep=",")
243     data.rows.sort(key=lambda r: disty(data, r))
244     for n,r1 in enumerate(data.rows):
245         if n>0:
246             r2=data.rows[n-1]
247             assert disty(data, r1) >= disty(data, r2)
248             if n%40==0: print(*r1, o(disty(data, r1)), sep=",")
249
250 def go_bins(file=the.file):
251     "FILE: show the rankings of a range"
252     data = Data(csv(file))
253     all_bins = (b for col in data.cols.x for b in cuts(col, data.rows, data))
254     for b in sorted(all_bins, key=lambda b: score(b.y)):
255         print(b.txt, b.xlo, b.xhi, o(mu=b.y.mu, sd=sd(b.y)), n=b.y.n,
256               scored=score(b.y)), sep="\n")
257
258 def go_xai(file=the.file):
259     "FILE: can we succinctly list main effects in a table?"
260     print("\n"+re.sub(r"^\s/", "", file))
261     xai(Data(csv(file)))
262
263 def xai(data, rows=None, loud=True):
264     if loud:
265         print("x:", len(data.cols.x))
266         print("y:", len(data.cols.y))
267         print("r:", len(data.rows))
268         print("b:", the.bins)
269     def goals(data, row): return [row[goal.at] for goal in data.cols.y]
270     if loud: print(*goals(data, data.cols.names), sep=",")
271     def show(n): return "\u221e" if n==BIG else "\u221e" if n==BIG else o(n)
272     def go(rows, lvl=0, prefix=""):
273         ys = Num(); rows.sort(key=lambda row: add(ys, disty(data, row)))
274         if loud:
275             print(f"[o(goals(data.mids(clone(data,rows))))]: {o(mu=ys.mu, n=ys.n, sd=sd(ys)):2s} {prefix}")
276         if rule := cut(data, rows):
277             rules.append(rule)
278             now = [row for row in rows if select(rule, row)]
279             if 2 < len(now) < len(rows):
280                 txt = rule.xlo if rule.xlo==rule.xhi \
281                     else f"[(show(rule.xlo)) .. {show(rule.xhi)}]"
282                 return go(now, lvl + 1, f"{rule.txt} is {txt}")
283         return rules, rows
284     rules=[]
285     return go(rows or data.rows, 0)
286
287 def go_lurch(file=the.file):
288     "FILE: can we succinctly list main effects in a table using random selection?"
289     print("\n"+re.sub(r"^\s/", "", file))
290     data = Data(csv(file))
291     ninety, few, br=Num(), Num(), Num()
292     Y= lambda row: disty(data, row)

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293 def learn(train, test):
294     labelled=clone(data, train)
295     _best= xai(labelled, loud=False)
296     bmid = mids(clone(data, best))
297     return sorted(test, key=lambda row: distx(labelled, row, bmid))
298
299 def poles(train, test):
300     train.sort(key=lambda row: disty(data, row))
301     n=int(sqrt(len(train)))
302     bmid, rmid = mids(clone(data, train[:n])), mids(clone(data, train[n:]))
303     seen=clone(data, train)
304     return sorted(test, key=lambda r: distx(seen, r, bmid) - distx(seen, r, rmid))
305
306 def check(rows): return Y(min(rows[:5], key=Y))
307
308 for _ in range(20):
309     rows = shuffle(data.rows)
310     train1 = rows[:int(0.9*len(rows))]
311     train2 = rows[:the.budget]
312     test = rows[len(rows)//2:]
313     add(ninety, check(learn(train1, test)))
314     add(few, check(learn(train2, test)))
315     add(br, check(learn(train2, test)))
316
317 all = adds(Y(row) for row in data.rows)
318 print("b", o(mu=all.mu, sd=sd(all)), sep="\n")
319 print("90%", o(mu=ninety.mu, sd=sd(ninety)), sep="\n")
320 print(f"rules[{the.budget+5}]", o(mu=few.mu, sd=sd(few)), sep="\n")
321 print("br", o(mu=br.mu, sd=sd(br)), sep="\n")
322
323 if __name__ == "__main__":
324     go_s(1)
325     for n, s in enumerate(sys.argv):
326         if fn := vars().get(f"go{s.replace('-', '_')}"):
327             fn(coerce(sys.argv[n+1])) if n < len(sys.argv) - 1 else fn()

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