graph_energy

March 12, 2024

1 Graph Based Spin Lattice

1.0.1 Find lowest ground state of simple Ising Hamiltonian

For a graph, $G = (E, V)$, defined by a set of edges, E, and vertices, V, we want to represent an Ising model, where the edge weights, w_{ij} are given by the spin interactions, i.e., $w_{ij} = J_{ij}$.

Given a configuration of spins (e.g., ↑↓↓↑↓) we can define the energy using what is referred to as an Ising Hamiltonian:

$$\hat{H} = \sum_{(i,j)\in E} J_{ij} s_i s_j$$

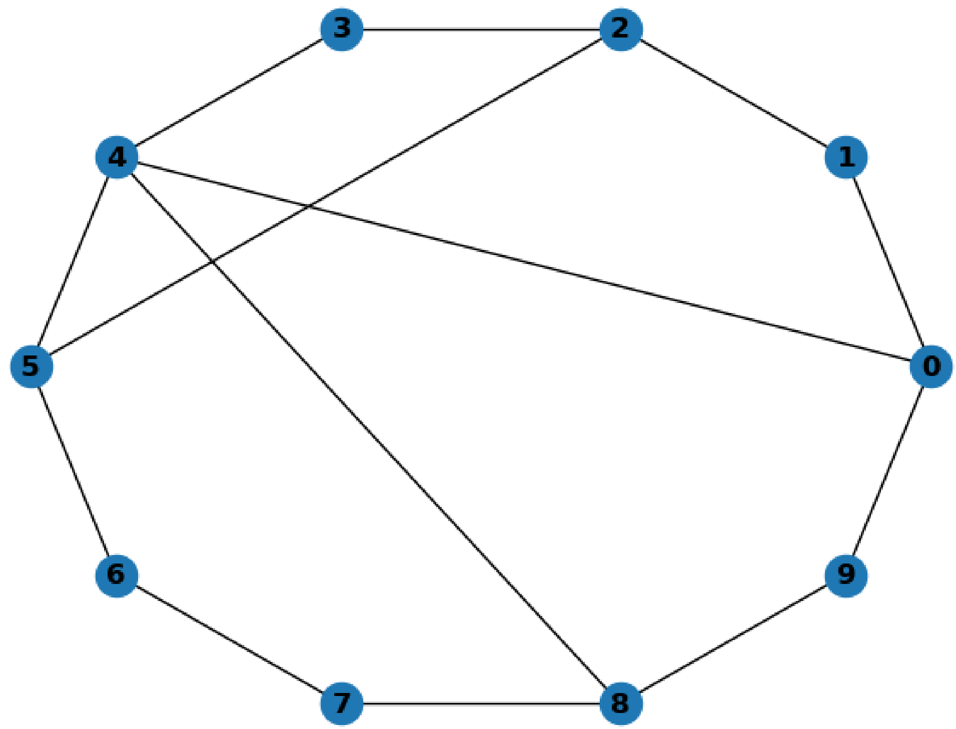
where, $s_i = 1$ if the i^{th} spin is `up` and $s_i = -1$ if it is `down`, and the sumation runs over all edges in the graph.

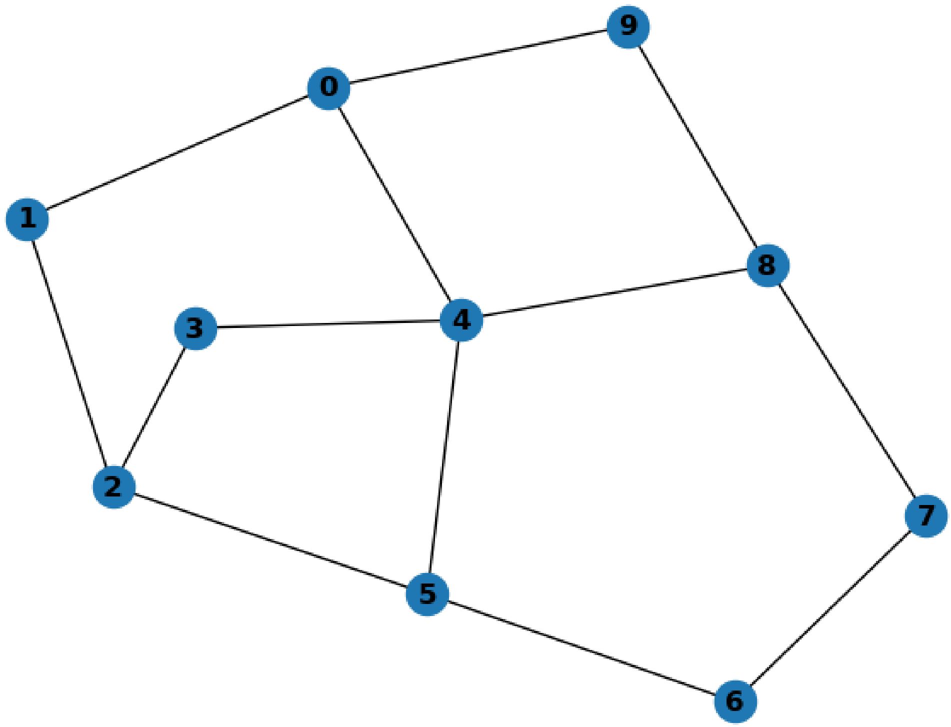
[ ]:
```
# Load relevant libraries. If you have errors you probably need to install them␣
↪into your conda env

import numpy as np
import networkx as nx
import matplotlib.pyplot as plt
import random
import scipy
random.seed(2)
```

1.0.2 Create a graph that defines the Ising interactions

[ ]:
```
G = nx.Graph()
G.add_nodes_from([i for i in range(10)])
G.add_edges_from([(i,(i+1)% G.number_of_nodes() ) for i in range(10)])
G.add_edge(2,5)
G.add_edge(4,8)
G.add_edge(4,0)
for e in G.edges:
    G.edges[e]['weight'] = 1.0

# Now Draw the graph. First we will draw it with the nodes arranged on the␣
↪circle, then we will draw the same graph
# with the position of the nodes optimized for easier visualization
```

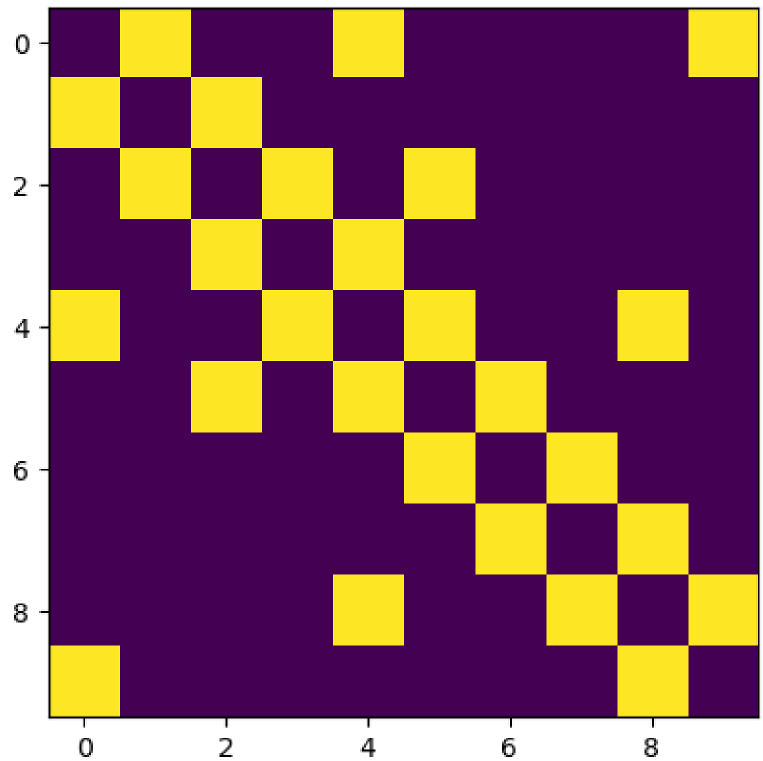
```
plt.figure(1)
nx.draw(G, with_labels=True, font_weight='bold', pos=nx.circular_layout(G))
plt.figure(2)
nx.draw(G, with_labels=True, font_weight='bold')
plt.show()
```





[ ]:
```
A = nx.adjacency_matrix(G).todense()
display(A)
plt.imshow(A);
```

```
array([[0., 1., 0., 0., 1., 0., 0., 0., 0., 1.],
       [1., 0., 1., 0., 0., 0., 0., 0., 0., 0.],
       [0., 1., 0., 1., 0., 1., 0., 0., 0., 0.],
       [0., 0., 1., 0., 1., 0., 0., 0., 0., 0.],
       [1., 0., 0., 1., 0., 1., 0., 0., 1., 0.],
       [0., 0., 1., 0., 1., 0., 1., 0., 0., 0.],
       [0., 0., 0., 0., 0., 1., 0., 1., 0., 0.],
       [0., 0., 0., 0., 0., 0., 1., 0., 1., 0.],
       [0., 0., 0., 0., 1., 0., 0., 1., 0., 1.],
       [1., 0., 0., 0., 0., 0., 0., 0., 1., 0.]])
```



1.0.3 Add your BitString class below

[ ]:
```python
class BitString:
    """
    Simple class to implement a config of bits
    """
    def __init__(self, N):
        self.N = N
        self.config = np.zeros(N, dtype=int)

    def __repr__(self):
        return np.array2string(self.config)

    def __eq__(self, other):
        #if every element between the two arrays is the same at all indexes,␣
 ↪they are the same
        return (self.config == other.config).all()

    def __len__(self):
        return self.N

    def on(self):
```

```
        count = 0
        for element in self.config:
            if element == 1:
                count += 1
        return count

    def off(self):
        count = 0
        for element in self.config:
            if element == 0:
                count += 1
        return count

    def flip_site(self,i):
        current_bit = self.config[i]
        if current_bit == 0:
            self.config[i] = 1
        elif current_bit == 1:
            self.config[i] = 0
        else:
            raise ValueError(f"Error: Bit is not a 1 or 0. At index {i}, the␣
↪value is {self.config[i]}")

    def int(self):
        decimal_number = 0
        length = len(self.config)
        for i in range(length):
            decimal_number += self.config[length - i - 1] * (2 ** i)
        return decimal_number

    def set_config(self, s:list[int]):
        try:
            self.config = np.array(s)
        except Exception as e:
            raise ValueError(f"Error: set_config failed {e}")

    def set_int_config(self, dec:int):
        #convert decimal to integer
        binary_representation = ''
        while dec > 0:
            remainder = dec % 2
            binary_representation = str(remainder) + binary_representation
            dec //= 2
        if not binary_representation:
            binary_representation = '0'

        #convert string to array
```

```
        #in order to add padding zeroes, create the correct dimension array of␣
↪all zeroes
        temp = np.zeros(self.N, dtype=int)
        #index should start with the correct amount of padding zeroes in the␣
↪front to ensure dimensions match
        index = self.N - len(binary_representation)
        #assign each digit in the string to an element of the array
        for digit in binary_representation:
            temp[index] = int(digit)
            index += 1
        #assign the internal array to this temporary array
        self.config = temp
```

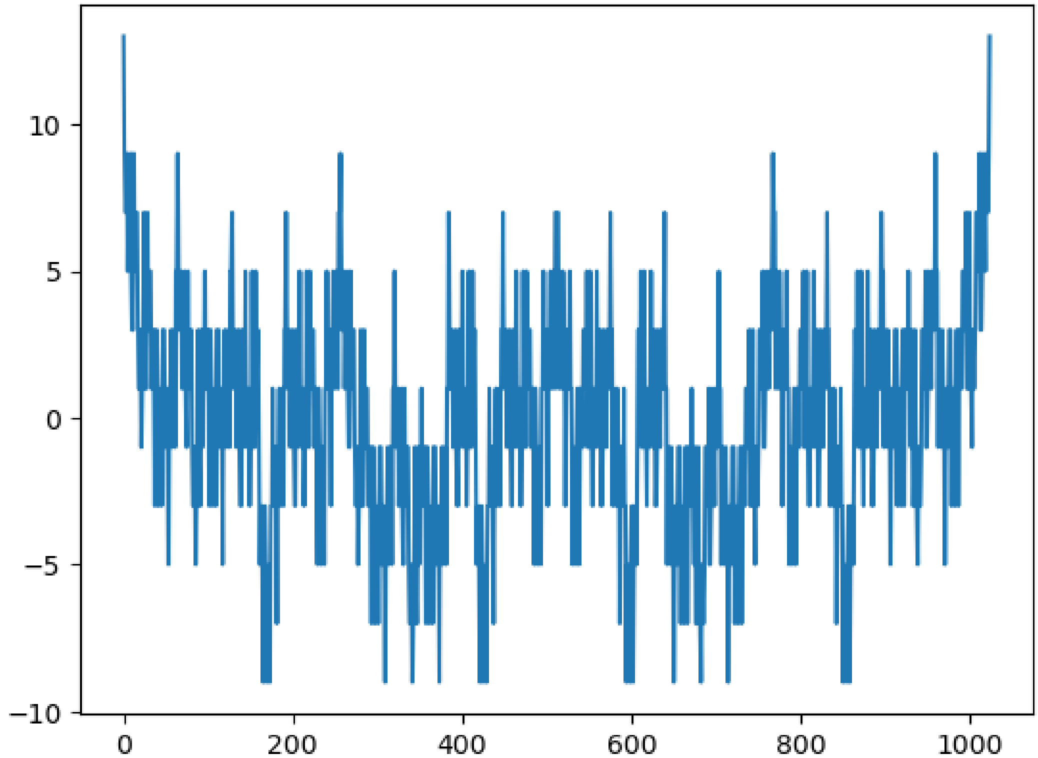
[ ]:
```
def energy(bs: BitString, G: nx.Graph):
    """Compute energy of configuration, `bs`

        .. math::
            E = \\left<\\hat{H}\\right>

    Parameters
    ----------
    bs    : Bitstring
        input configuration
    G     : Graph
        input graph defining the Hamiltonian
    Returns
    -------
    energy  : float
        Energy of the input configuration
    """

    energy = 0.0
    for edge in G.edges():
        i, j = edge
        si = 1
        if bs.config[i] == 0:
            si = -1
        sj = 1
        if bs.config[j] == 0:
            sj = -1
        energy += G.edges[edge]['weight'] * si * sj

    return energy
```

1.0.4 Naive minimization

Loop over all configurations and compute energies to find the lowest

[ ]:
```
x = [] # Store list of indices
y = [] # Store list of energies
xmin = None # configuration of minimum energy configuration
emin = float('inf') # changed to allow algorithm to find the lowest energy by␣
 ↪initially comparing it to largest amount
my_bs = BitString(10)

#iterate over all possible combinations of the bitstring, 2^n possibilities,␣
 ↪where n is length of bitstring
for index in range(2**len(my_bs)):
    my_bs.set_int_config(index)

    # Compute energy for this configuration
    en = energy(my_bs, G)

    # Update minimum energy and bitstring if it is the smallest energy found so␣
 ↪far
    if en < emin:
        emin = en
        xmin = index

    #Append appropriate values
    x.append(index)
    y.append(en)

# Print out all the energies
plt.plot(x,y)

# Print out the lowest energy configuration
my_bs.set_int_config(xmin)

print(" Lowest energy %12.8f: %s" %(emin, my_bs))
assert(abs(energy(my_bs, G) - -9) < 1e-12)
```

```
 Lowest energy  -9.00000000: [0 0 1 0 1 0 0 1 0 1]
```



1.0.5 Visualize ground state

Print out the graph again, this time coloring each node according to it's state (0 or 1)

[ ]:
```
print("Configuration: %s" %my_bs)
nx.draw(G, node_color=my_bs.config)
```

```
Configuration: [0 0 1 0 1 0 0 1 0 1]
```