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1
2 from importlib.resources import path
3 from math import ceil
4 from struct import unpack
5 from qiskit import QuantumCircuit
6 from qiskit.visualization import circuit_drawer
7 from matplotlib import pyplot as plt
8 import datetime
9 import numpy as np
10
11 N = 4
12 WIRES = 10
13 TEST = "NOT"
14 RANDOMSTACTICS = True
15 STRATEGY = "PRODUCT"
16 OUTSIDE_OF_CIRCUIT = WIRES + 1
17 PATHFILE = {
18     "NOT" : "./LiH",
19     "YES" : "./LiH_test",
20     "PRODUCT" : "./LiH_test_product_space"
21 }[TEST]
22
23
24 class local_Hamiltonian():
25     def __init__(self, tensor, weight) -> None:
26         self.tensor = tensor
27         self.weight = weight
28         self.parent = self
29
30     def tensorspace(self, other) -> bool:
31         for A,B in zip( list(self.tensor), list(other.tensor)):
32             if "I" not in [A, B]:
33                 return False
34         return True
35
36     def dis(self, other) -> int:
37         ret = 0
38         for A,B in zip(list(self.tensor), list(other.tensor)):
39             if A != B:
40                 ret += 1
41         return ret
42
43     def solid_product(self, other):
44         indices = []
45         for j in range(1,WIRES):
46             l= "X" * j + "I" * (WIRES-j)
47             r = "I" * j + "X" * (WIRES-j)
48             if local_Hamiltonian(l,0).tensorspace(self) and\
49                 local_Hamiltonian(r,0).tensorspace(other):
50                 indices.append(j)
51
52         if len(indices) > 0:
53             return True, indices
54         return False, []
55
56     def newbase(self, perm):
57         tensor = [ "" ] * len(self.tensor)
58         for i in range(len(perm)):
59             tensor[i] = self.tensor[perm[i]]
60         ret = local_Hamiltonian(tensor,self.weight)
61         ret.parent = self.parent
62         return ret
63

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64     def median(self):
65         support = list(filter( lambda x : self.tensor[x] != 'I', range(WIRES)))
66         if len(support) != 0:
67             return support[int(len(support)/2)]
68         return 0
69
70     def seconed_wires(self):
71         j = self.median()
72
73         def find_nearset_nontrival(sign):
74
75
76             gen = [ (i,v) for i,v in list(enumerate(self.tensor))[j+1:]] if sign ==1\
77                     else [ (i,v) for i,v in list(enumerate(self.tensor))[j-1::-1]]
78
79             for i,v in gen:
80                 if v != "I":
81                     return i
82             return j
83
84             pos_wire = j
85             neg_wire = j
86             if j + 1 < WIRES:
87                 pos_wire = find_nearset_nontrival(1)
88             if j - 1 >= 0:
89                 neg_wire = find_nearset_nontrival(-1)
90
91             return neg_wire, pos_wire
92
93     def parser_line(line) -> local_Hamiltonian:
94         line = line.split()
95         return local_Hamiltonian( list(line[-1]),
96             { "-" : -1 , "+" : 1 }[line[0]] * np.float64(line[1]) / N )
97
98     def parser() -> None:
99         hamiltonians = [ ]
100         for line in open(PATHFILE).readlines():
101             if len(line) > 1:
102                 hamiltonians.append(parser_line(line))
103         return hamiltonians
104
105     def donothing(_):
106         pass
107
108     def rotateY(cir):
109         def _func(wire):
110             cir.s(wire)
111             cir.h(wire)
112         return _func
113
114     def unrotateY(cir):
115         def _func(wire):
116             cir.h(wire)
117             cir.sdg(wire)
118         return _func
119
120     def MulByterm (circuit : QuantumCircuit, term ,next_terms = [], last_terms = [],
121         main_wire = WIRES-1) -> QuantumCircuit:
122
123         def reqursive_manner(tensor, wire, weight, last_wire, _sign, first_not_trival=True):
124
125             if wire < 0 or wire == WIRES:
126                 return QuantumCircuit(WIRES),QuantumCircuit(WIRES)
127

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128     compute = {
129         "X" : lambda cir : cir.h,
130         "Y" : lambda cir : rotateY(cir),
131         "Z" : lambda cir : donothing,
132         "I" : lambda cir : donothing }
133
134
135     uncompute = {
136         "X" : lambda cir : cir.h,
137         "Y" : lambda cir : unrotateY(cir),
138         "Z" : lambda cir : donothing,
139         "I" : lambda cir : donothing }
140
141     pauli = tensor[wire]
142     if wire == main_wire:
143         circuit_node = QuantumCircuit(WIRES)
144         LU, RU = reursive_manner(tensor, wire-1, weight, last_wire, -1, first_not_trival = True)
145         LD, RD = reursive_manner(tensor, wire+1, weight, last_wire, 1, first_not_trival = True)
146
147         compute[pauli](circuit_node)(wire)
148         for L in [ LD, LU]:
149             circuit_node = circuit_node.compose(L)
150         circuit_node.rz(2*weight, main_wire)
151         for R in [ RD, RU]:
152             circuit_node = circuit_node.compose(R)
153         uncompute[pauli](circuit_node)(wire)
154         return circuit_node
155
156     if pauli == 'I':
157
158
159         # temp_wire = last_wire + _sign if first_not_trival else last_wire
160         return reursive_manner(tensor, wire + _sign, weight,
161             last_wire, _sign, first_not_trival = first_not_trival)
162
163     else:
164
165         temp_wire = wire if first_not_trival else last_wire
166         parity_collector = False
167         if first_not_trival:
168             parity_collector = True
169
170
171         L, R = reursive_manner(tensor, wire + _sign, weight, temp_wire, _sign, first_not_trival =
False)
172         circuit_left, circuit_right = QuantumCircuit(WIRES), QuantumCircuit(WIRES)
173
174         if (parity_collector) or not ( \
175             (last_terms[wire][0] == pauli) and \
176             (last_terms[wire][1][ { 1 : 1 , -1 : 0 }[_sign] ] == last_wire)):
177
178             compute[pauli](circuit_left)(wire)
179             circuit_left = circuit_left.compose(L)
180             circuit_left.cx(wire, last_wire)
181
182         else:
183             circuit_left = L
184
185         if (parity_collector) or not ( \
186             (next_terms[wire][0] == pauli) and \
187             (next_terms[wire][1][ { 1 : 1 , -1 : 0 }[_sign] ] == last_wire)):
188
189             circuit_right.cx(wire, last_wire)
190             circuit_right = circuit_right.compose(R)

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191         uncompute[pauli](circuit_right)(wire)
192     else:
193         circuit_right = R
194     return circuit_left, circuit_right
195
196 circuit = circuit.compose(reursive_manner(term.tensor, main_wire, term.weight, main_wire, 0))
197 return circuit
198
199
200
201 def cutting(circuit : QuantumCircuit):
202     '''Second optimization, cuts the gates which are followed by their
203     uncompute '''
204     def filter_by_wire(wire):
205         return list(filter( lambda item :\
206             any( [register.index == wire for register in item[1][1]] ), enumerate(circuit.data) ))
207
208
209     UNCOMPTE = {
210         "h" : "h",
211         "cx" : "?",
212         "rz" : "?",
213         "s" : "sdg",
214         "sdg" : "s",
215         "sxdg" : "?" }
216
217     indices_todelete = []
218     for wire in range(WIRES):
219         operators = filter_by_wire(wire)
220
221         j = 0
222         while (j < len(operators) - 1 ):
223             if ( UNCOMPTE[operators[j][1][0].name] == operators[j+1][1][0].name ):
224                 indices_todelete.append( operators[j][0] )
225                 indices_todelete.append( operators[j+1][0] )
226             j += 1
227
228     for index in reversed(sorted(indices_todelete)):
229         circuit.data.pop(index)
230
231     return circuit
232
233
234 def genreate_circuit(terms = None):
235     circuit = QuantumCircuit(WIRES)
236     terms = parser() if terms == None else terms
237     print(len(terms))
238     for i, term in enumerate(terms):
239
240         main_wire = term.median()
241         next_terms,last_terms = [],[]
242
243         for _j in range(WIRES):
244             found = False
245             if i+1 < len(terms):
246                 for _term in terms[i+1:]:
247                     if _term.tensor[_j] != 'I':
248                         next_terms.append( (_term.tensor[_j], _term.seconed_wires() ))
249                         found = True
250                     break
251             if not found:
252                 next_terms.append( ('I', OUTSIDE_OF_CIRCUIT ))
253
254         found = False

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255         if i > 0:
256             for _term in terms[i-1::-1]:
257                 if _term.tensor[_j] != 'I':
258                     last_terms.append( (_term.tensor[_j], _term.seconed_wires() ))
259                     found = True
260                     break
261             if not found:
262                 last_terms.append( ('I', OUTSIDE_OF_CIRCUIT ))
263
264         circuit = MulByterm(circuit, term, main_wire=main_wire,
265                             next_terms=next_terms, last_terms=last_terms )
266
267     return circuit
268
269 def genreate_optimized_circut(circuit, terms, svg =False, entire = False):
270     circuit = cutting(cutting(circuit))
271
272     if entire:
273         for _ in range(ceil(np.log(N))):
274             circuit = circuit.compose(circuit)
275             circuit = cutting(circuit)
276
277     print(f"TERMS: {len(terms)}, DEPTH:{circuit.depth()}")
278
279     if svg:
280         circuit_drawer(circuit, output='mpl',style="bw", fold=-1)
281         plt.title( f"TERMS: {len(terms)}, DEPTH:{circuit.depth()}")
282         plt.tight_layout()
283         plt.savefig(f'Ham_{STRATEGY}-{datetime.datetime.now()}.svg')
284
285     if entire:
286         open(f"Ham_{STRATEGY}-{datetime.datetime.now()}.qasm", "w+").write(circuit.qasm())
287
288     return circuit.depth()
289
290
291

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```

1 from copy import deepcopy
2 import networkx as nx
3 from Hamiltonian_parser import WIRES, parser, local_Hamiltonian, generate_circuit, generate_optimized_circuit
4 from itertools import permutations, product, combinations
5 from random import choice
6 import pickle as pkl
7
8 from matplotlib import pyplot as plt
9
10
11 class Permutation_Base():
12     def __init__(self, arr) -> None:
13         self.arr = arr
14         self.parent = self
15
16
17 def generated_the_product_graph(terms = parser()):
18     def generated_the_product_graph_by_base(_terms, number_premu=0):
19
20         G = nx.Graph()
21         Gproduct = nx.Graph()
22
23         edges_set = set()
24
25         for (H1, H2) in product(_terms, _terms):
26             if H1.tensorspace(H2):
27                 G.add_edge(H1, H2)
28                 edges_set.add( (H1,H2) )
29                 G.edges[(H1, H2)]['weight'] = H1.dis(H2)
30                 G.edges[(H1, H2)]['solid'] = True
31                 G.edges[(H1, H2)]['permutation'] = j
32
33         for e in G.edges():
34             H1,H2 = e
35             for H3,H4 in \
36                 product(list(G.adj[H1]),list(G.adj[H2])):
37                 if (H1,H4) in edges_set and\
38                     (H3,H4) in edges_set and\
39                     (H2,H3) in edges_set:
40                     Gproduct.add_edge((H1,H2), (H3, H4))
41                     Gproduct.edges[(H1, H2), (H3, H4)]['weight'] = max(H1.dis(H3), H2.dis(H4))
42                     Gproduct.edges[(H1, H2), (H3, H4)]['solid'] = True
43                     Gproduct.edges[(H1, H2), (H3, H4)]['permutation'] = j
44
45         for (H1, H2) in product(_terms, _terms):
46             if (H1,H2) not in edges_set:
47                 G.add_edge(H1, H2)
48                 G.edges[(H1, H2)]['weight'] = H1.dis(H2)
49                 G.edges[(H1, H2)]['solid'] = False
50                 G.edges[(H1, H2)]['permutation'] = j
51
52         print(f"vertices:{Gproduct.number_of_nodes()}\t edges: ~{Gproduct.number_of_edges()}")
53         return Gproduct, G, _terms
54
55     return pkl.load( open(f"mainG-276-1.pkl", "br"))
56
57 permutations = list(map(lambda x: Permutation_Base(x) , [
58     # [0,2,4,6,8,1,3,5,7,9],
59     [0,1,2,3,4,5,6,7,8,9]
60     # [0,7,4,6,8,9,3,5,2,1]
61 ]))
62 graphs = []
63 perm_terms = []

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64     mainG = nx.Graph()
65     mainProductG = nx.Graph()
66     for j, permutation in enumerate(permutations):
67         perm_terms = list(map( lambda x : x.newbase(permutation.arr), terms))
68         productG, G, _ = generated_the_product_graph_by_base(perm_terms, number_premu=j)
69
70         if mainG.number_of_nodes() == 0:
71             mainG = nx.compose(mainG, G)
72             mainProductG = nx.compose(mainProductG, productG)
73
74     pickle.dump((mainG, mainProductG, terms ,permutations), open(f"mainG-{len(terms)}-
{len(permutations)}.pkl", "bw+"))
75     return mainG, mainProductG, terms, permutations
76
77 def select(_list, v, G, flag = True):
78     minimal = min(_list, key =lambda u : G.edges[v,u]['weight'] )
79     return choice( [r for r in _list if G.edges[v,r]['weight'] == \
80         G.edges[v,minimal]['weight'] ])
81
82 def notcolorized(node, _set):
83     if isinstance(node, tuple):
84         term1, term2 = node
85         if (term1.parent in _set) or (term2.parent in _set):
86             return False
87         return True
88     else:
89         return node.parent not in _set
90
91 def colirize(node, _set):
92     if isinstance(node, tuple):
93         term1, term2 = node
94
95         if (term1.parent in _set) or (term2.parent in _set):
96             return False, _set, 1
97         _set.add(term1.parent)
98         _set.add(term2.parent)
99         return True
100    else:
101        if node.parent in _set:
102            return False
103        else:
104            _set.add(node.parent)
105            return True
106
107
108 #randomized DFS.
109 def sample_path(G, terms) -> tuple((nx.Graph, set)):
110     print("sample_path")
111     color = set()
112
113     def DFS(v, T, _color, sign=0, flag =True):
114
115         if not colirize(v, _color):
116             return _color, sign
117
118         can_packed = [None]
119         while len(can_packed) > 0 :
120             can_packed = list(filter(lambda x :\
121                 notcolorized(x, _color), G.adj[v]))
122
123             if len(can_packed) > 0:
124                 u = select( can_packed, v, G, flag=flag)
125                 T.add_edge(v,u)
126                 if 'permutation' in G.edges[v,u]:

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127         T.edges[v,u]['permutation'] = G.edges[v,u]['permutation']
128         T.edges[v,u]['sign'] = sign
129         _color, sign = DFS(u, T, _color, sign=sign+1, flag=flag)
130     return _color, sign
131
132     T = nx.DiGraph()
133     l = []
134
135     for v in G.nodes():
136         T.add_node(v)
137         l.append(v)
138
139     _sign = 0
140     for v in G.nodes():
141         color, _sign = DFS(v, T, color, sign=_sign, flag=False)
142
143     return T, color
144
145 def get_Diameter(Tree: nx.Graph) -> tuple((tuple([], int)), tuple([], int))) :
146
147     def DFS_tree_depth(G, v):
148
149         if len(list(G.adj[v])) == 0 :
150             return ([v], 1), ([v], 1)
151
152         branches = []
153         maxinnerpath, maxinnerdepth = [], 0
154         for u in list(G.adj[v]):
155             ((temppath, tempdepth), \
156              (tempinnerpath, tempinnerdepth)) = DFS_tree_depth(G, u)
157
158             if maxinnerdepth < tempinnerdepth:
159                 maxinnerpath, maxinnerdepth = tempinnerpath, tempinnerdepth
160
161             branches.append((temppath, tempdepth))
162
163         maxpath, maxdepth = [], 0
164
165         for (b1, d1), (b2, d2) in combinations(branches, r=2):
166             if 1 + d1 + d2 > maxinnerdepth:
167                 maxinnerpath = b1 + [v] + b2
168                 maxinnerdepth = 1 + d1 + d2
169
170         for b, d in branches:
171             if 1 + d > maxdepth:
172                 maxpath = [v] + b
173                 maxdepth = 1 + d
174         return ((maxpath, maxdepth), (maxinnerpath, maxinnerdepth))
175
176     ((maxpath, maxdepth), (maxinnerpath, maxinnerdepth)) = DFS_tree_depth(Tree, list(Tree.nodes)[0])
177     print(maxdepth, maxinnerdepth)
178     return maxpath if maxdepth > maxinnerdepth else maxinnerpath
179
180
181 def generate_simple_graph(_terms):
182     G = nx.Graph()
183     for (H1, H2) in product(_terms, _terms):
184         G.add_edge(H1, H2)
185         G.edges[(H1, H2)]['weight'] = H1.dis(H2)
186     return G
187
188 def greedy_path( terms ):
189     G = generate_simple_graph(terms )
190

```



```

191 def reursive_form( _terms ):
192     if len(_terms) < 3:
193         return _terms
194     else:
195
196         T, _ = sample_path(G, _terms)
197
198         Q = get_Diameter(T)
199         color = set()
200
201         ret = []
202         for H in Q:
203             if H.parent not in color:
204                 color.add(H.parent)
205                 ret.append(H.parent)
206                 G.remove_node(H)
207
208         remain_terms = [ term for term in _terms if term not in color ]
209         return ret + reursive_form(remain_terms)
210 return reursive_form(terms)
211
212 def Hamiltonian_sorting(hamiltonians):
213     groups = [[] for _ in product(range(WIRES), range(WIRES))]
214     for term in hamiltonians:
215         x,y = term.seconed_wires()
216         groups[x + WIRES*y].append(term)
217
218     ret = [ ]
219     for group in groups:
220         group = greedy_path(group)
221         ret += group
222     return ret
223
224 def enforce_seapration(hamiltonians):
225
226     def seperate(terms):
227
228         def sort_tensor_by_geometrical_support(tensor, up = True):
229
230
231             for j,pauli in enumerate( { True: tensor, False: reversed(tensor) }[up] ):
232                 if pauli != "I":
233                     if up:
234                         return 10 - j
235                     else:
236                         return 10 - j
237             else:
238                 return 10
239
240         above = sorted(terms,\
241             key=lambda x : sort_tensor_by_geometrical_support(x.tensor, up=True))
242         beneath = sorted(terms,\
243             key=lambda x : sort_tensor_by_geometrical_support(x.tensor, up=False))
244
245         contact_point = min( range(len(terms)),\
246             key = lambda i : above[i].tensorspace(beneath[i]))
247
248         print(f"contact point: {contact_point}")
249         path = []
250         for x,y in zip( sorted(above[:contact_point], key = lambda z : z.tensor),\
251             sorted(beneath[:contact_point], key = lambda z : z.tensor)):
252             path.append(x)
253             path.append(y)
254

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255     new_terms = []
256     for x in above[contact_point:]:
257         if x not in beneath[:contact_point]:
258             new_terms.append(x)
259     return new_terms, path
260 path = [ ]
261 terms ,temppath = seperate(deepcopy(hamiltonians))
262 path += temppath
263
264 print(f"terms:{len(terms)}")
265 return path, terms
266
267 def alternate_path_v2(mG : nx.Graph, G : nx.Graph,\
268     terms, permutations, single_iteration = False):
269     other_color = set()
270
271     T, _ = sample_path(G, terms)
272     Q = get_Diameter(T)
273     ret = []
274
275     for (u,v) in Q:
276         for H in [u,v]:
277             if H not in other_color:
278                 other_color.add(H)
279                 ret.append(H)
280
281     made_progress = True
282     _single_iteration = True
283     while _single_iteration and (len(Q) > 2 and made_progress):
284         made_progress = False
285         for u,v in Q:
286             for H in [u,v]:
287                 if H.parent not in other_color:
288                     ret.append(H)
289                     other_color.add(H.parent)
290                 for w in list(G.nodes()):
291                     if H in w:
292                         G.remove_node(w)
293                         made_progress = True
294
295                 if mG.has_node(H):
296                     mG.remove_node(H)
297
298     T, _ = sample_path(G, terms)
299     if T.number_of_edges() > 1:
300         Q = get_Diameter(T)
301     else:
302         break
303     _single_iteration = not single_iteration
304
305     if not single_iteration:
306         for term in terms:
307             if term.parent not in other_color:
308                 ret.append(term)
309
310     return ret, terms, other_color
311
312 def main_enforce(hamiltonians):
313     path, terms = enforce_seapration(hamiltonians)
314     path += Hamiltonian_sorting(terms)
315     circuit = genreate_circut(path)
316     depth = genreate_optimized_circut(circuit, hamiltonians, svg=False, entire=False)
317     return circuit
318

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```

319 def compose_alternate_enforce():
320     G, mainProductG, terms, permus = generated_the_product_graph()
321     canidates = [ ]
322     for _ in range(5):
323         path, terms, color = alternate_path_v2( deepcopy(G), deepcopy(mainProductG), terms, permus,
single_iteration=True)
324         circuit = genreate_circuit(path)
325         genreate_optimized_circuit(circuit, terms, svg=False, entire=False)
326         remain_terms = [ term for term in terms if term not in color ]
327         circuit = circuit.compose( main_enforce( remain_terms ) )
328         depth = genreate_optimized_circuit(circuit, terms, svg = False, entire=False )
329         canidates.append( (depth, circuit) )
330         print(f"DEPTH: {depth}")
331         depth, circuit = min( canidates, key = lambda x : x[0] )
332         depth = genreate_optimized_circuit(circuit, terms, svg = False, entire=True)
333         # depth = genreate_optimized_circuit(circuit, terms, entire=True)
334         return circuit,terms
335
336
337
338
339 def demonstrate_fig( ):
340     path = [ local_Hamiltonian( "XIXZZIIIII", 0.5 ),
341             local_Hamiltonian( "XXXZIIIII", 0.5 ),
342             local_Hamiltonian( "IIIIIXXZX", 0.5 ),
343             local_Hamiltonian( "IIIIIZIZX", 0.5 ),
344             local_Hamiltonian( "IIXIIZIZX", 0.5 ) ]
345
346     path, terms = enforce_seapration(path)
347     circuit = genreate_circuit(path)
348     genreate_optimized_circuit(circuit ,path, svg=True, entire=False)
349
350
351 if __name__ == "__main__":
352
353     circuit, terms = compose_alternate_enforce()
354
355
356

```