Project 1: Bayesian Network Learning

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1. Algorithm Description

In my implementation of the Bayesian network learning, I choose the K2 Search algorithm to find the possible network structure. The reason I choose K2 Search is based on the following reasons:

- 1. It begins with a graph with no directed edges, which is straightforward to implement
- 2. It runs in polynomial time
- 3. Greedily adding parents

However, it cannot guarantee a globally optimal solution, so I iterate K2 Search through different initial ordering. This part is implemented in iterative_K2_fit(), which essentially run K2 Search function K2_fit() multiple times with random initial ordering. The iteration terminates when the iteration times exceed the maximum iteration (max_iter) time or the improvement of the Bayesian score is lower than the improvement threshold (improvement_threshold).

In the K2 search algorithm, the most essential function is calculating the Bayesian score, and here, I use equation 5.5 from the textbook to calculate the Bayesian Score in function Bayesian_score(). Assuming prior equal to 1, the alpha is calculated in compute_a(). Another unknown in the log Bayesian Score function is m, and it is calculated in compute_m(). One thing to notice is that the DataFrame datatype needs to be converted into an Integer Matrix before doing a row broadcast in Julia; the df_to_matrix() achieves this goal.

Pseudo Code for Iterative K2 Search:

```
Iterative_K2_Search(Data, max_iter, improve_threshold):
    s = shuffle_order()
    Graph = K2_fit(s,Data)
    if(iter > max_iter || improve< improve_threshold):
    break
    return G_best, Score_best
```

Below is the Bayesian score and their run time I test for 1, 10, 100 iteration:

B_Score/runtime	1 iteration	10 iterations	100 iterations
small.csv	-3839.05 (0.062s)	-3818.33 (0.152s)	-3801.09 (2.984s)
medium.csv	-96945.66 (1.479s)	-97333.55 (18.31s)	-96652.33 (155.592s)
large.csv	-426687.06 (158.532 s)		

I didn't run an iterative K2 Search for large.csv; this is because it will take too much time; the reason should be that I do not set the upper bound on the number of parents, so the structure becomes complex. However, K2 Search is a greedy algorithm, so a one-time search will have guaranteed output.

Data preprocess include calculating the number of instantiations for each node, and I use max() in each row of DataFrame to find out in construct_vars(). Also, I customize a struct Node with names{String} and $r{Int}$ attributes.

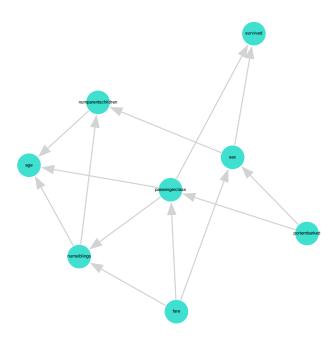


Figure 1. small.gph (1 Iteration)

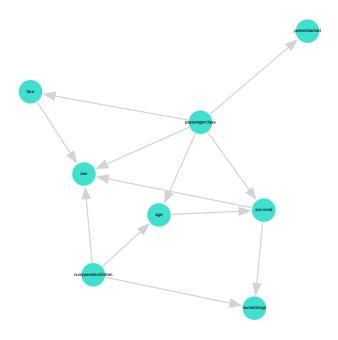


Figure 2. small.gph (10 Iterations)

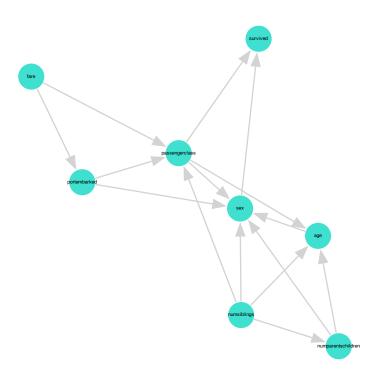


Figure 3. small.gph (100 Iterations)

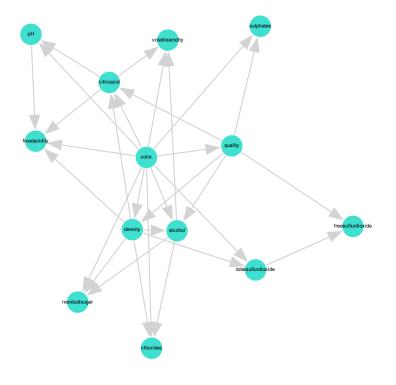


Figure 4. medium.gph (1 Iteration)

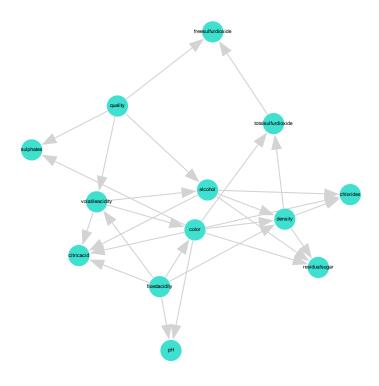


Figure 5. medium.gph (10 Iterations)

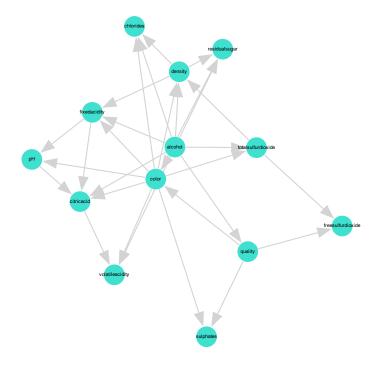


Figure 6. medium.gph (100 Iterations)

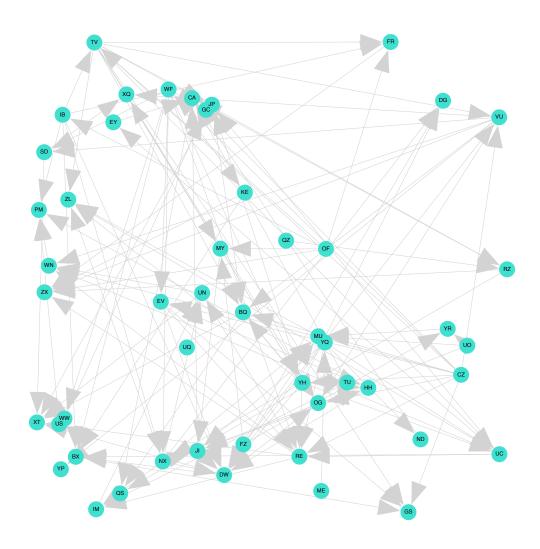


Figure 7. large.gph (1 Iteration)

```
Project.jl

using Printf

using Pkg

Pkg.add("DataFrames")

Pkg.add("CSV")

Pkg.add("Graphs")

Pkg.add("GraphPlot")

Pkg.add("Compose")

Pkg.add("Cairo")

Pkg.add("Fontconfig")

Pkg.add("SpecialFunctions")

using DataFrames

using CSV
```

```
using Graphs
using LinearAlgebra
using GraphPlot
using Compose, Cairo, Fontconfig
using Random
using SpecialFunctions
using Profile
mutable struct Node
   names::String
    r::Int
end
# Establish r for every node
function construct_vars(df)
   node_names = names(df)
    n = length(node_names)
   vars = Node[]
    for i in 1:n
       r = maximum(df[:,i])
       names = node_names[i]
        push!(vars,Node(names,r))
    end
    return vars
end
# Linear Indice
function sub2ind(siz,x)
    k = vcat(1,cumprod(siz[1:end-1]))
    return dot(k, x - 1) + 1
end
function compute_a(vars,G)
   n = length(vars)
    r = [vars[i].r for i in 1:n]
    q = [prod([r[j] for j in inneighbors(G,i)]) for i in 1:n]
    return [ones(q[i],r[i]) for i in 1:n]
end
# Convert DataFrame to Integer Matrix
function df_to_matrix(df::DataFrame)
    return Matrix{Int}(df)
end
function compute_m(vars, G, D::DataFrame)
```

```
D_matrix = df_to_matrix(D)
    return compute_m(vars, G, D_matrix)
end
function compute_m(vars, G, D::Matrix{Int})
    n = size(D, 2)
    r = [vars[i].r for i in 1:n] # r = # instantiation of X_i
    q = [prod([r[j] for j in inneighbors(G,i)]) for i in 1:n] # q = # instantiation of
Parent Nodes
    m = [zeros(q[i],r[i]) for i in 1:n]
    for o in eachrow(D)
        for i in 1:n
            k = o[i]
            parents = inneighbors(G,i)
            if !isempty(parents)
                j = sub2ind(r[parents],o[parents])
            end
            m[i][j,k] += 1.0
        end
    end
    return m
end
function bayesian_score_component(m,a)
    p = sum(loggamma.(m+a))
    p -= sum(loggamma.(a))
    p += sum(loggamma.(sum(a,dims = 2)))
    p -= sum(loggamma.(sum(a,dims = 2)+sum(m,dims=2)))
    return p
end
function bayesian_score(vars, G, D::DataFrame)
    D_matrix = df_to_matrix(D)
    return bayesian_score(vars, G, D_matrix)
end
function bayesian_score(vars,G,D)
   n = length(vars)
   # Compute statistic
   m = compute_m(vars,G,D)
    # Compute prior
   a = compute_a(vars,G)
    return sum(bayesian_score_component(m[i],a[i]) for i in 1:n)
end
struct K2Search
```

```
ordering::Vector{Int}
end
function K2_fit(method::K2Search, vars,D)
    G = SimpleDiGraph(length(vars))
    for (k,i) in enumerate(method.ordering[2:end])
        # Calculate bayesian score
        y = bayesian_score(vars,G,D)
        while true
            y_best, j_best = -Inf, 0
            for j in method.ordering[1:k]
                # Try add adge
                if !has_edge(G,j,i)
                    add_edge!(G,j,i)
                    y_h = bayesian_score(vars,G,D)
                    if y_h > y_best
                        y_best, j_best = y_h, j
                    end
                    rem_edge!(G,j,i)
                end
            end
            if y_best > y
                y = y_best
                add_edge!(G,j_best,i)
            else
                break
            end
        end
    end
    return G
end
function iterative_K2_fit(vars,D,max_iter,improvement_threshold)
    best_G = nothing
    best_score = -Inf
    for iter in 1: max_iter
        # Shuffle random order for search
        order = shuffle(1:length(vars))
        method = K2Search(order)
        G = K2_fit(method, vars,D)
        b_score = bayesian_score(vars,G,D)
        if b_score > best_score
            # Break if improve is slow
            if (iter > 1 && (b_score-best_score)/abs(best_score) < improvement_threshold)
```

```
best_score = b_score
                best_G = G
                println("Iter"*string(iter)*": "*string(best_score))
                break
            end
            best_score = b_score
            best G = G
            println("Iter"*string(iter)*": "*string(best_score))
        end
    end
    return best_G, best_score
end
   write_gph(dag::DiGraph, idx2names, filename)
Takes a DiGraph, a Dict of index to names and a output filename to write the graph in `gph`
format.
function write gph(dag::DiGraph, idx2names, filename)
    open(filename, "w") do io
        for edge in edges(dag)
            @printf(io, "%s,%s\n", idx2names[src(edge)], idx2names[dst(edge)])
        end
   end
end
function compute(infile, outfile)
   # Set timer
    total_time = @elapsed begin
       # Read CSV
       df = CSV.read(infile,DataFrame)
        # Setup vars
        vars = construct_vars(df)
        idx2names = Dict(i => vars[i].names for i in 1:length(vars))
        learning_time = @elapsed begin
            # iterative K2 Search
            G,score = iterative_K2_fit(vars,df,1,0.0001)
        end
        # Plot graph
        node_labels = [idx2names[i] for i in 1:nv(G)]
        p = gplot(G; nodelabel=node_labels, NODELABELSIZE=10.0,layout=spring_layout)
```

```
draw(PDF(string(outfile)*".pdf", 100cm, 100cm), p)
        write_gph(G,idx2names,outfile)
    end
    println("Final Score: "*string(score))
    println("Structure learning time: $(round(learning_time, digits=3)) seconds")
    println("Total runtime: $(round(total_time, digits=3)) seconds")
end
function main()
    if length(ARGS) != 2
        error("usage: julia project1.jl <infile>.csv <outfile>.gph")
    end
    inputfilename = ARGS[1]
    outputfilename = ARGS[2]
    compute(inputfilename, outputfilename)
end
main()
# @profile main()
# Profile.print()
```