Machine Learning the Ising Transition

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```julia
const IsingTc = 1/(1/2*log(1+sqrt(2))) # Exact Onsager solution
```

```
2.269185314213022
```

1 Monte Carlo simulation

```julia
using Printf, Dates

up(neighs, i) = neighs[1, i]
right(neighs, i) = neighs[2, i]
down(neighs, i) = neighs[3, i]
left(neighs, i) = neighs[4, i]

function montecarlo(; L, T)
    # set parameters & initialize
    nsweeps = 10^7
    measure_rate = 5_000
    beta = 1/T
    conf = rand([-1, 1], L, L)
    confs = Matrix{Int64}[] # storing intermediate configurations
    # build nearest neighbor lookup table
    lattice = reshape(1:L^2, (L, L))
    ups     = circshift(lattice, (-1,0))
    rights  = circshift(lattice, (0,-1))
    downs   = circshift(lattice,(1,0))
    lefts   = circshift(lattice,(0,1))
    neighs = vcat(ups[:]',rights[:]',downs[:]',lefts[:]')

    start_time = now()
    println("Started:  ", Dates.format(start_time, "d.u yyyy HH:MM"))

    for i in 1:nsweeps
        # sweep
        for i in eachindex(conf)
            # local update
            ΔE = 2.0 * conf[i] * (conf[up(neighs, i)] + conf[right(neighs, i)] +
                                  + conf[down(neighs, i)] + conf[left(neighs, i)])
            # Metropolis
            if ΔE <= 0 || rand() < exp(- beta*ΔE)
                conf[i] *= -1 # flip spin
            end
        end
        # measure
        iszero(mod(i, measure_rate)) && push!(confs, copy(conf))
    end

    end_time = now()
    println("Ended:  ", Dates.format(end_time, "d.u yyyy HH:MM"))
    @printf("Duration:  %.2f minutes", (end_time - start_time).value / 1000. /60.)
    return confs
end
```

```
montecarlo (generic function with 1 method)
```

```
montecarlo(L=8, T=5)
```

```
Started: 5.Aug 2019 11:33
Ended: 5.Aug 2019 11:33
Duration: 0.24 minutes2000-element Array{Array{Int64,2},1}:
 [-1 -1 ... 1 -1; -1 -1 ... -1 1; ... ; -1 -1 ... -1 -1; -1 1 ... -1 -1]
 [-1 1 ... -1 -1; 1 -1 ... -1 -1; ... ; 1 1 ... -1 -1; 1 1 ... 1 1]
 [-1 1 ... -1 -1; -1 1 ... 1 1; ... ; 1 1 ... 1 1; 1 1 ... 1 1]
 [-1 1 ... 1 1; -1 -1 ... -1 1; ... ; 1 -1 ... 1 1; 1 1 ... 1 -1]
 [-1 1 ... -1 -1; 1 1 ... 1 1; ... ; 1 -1 ... -1 1; -1 1 ... -1 -1]
 [1 1 ... 1 1; 1 -1 ... 1 1; ... ; 1 1 ... 1 1; 1 -1 ... -1 1]
 [1 -1 ... -1 1; 1 1 ... -1 1; ... ; 1 1 ... 1 1; 1 1 ... -1 1]
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 [-1 1 ... -1 -1; 1 1 ... -1 1; ... ; 1 1 ... -1 1; 1 1 ... -1 -1]
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 [-1 -1 ... 1 1; -1 1 ... 1 -1; ... ; -1 1 ... -1 -1; -1 -1 ... 1 1]
 [-1 1 ... 1 -1; -1 1 ... 1 -1; ... ; -1 1 ... 1 1; -1 -1 ... 1 1]
 [-1 -1 ... -1 -1; -1 -1 ... -1 1; ... ; -1 -1 ... -1 -1; 1 -1 ... -1 1]
 [-1 1 ... 1 -1; 1 -1 ... -1 -1; ... ; 1 1 ... 1 1; -1 -1 ... 1 -1]
 [-1 -1 ... 1 -1; -1 -1 ... 1 -1; ... ; 1 -1 ... 1 -1; -1 1 ... 1 -1]
 [-1 1 ... 1 1; -1 -1 ... -1 -1; ... ; 1 -1 ... 1 1; 1 1 ... 1 1]
 [-1 -1 ... 1 -1; -1 -1 ... -1 -1; ... ; -1 1 ... 1 -1; -1 -1 ... 1 -1]
 [1 1 ... 1 1; 1 1 ... 1 1; ... ; -1 -1 ... 1 1; -1 -1 ... -1 1]
 [1 1 ... 1 1; -1 1 ... 1 -1; ... ; 1 -1 ... 1 1; 1 1 ... 1 -1]
```
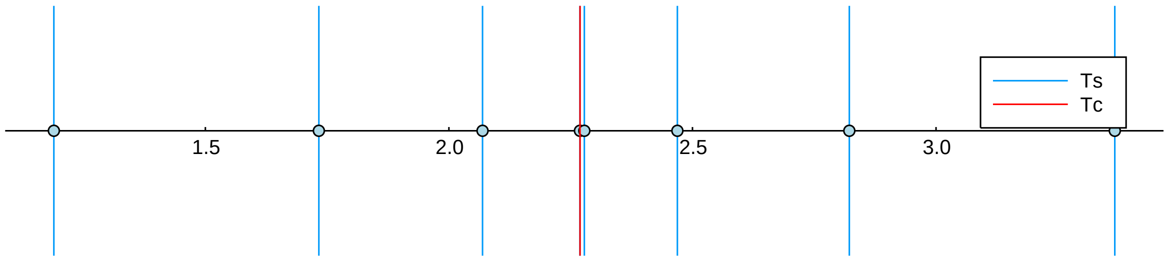

1.0.1 Simulate an $L = 8$ system at a couple of temperatures

```
Ts = [1.189, 1.733, 2.069, 2.269, 2.278, 2.469, 2.822, 3.367]
```

```
8-element Array{Float64,1}:
 1.189
 1.733
 2.069
 2.269
 2.278
 2.469
 2.822
 3.367
```

```
# visualize temperatures
using Plots
vline(Ts, grid=false, axis=:x, framestyle=:origin, xlim=(minimum(Ts)-0.1,
    maximum(Ts)+0.1), size=(800,200), label="Ts")
scatter!(Ts, fill(0, length(Ts)), color=:lightblue, label="")
vline!([IsingTc], color=:red, label="Tc")
```



```
confs = Dict{Float64, Array{Float64,3}}() # key:  T, value:  confs
for T in Ts
    println("T = $T"); flush(stdout);
    c = montecarlo(L=8, T=T)
    confs[T] = cat(c..., dims=3)
    println("Done.\n")
end
```

```
T = 1.189
Started: 5.Aug 2019 11:33
Ended: 5.Aug 2019 11:33
Duration: 0.28 minutesDone.

T = 1.733
Started: 5.Aug 2019 11:33
Ended: 5.Aug 2019 11:34
Duration: 0.30 minutesDone.

T = 2.069
Started: 5.Aug 2019 11:34
Ended: 5.Aug 2019 11:34
Duration: 0.31 minutesDone.

T = 2.269
Started: 5.Aug 2019 11:34
Ended: 5.Aug 2019 11:34
Duration: 0.30 minutesDone.

T = 2.278
Started: 5.Aug 2019 11:34
Ended: 5.Aug 2019 11:35
Duration: 0.30 minutesDone.

T = 2.469
Started: 5.Aug 2019 11:35
Ended: 5.Aug 2019 11:35
Duration: 0.29 minutesDone.

T = 2.822
Started: 5.Aug 2019 11:35
Ended: 5.Aug 2019 11:35
Duration: 0.27 minutesDone.

T = 3.367
Started: 5.Aug 2019 11:35
Ended: 5.Aug 2019 11:35
Duration: 0.26 minutesDone.
```

2 Machine learning the magnetic phase transition

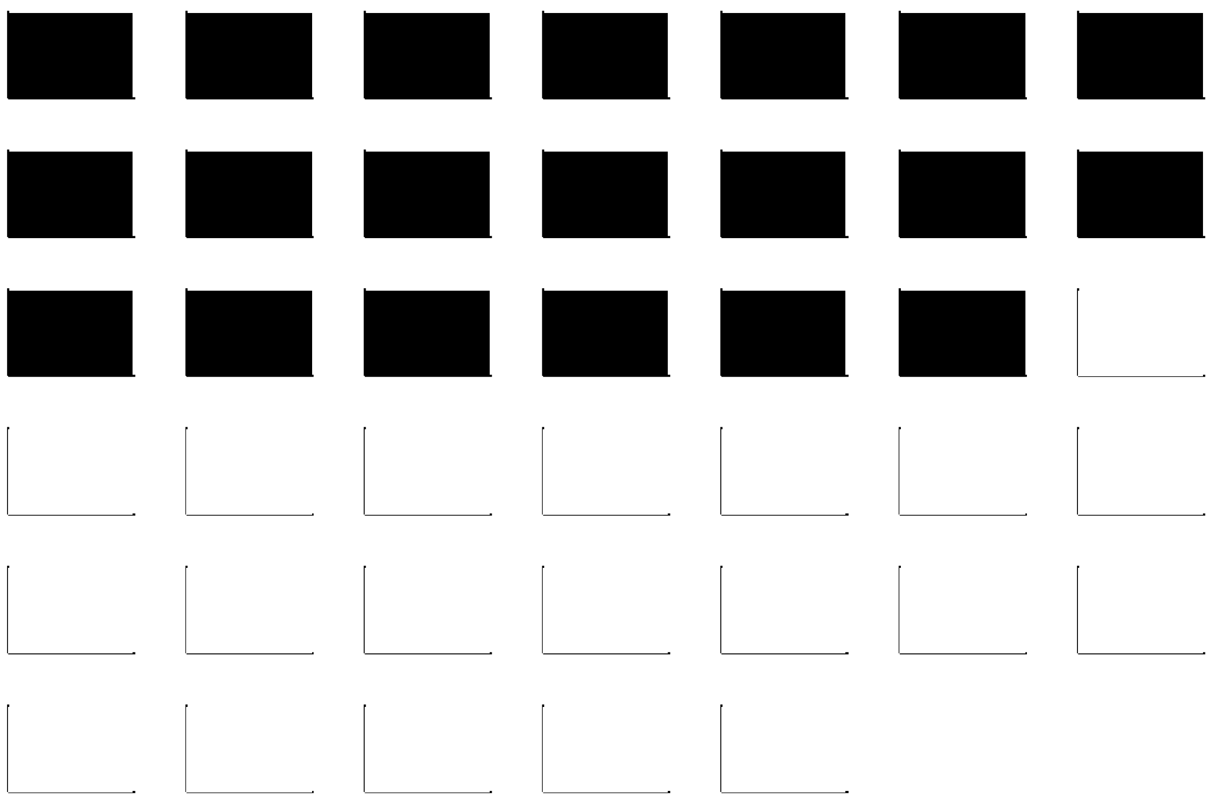
```
using Flux
using Flux: crossentropy, onecold, onehotbatch, params, throttle, @epochs
using Statistics, Random

function flatten_and_Z2(confs, T)
    c = confs[T]
    cs = Float64.(reshape(c, (64,:))) # flatten space dimension
    cs = hcat(cs, -one(eltype(cs)) .* cs) # concatenate Z2 (spin flip) symmetry partners
    return cs
end
```

```
flatten_and_Z2 (generic function with 1 method)
```

```
L = 8
Tleft = 1.189
Tright = 3.367

confs_left = flatten_and_Z2(confs, Tleft)
confs_right = flatten_and_Z2(confs, Tright);

# visualize configurations
printconfs(confs) = plot([heatmap(Gray.(reshape(confs[:,i], (L,L))), ticks=false) for i
    in 1:100:size(confs, 2)]...)
```

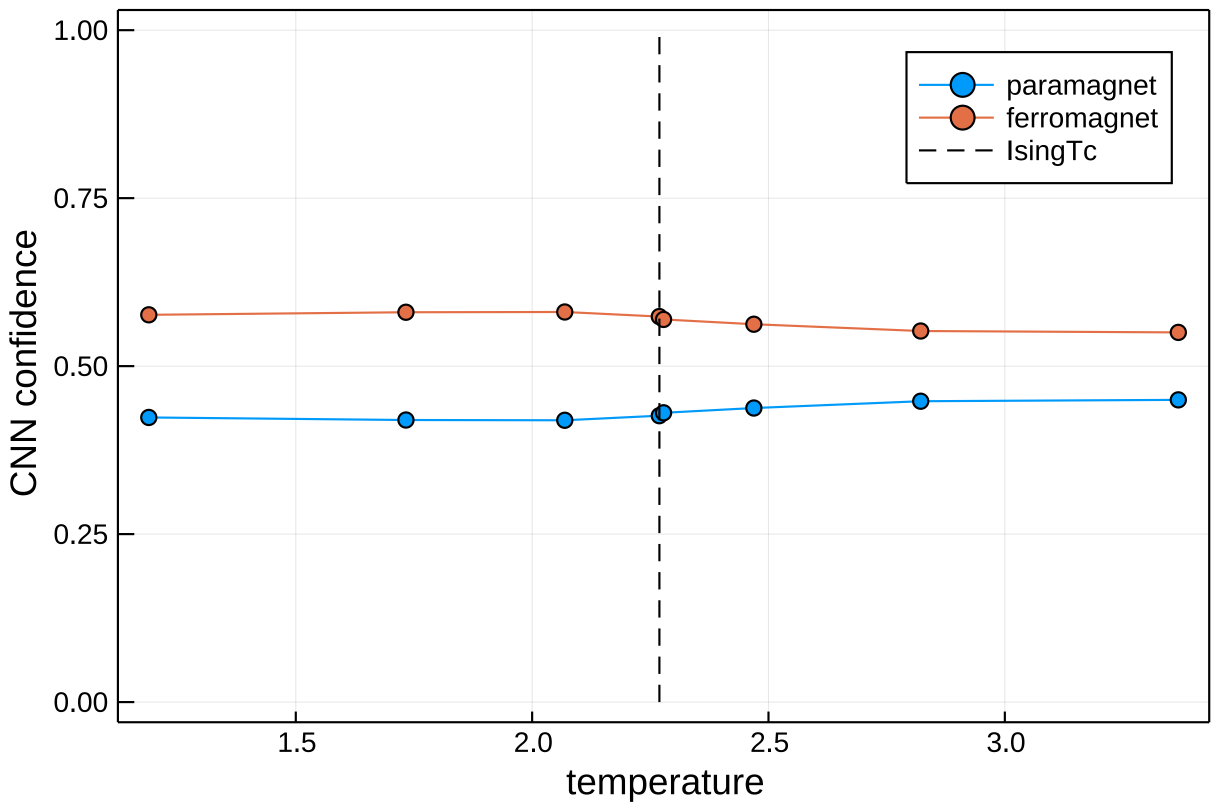
```
printconfs (generic function with 1 method)
```

```
printconfs(confs_left)
```

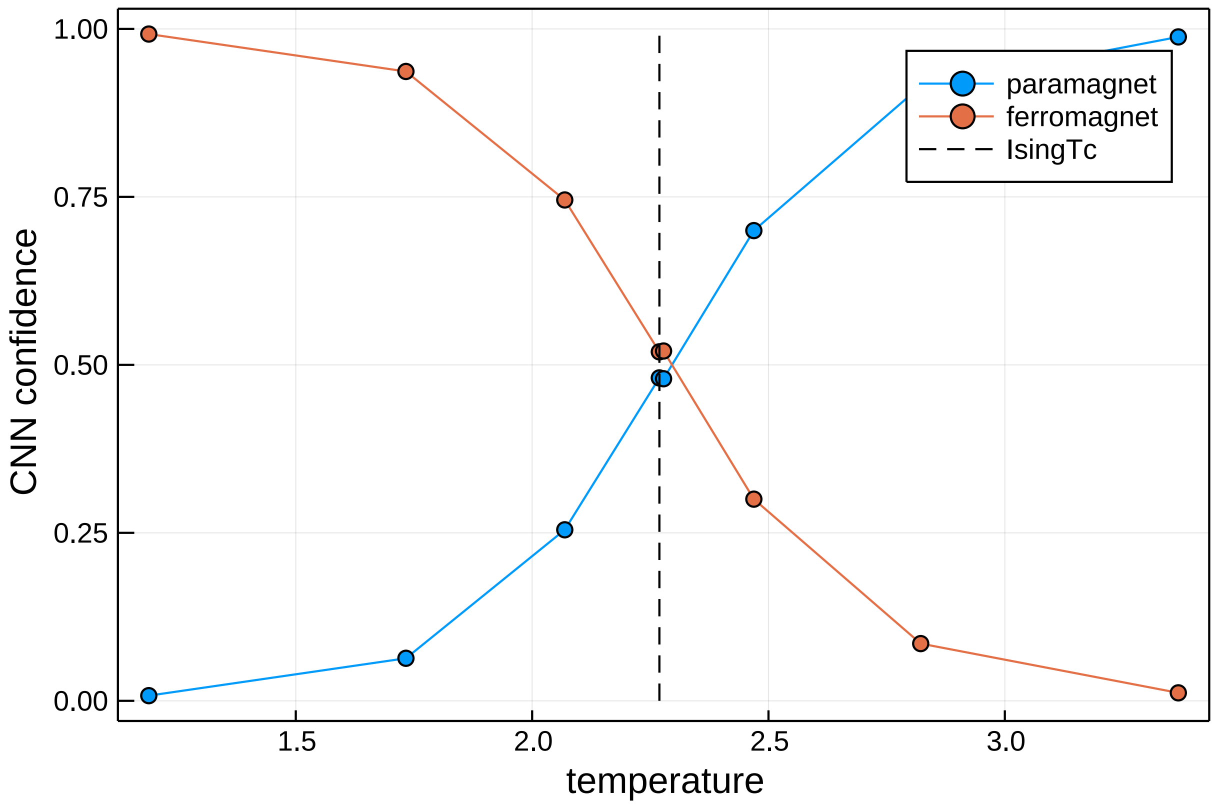


```
printconfs(confs_right)
```

```
# set up as training data
neach = size(confs_left, 2)
X = hcat(confs_left, confs_right)
labels = vcat(fill(1, neach), fill(0, neach))
Y = onehotbatch(labels, 0:1)
dataset = Base.Iterators.repeated((X, Y), 10); # repeat dataset 10 times

# create neural network with 10 hidden units and 2 output neurons
Random.seed!(123)

m = Chain(
    Dense(L^2, 10, relu),
    Dense(10, 2),
    softmax)

Chain(Dense(64, 10, NNlib.relu), Dense(10, 2), NNlib.softmax)

# classify phases at all intermediate temperatures
function confidence_plot()
    results = Dict{Float64, Vector{Float32}}()
    for T in Ts
      c = flatten_and_Z2(confs, T);
      results[T] = vec(mean(m(c), dims=2).data)
    end
    results = sort(results)

    p = plot(keys(results) |> collect, reduce(hcat, values(results))',
      marker=:circle,
      xlab="temperature",
      ylabel="CNN confidence",
      labels=["paramagnet", "ferromagnet"],
      frame=:box)
    plot!(p, [IsingTc, IsingTc], [0, 1], ls=:dash, color=:black, label="IsingTc")
    if (@isdefined IJulia)
        # "animation" in jupyter
        IJulia.clear_output(true)
    end
    display(p)
end

confidence_plot()
```

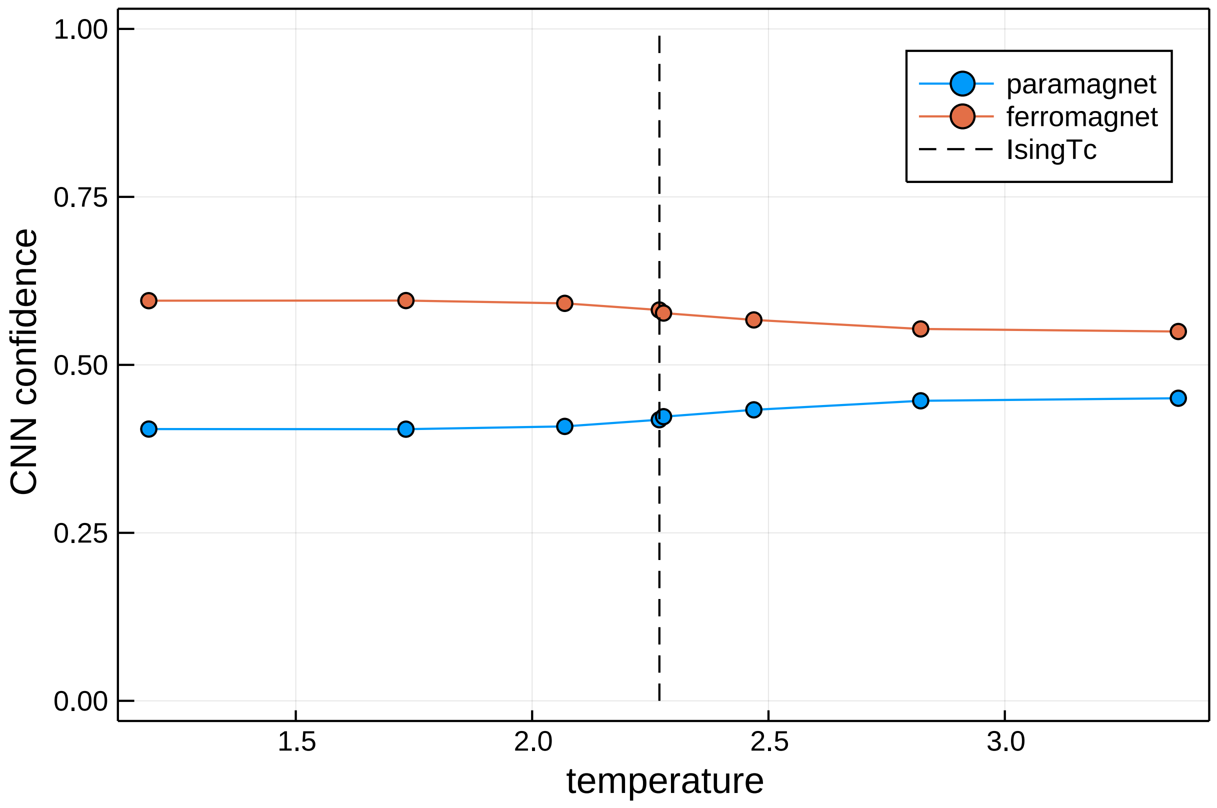


```
# define cost-function
loss(x, y) = crossentropy(m(x), y)

# define optimizer
opt = ADAM()

# train for 100 epochs
for i in 1:100
    Flux.train!(loss, params(m), dataset, opt)
end

#
confidence_plot()
```



In Jupyter notebooks or Juno you should see an "animation" of the confidence plot across training.

```
# Define a callback
evalcb = () -> begin
# @show(loss(X, Y))
# @show(accuracy(X, Y))
    confidence_plot()
end

# Reset the network and the optimizer
Random.seed!(123)
m = Chain(
    Dense(L^2, 10, relu),
    Dense(10, 2),
    softmax)
opt = ADAM()

# Train for 100 epochs (with "animation")
for i in 1:100
    Flux.train!(loss, params(m), dataset, opt, cb = throttle(evalcb, 50))
end
```



1.00
0.75
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CNN confidence
1.5
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2.5
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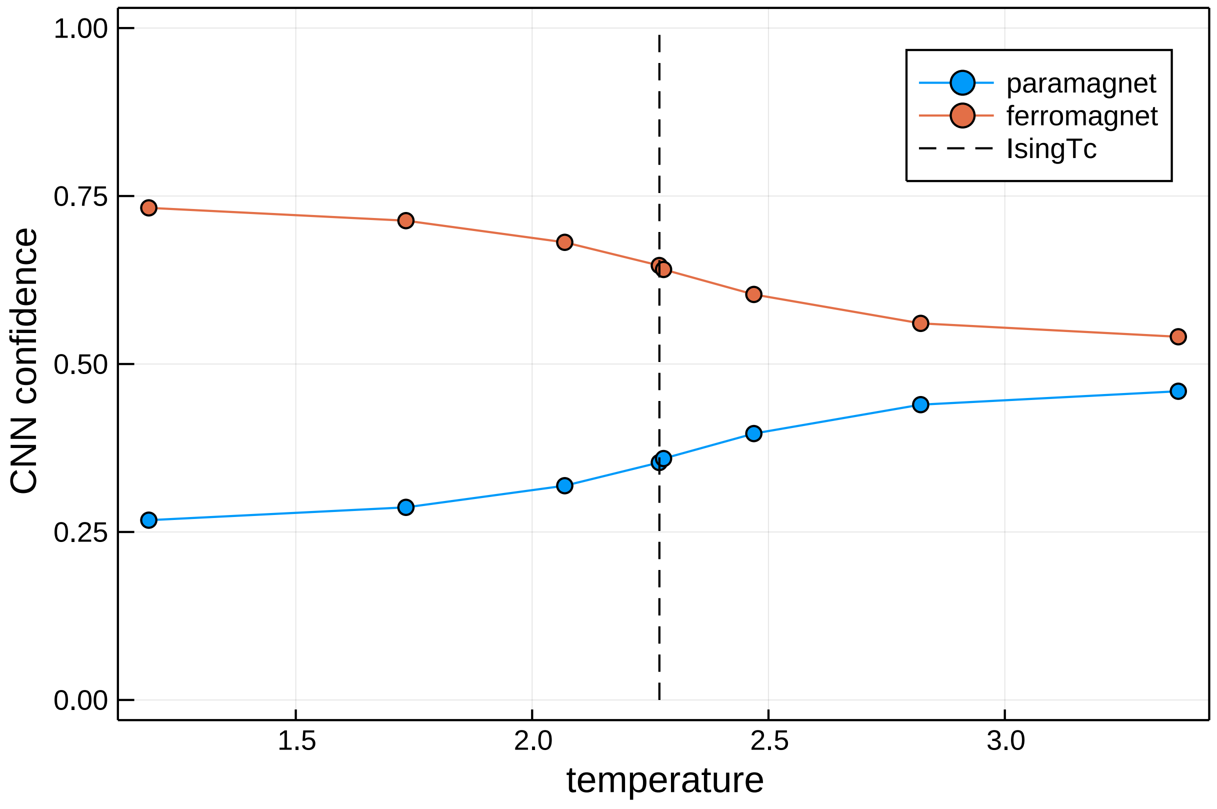
temperature
paramagnet
ferromagnet
IsingTc



1.00
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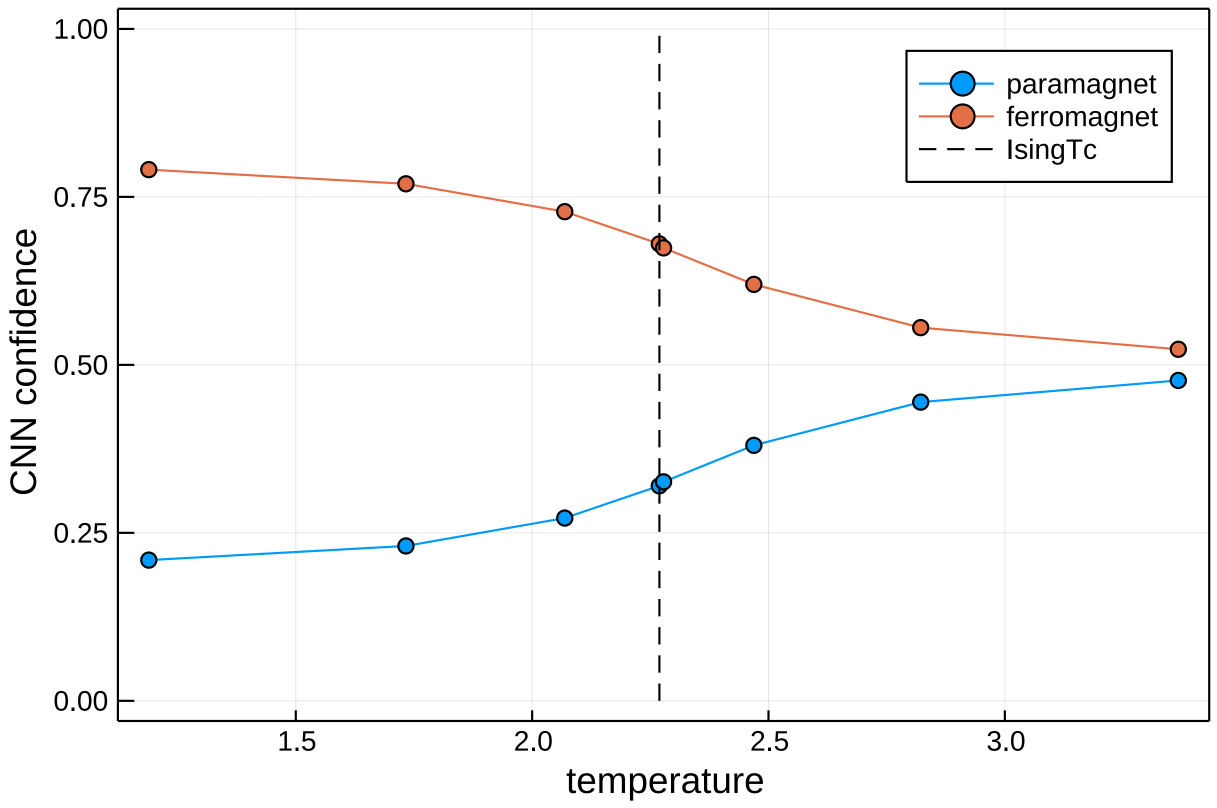
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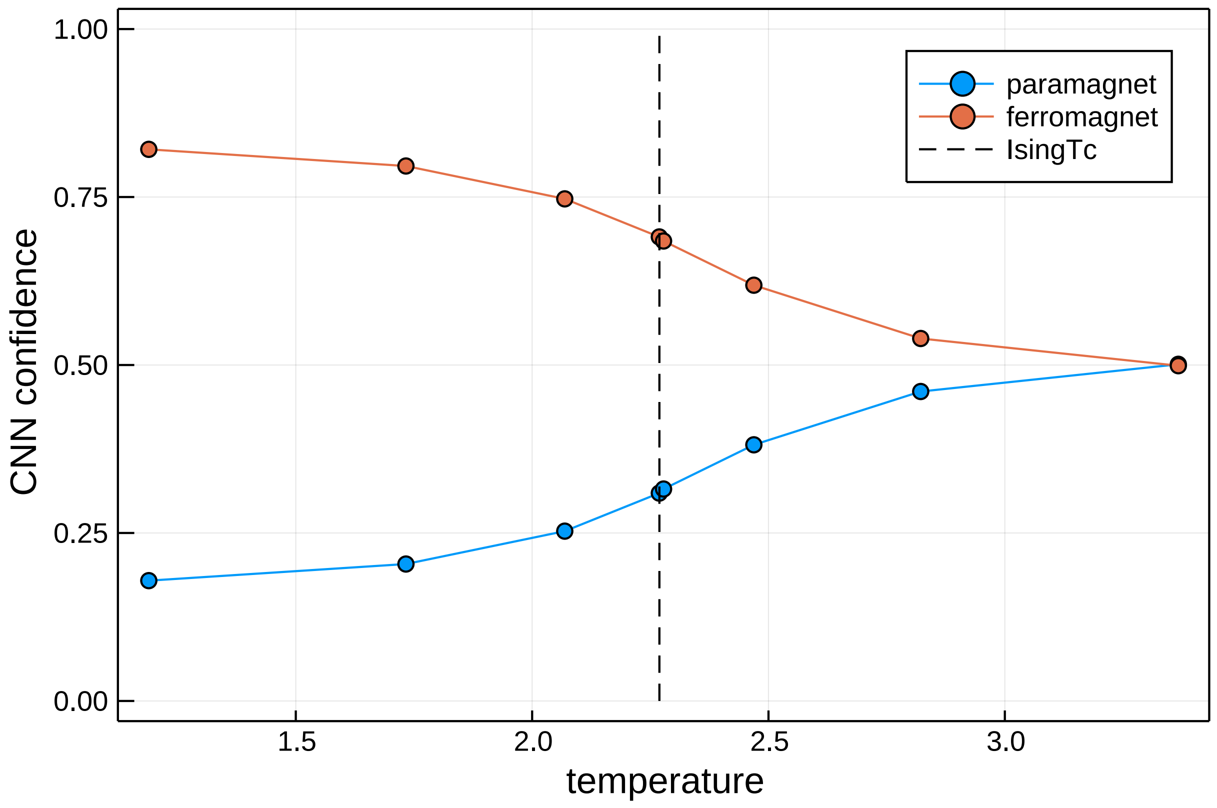
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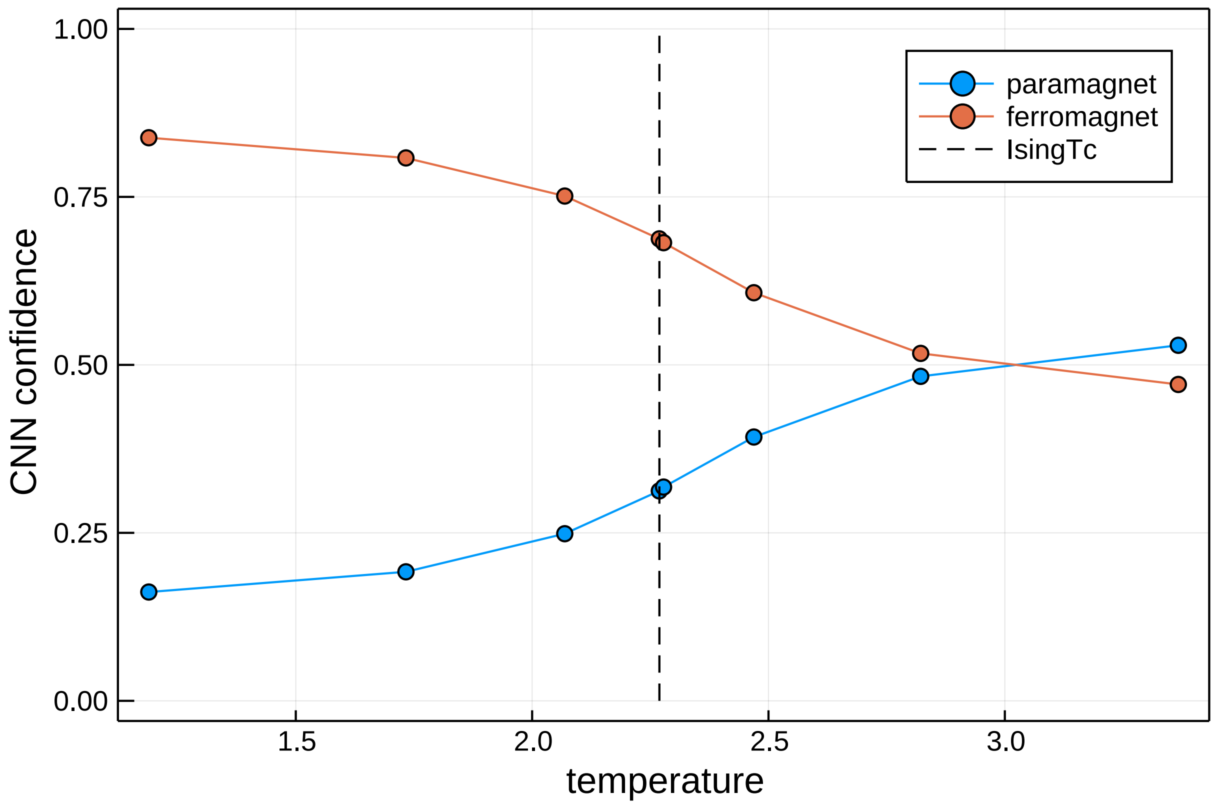
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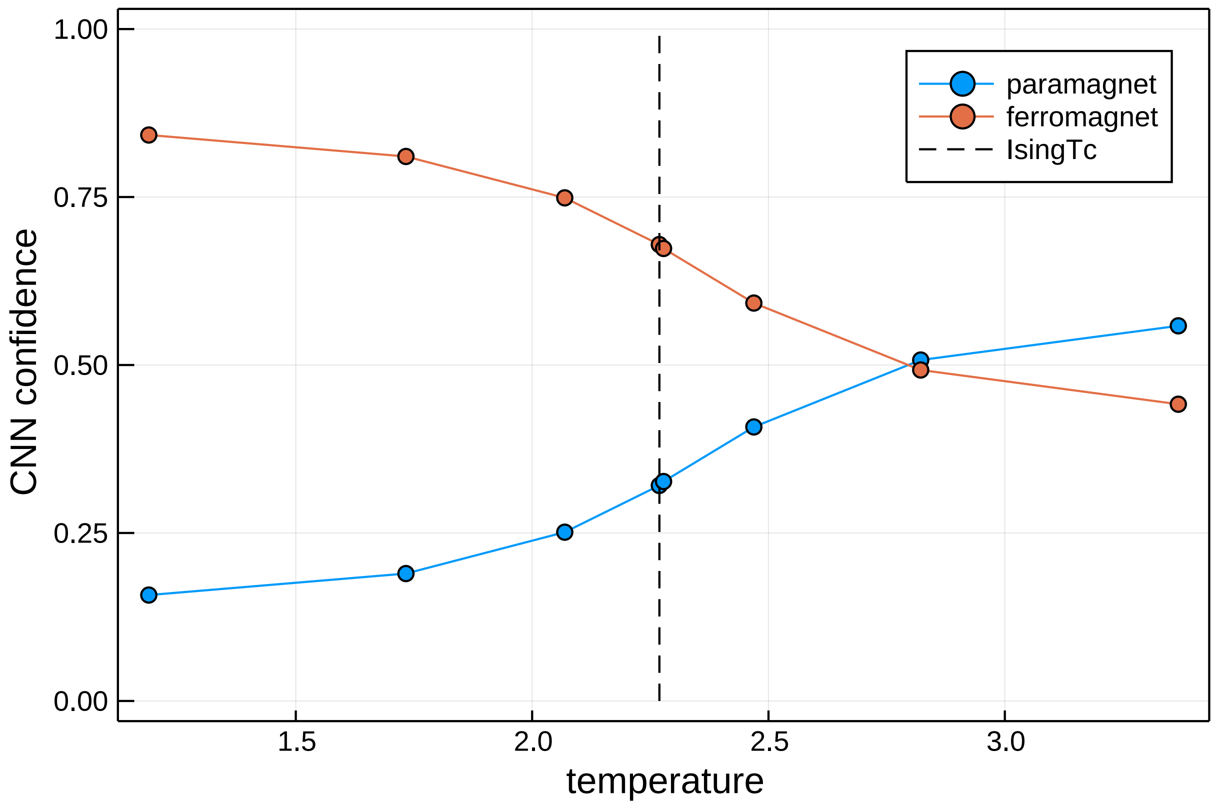
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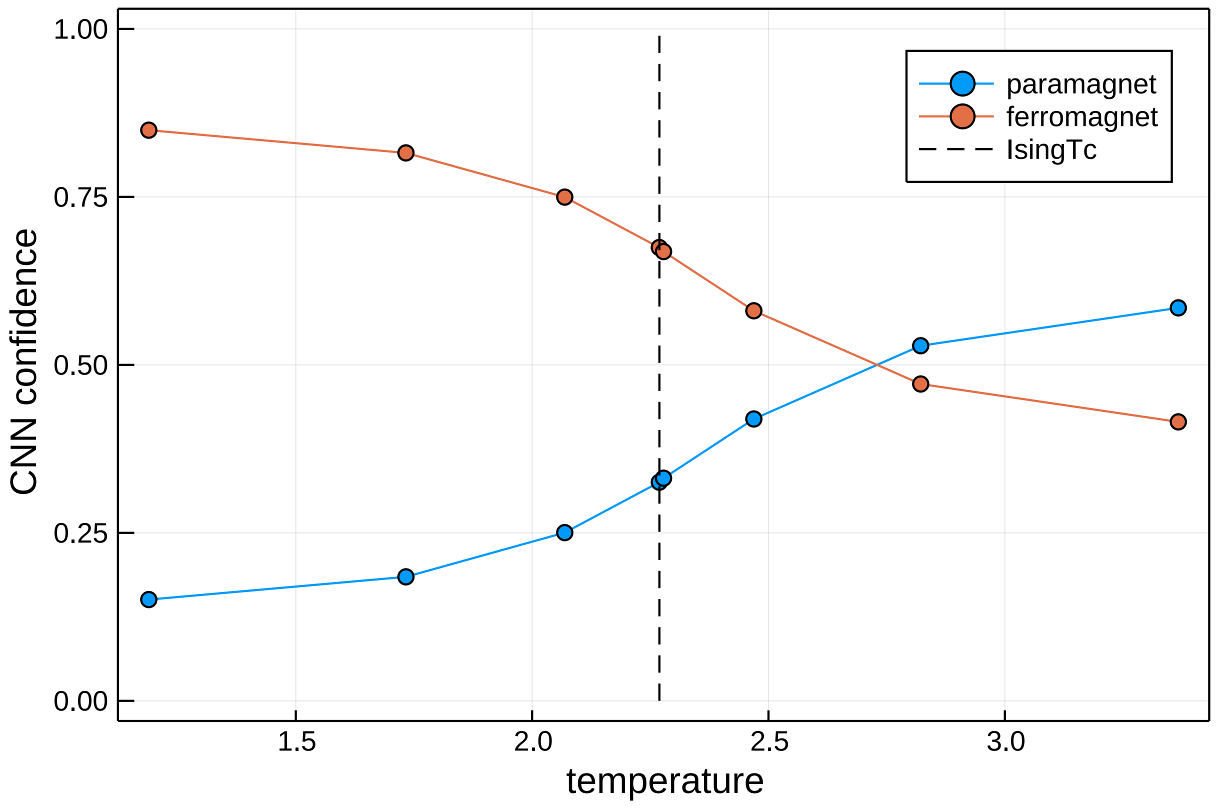

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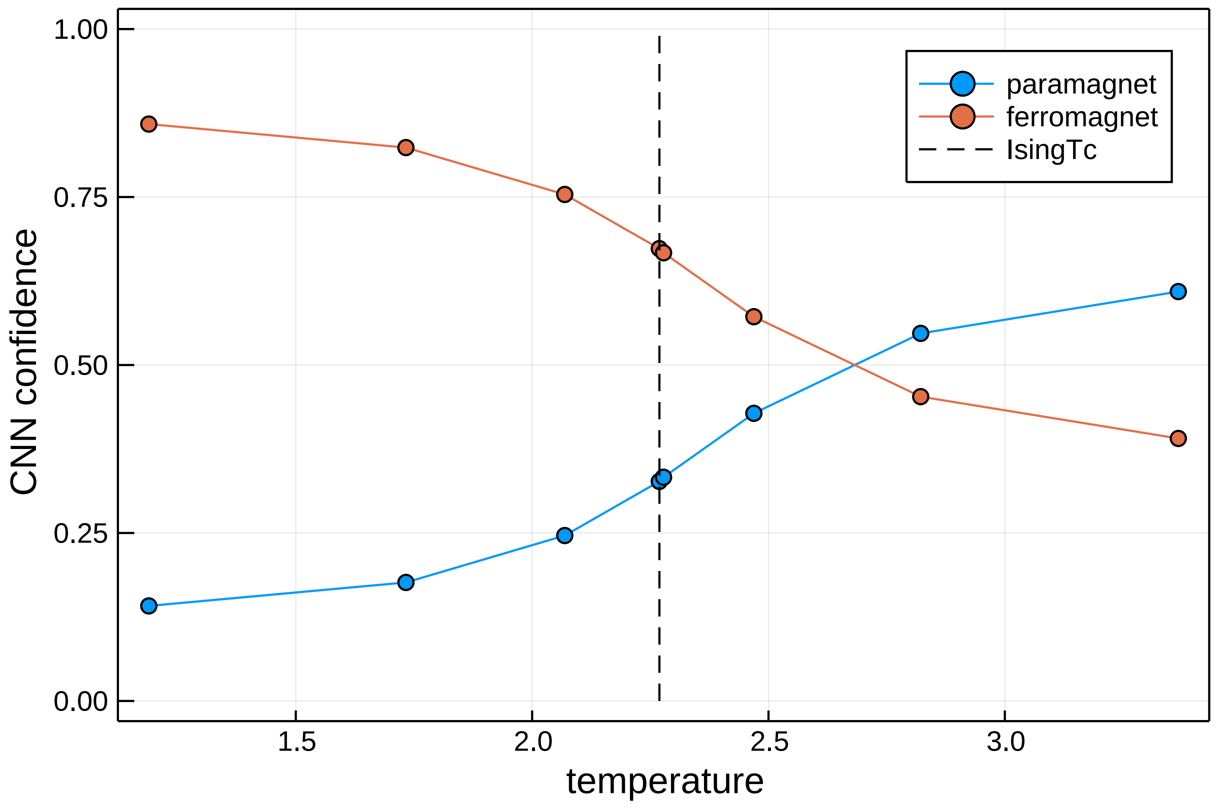

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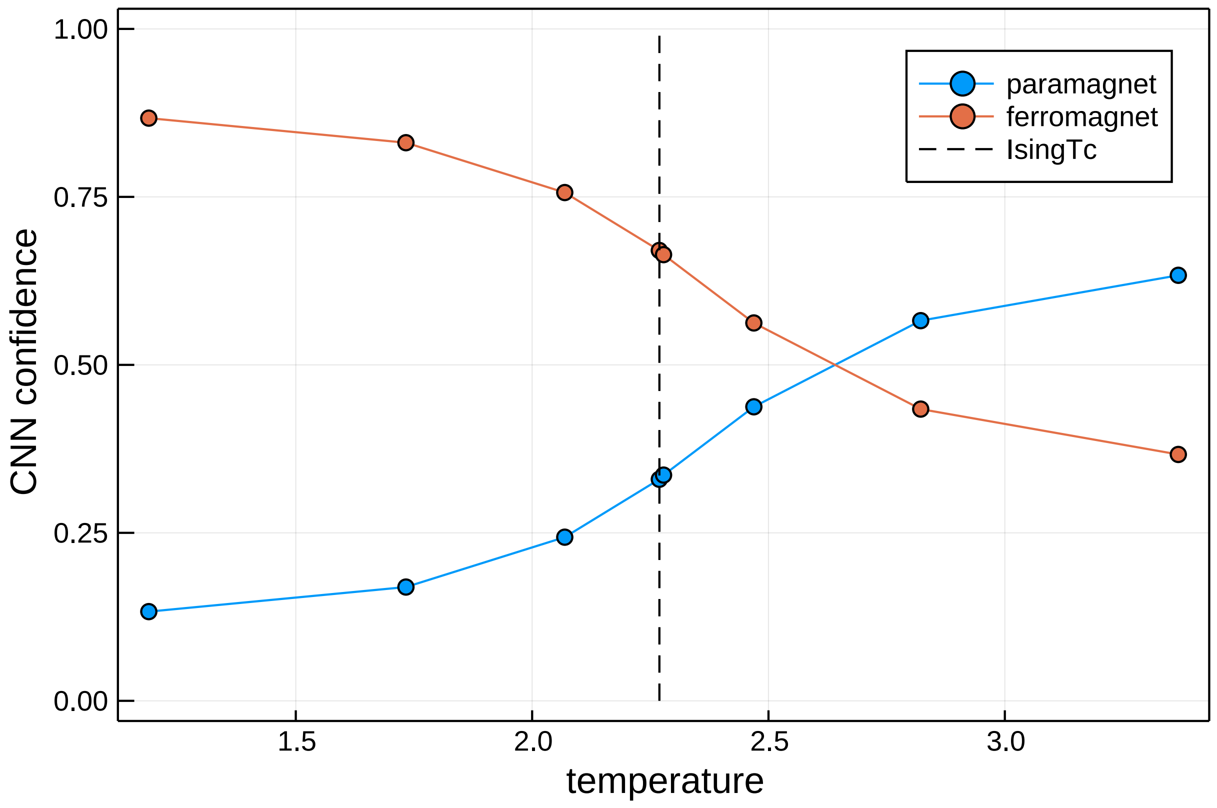
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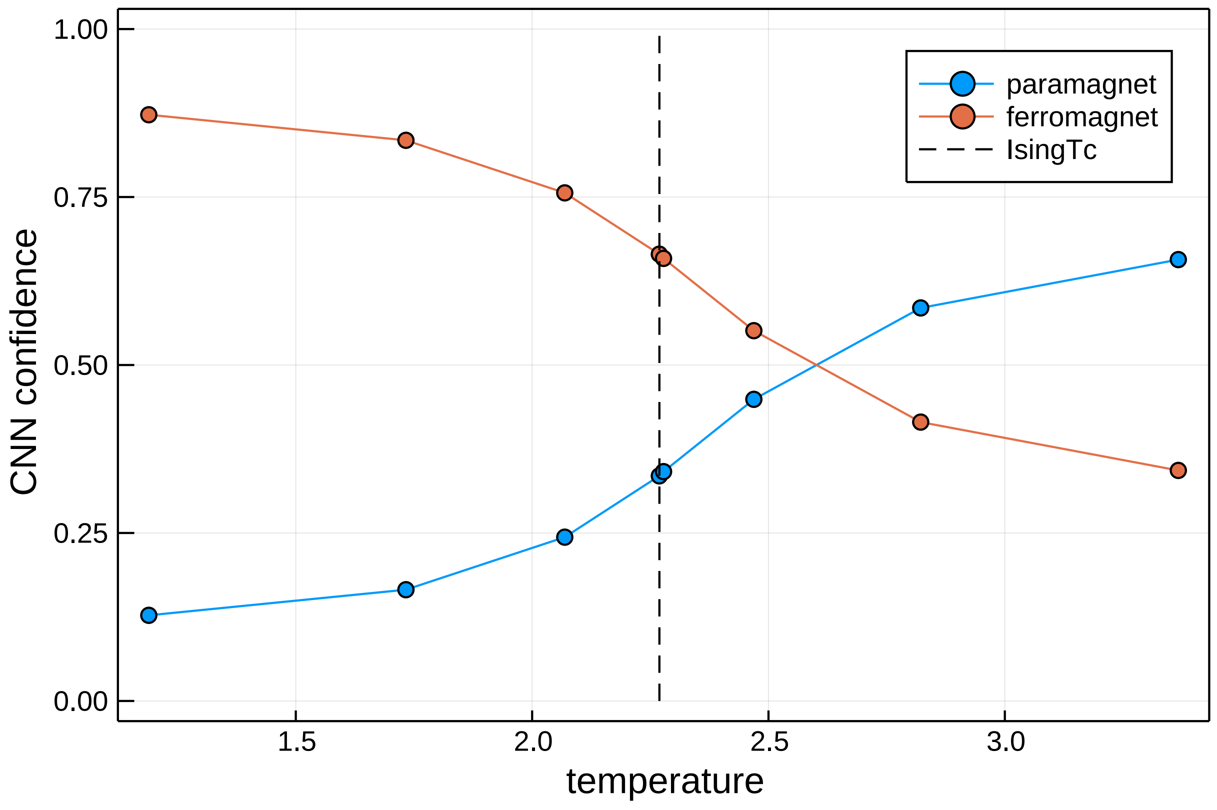
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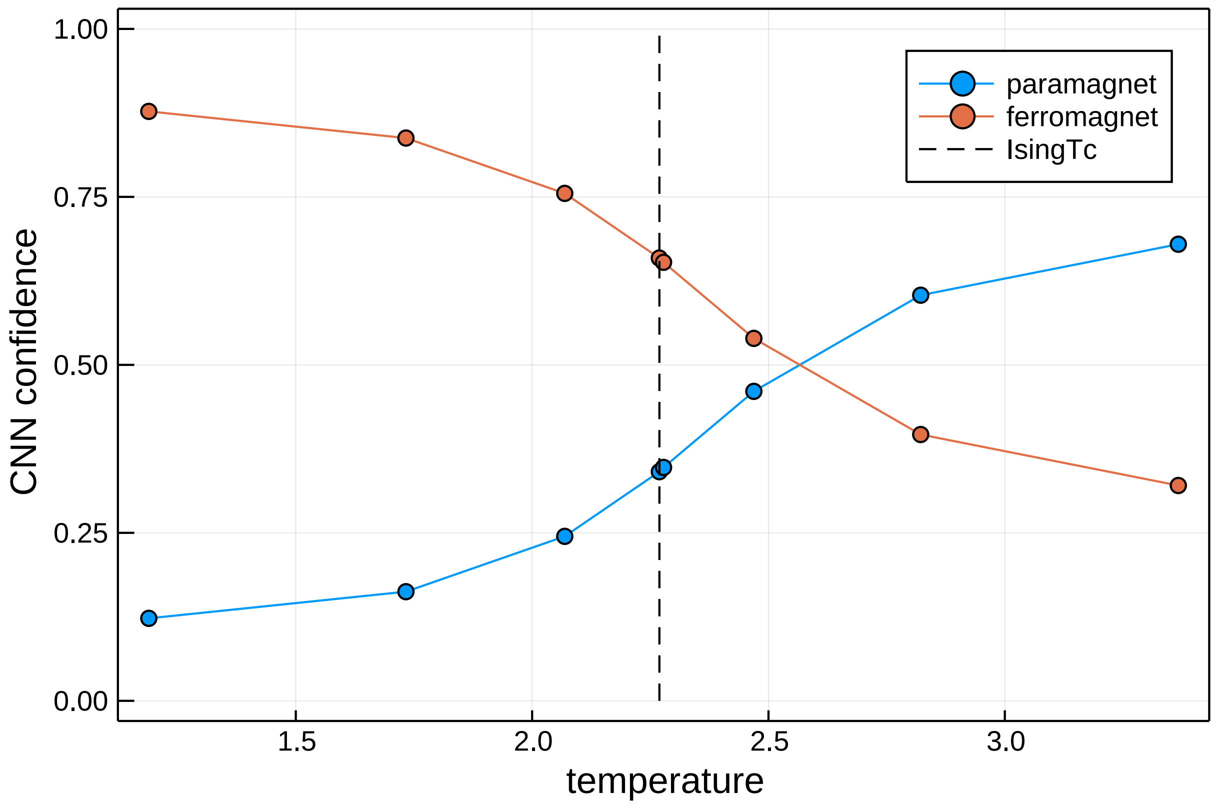

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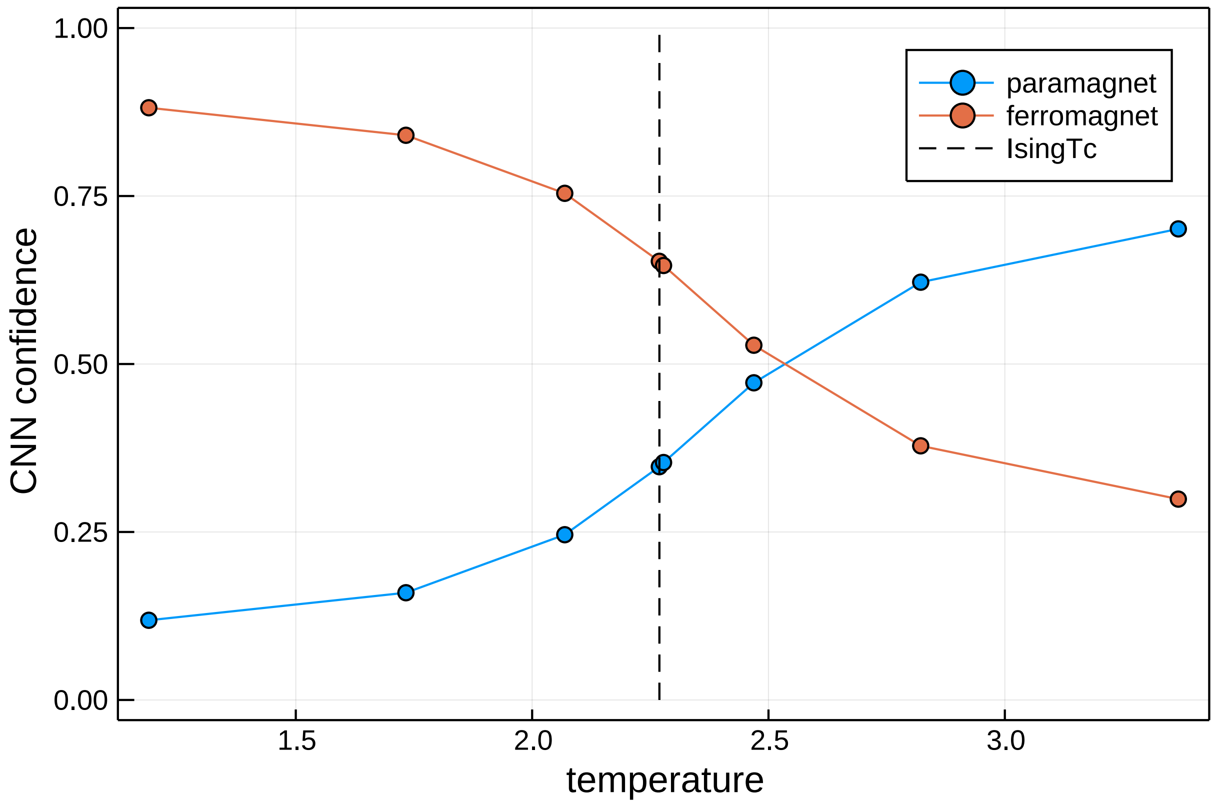

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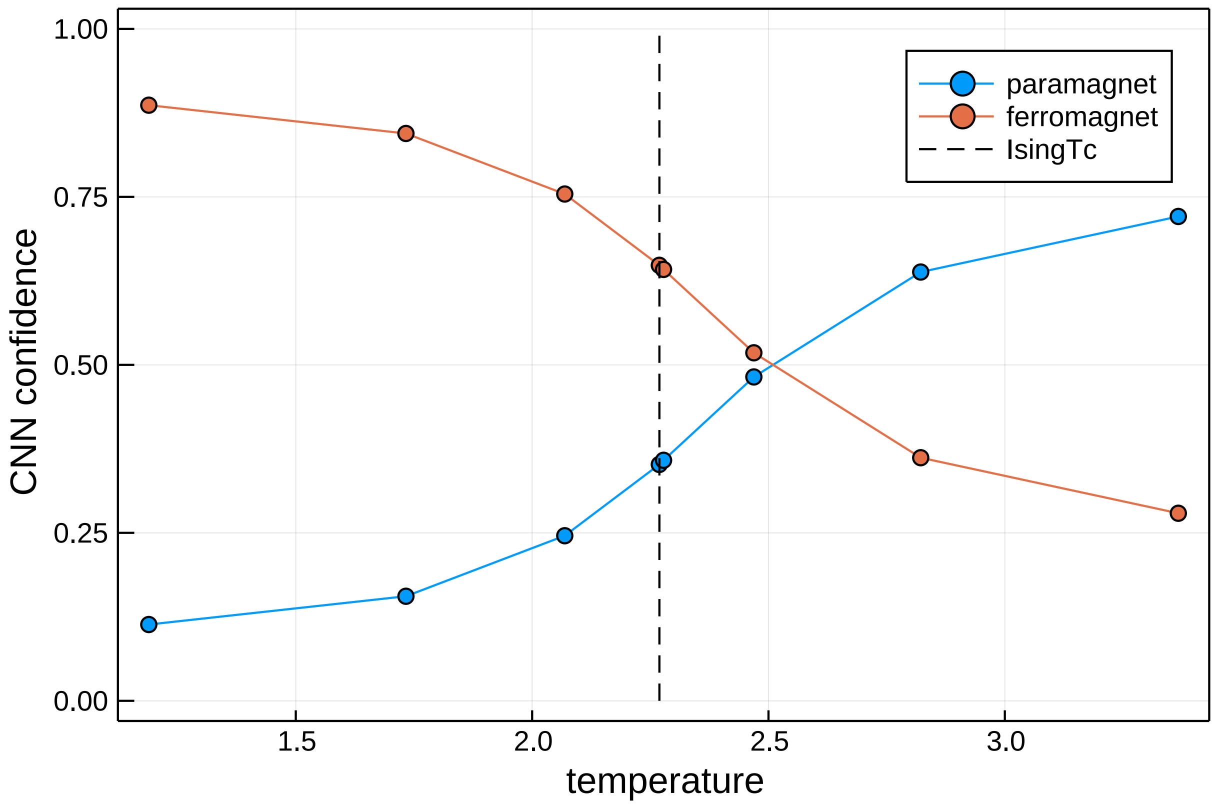

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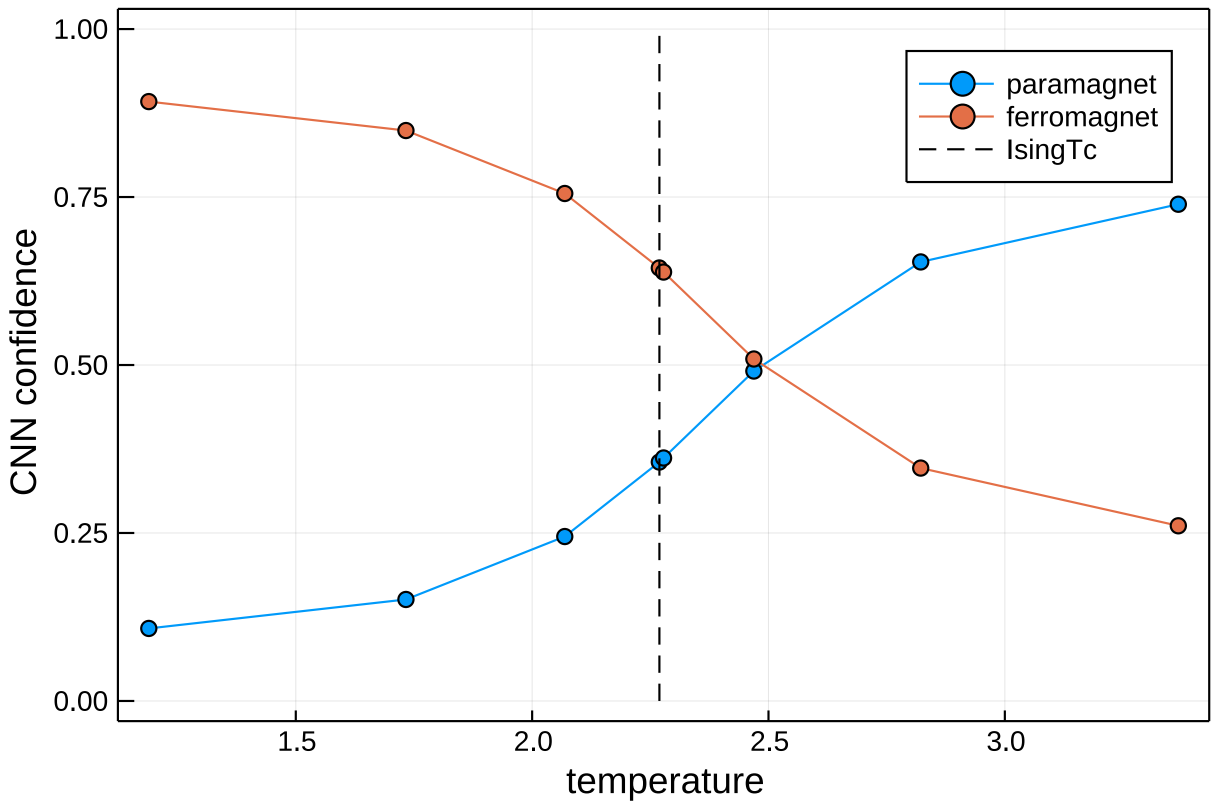

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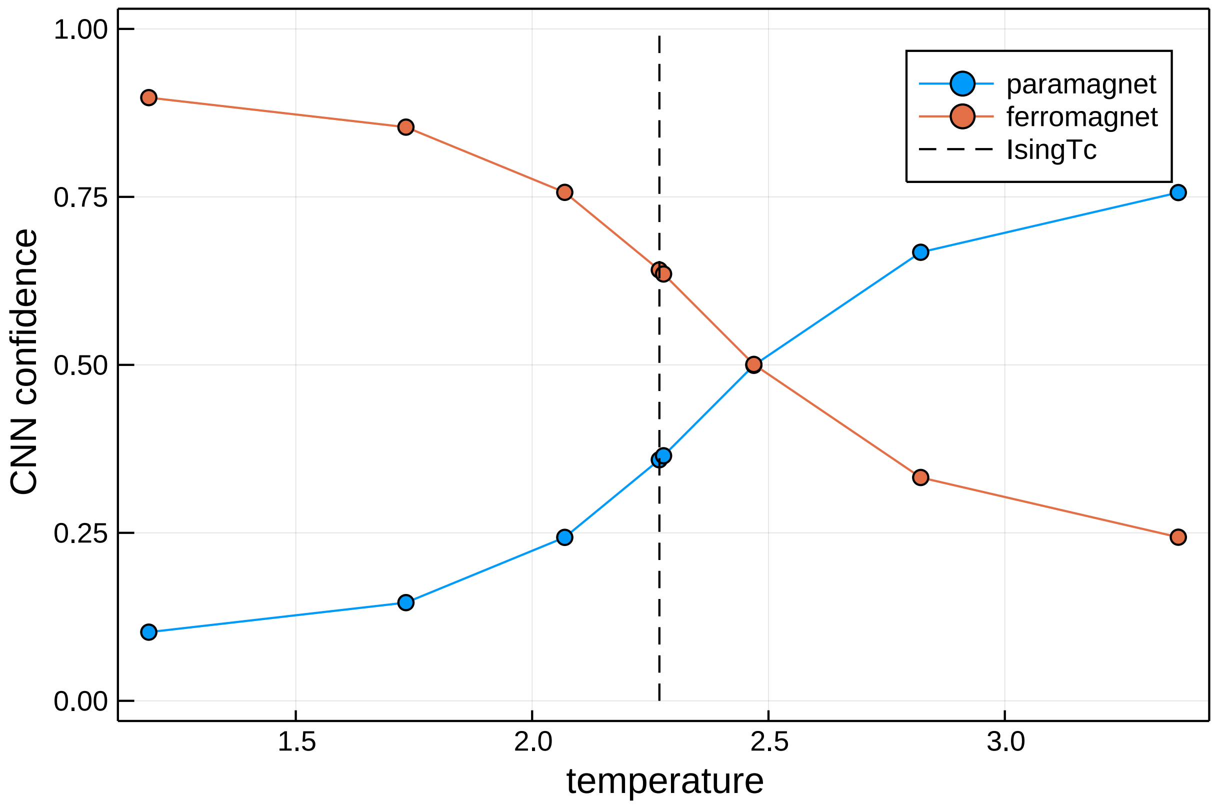
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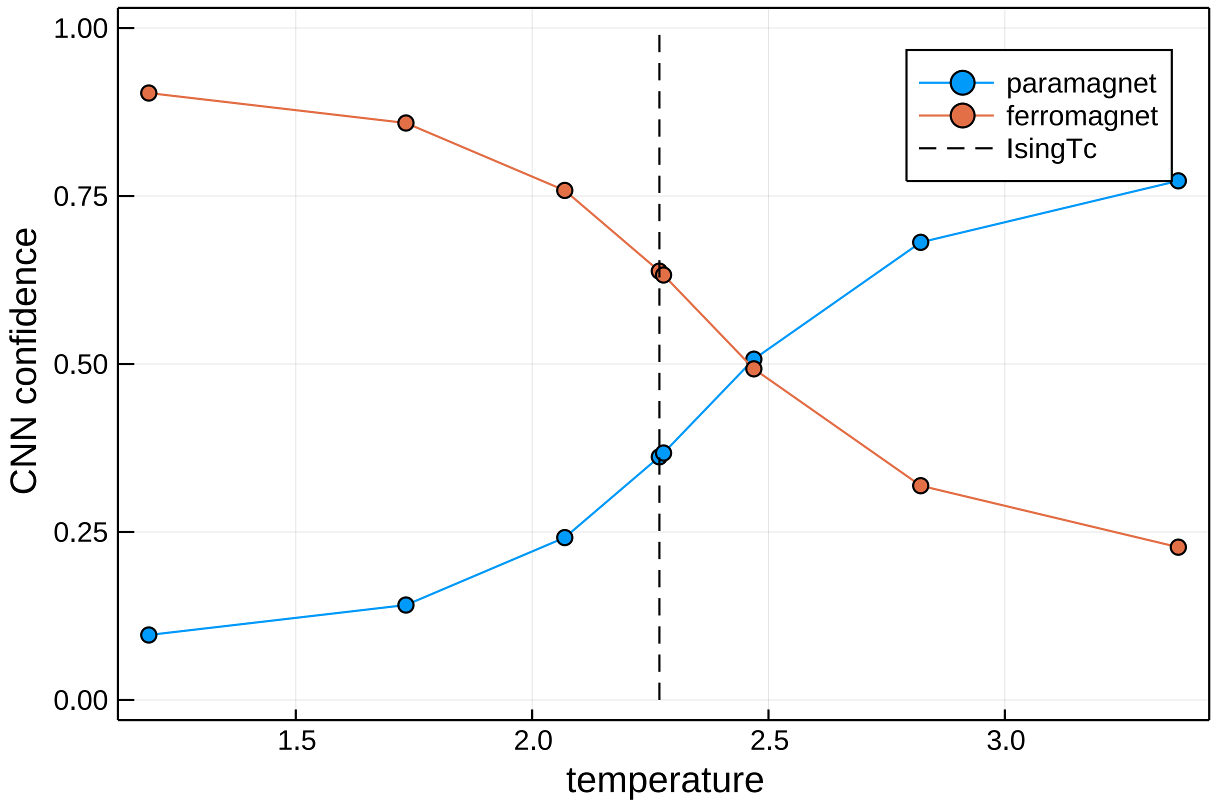
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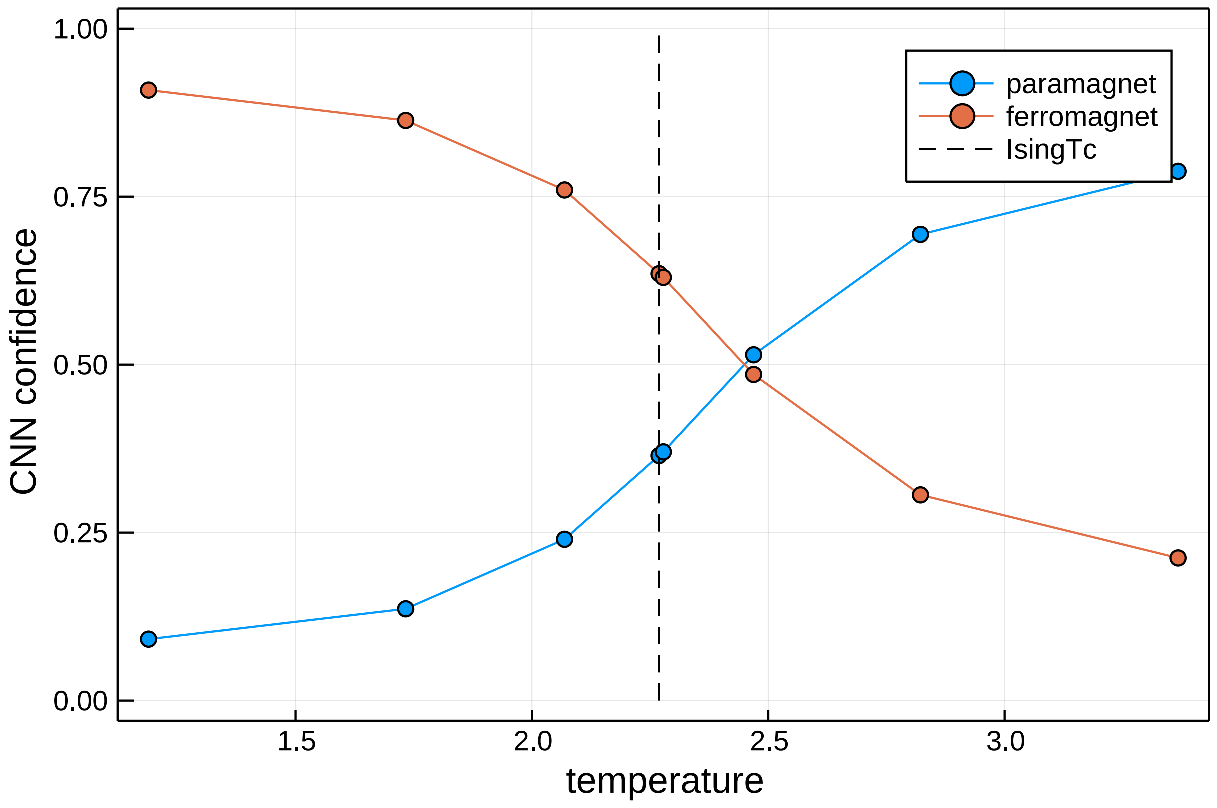
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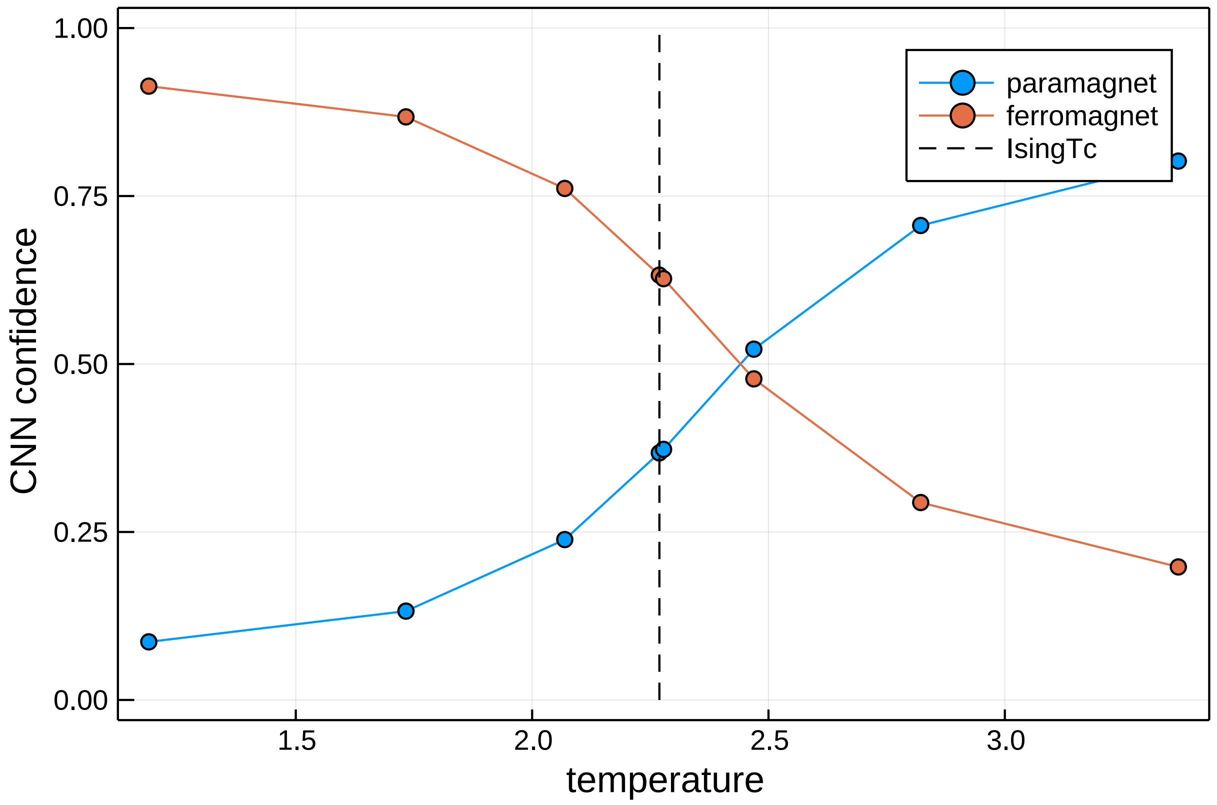
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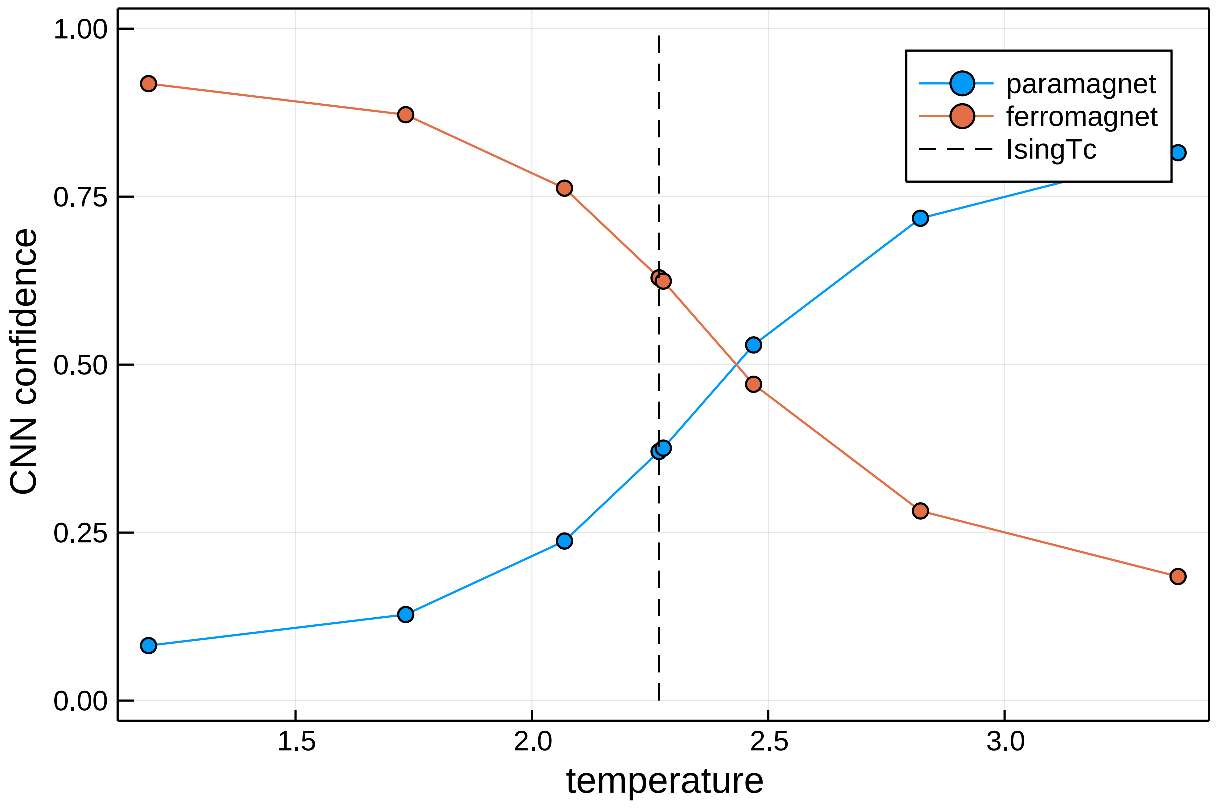

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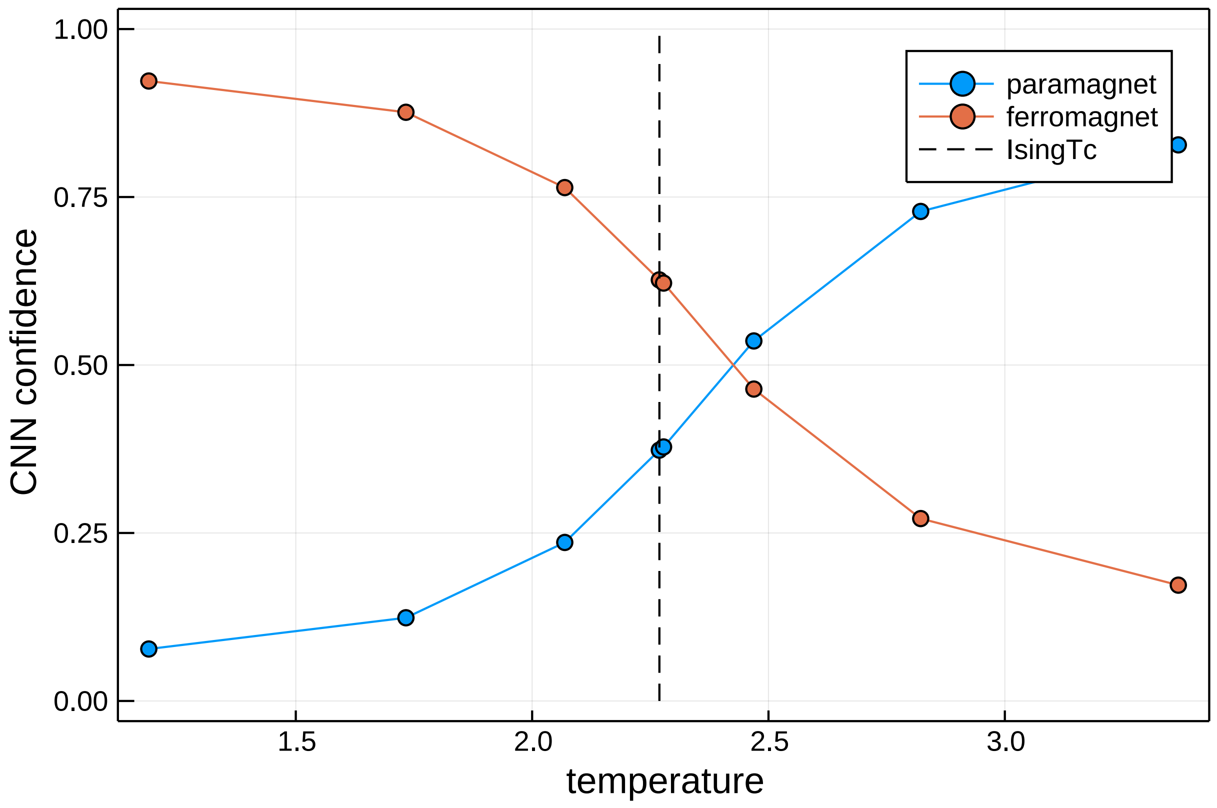

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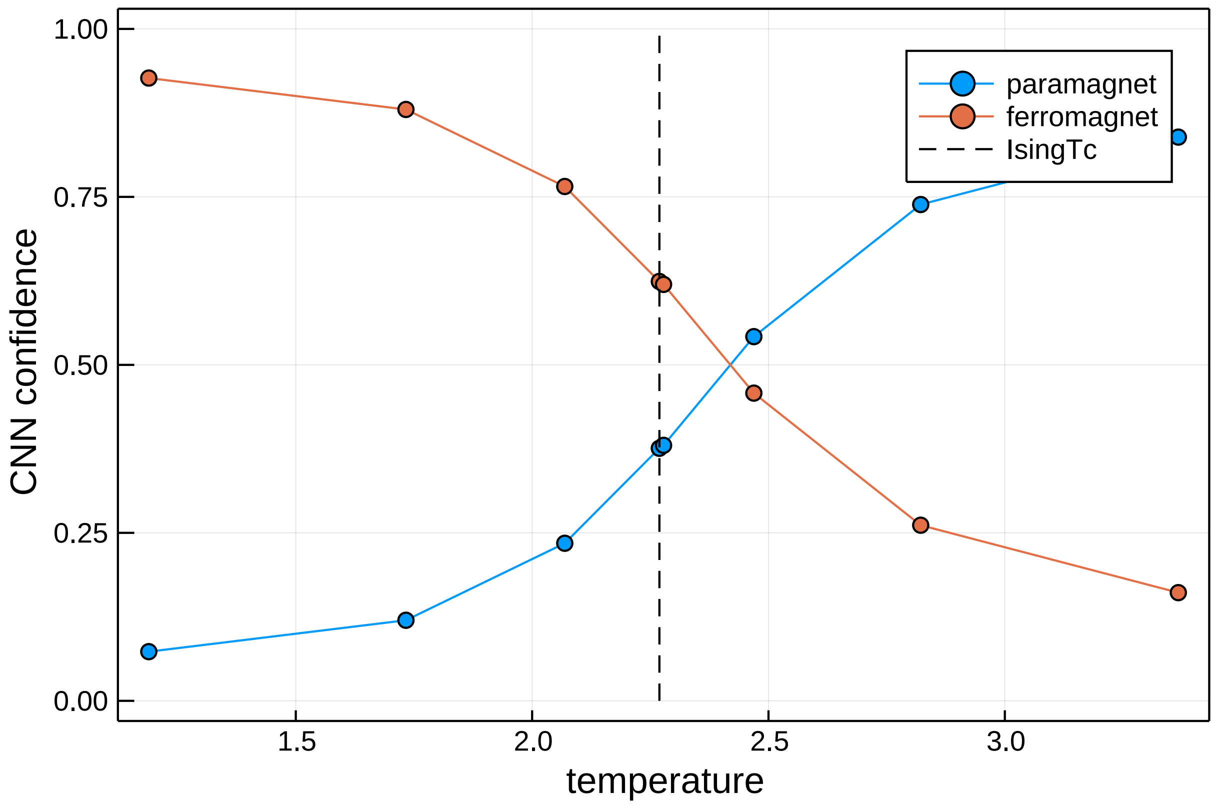

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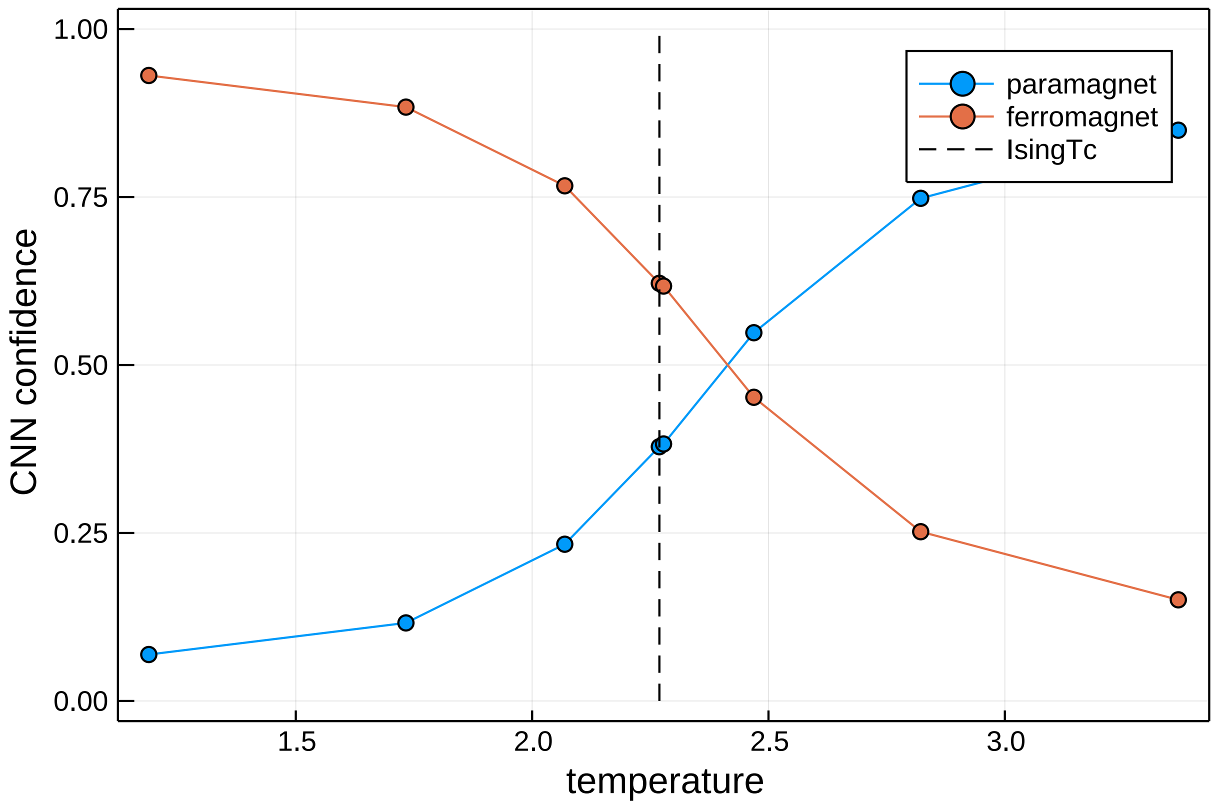

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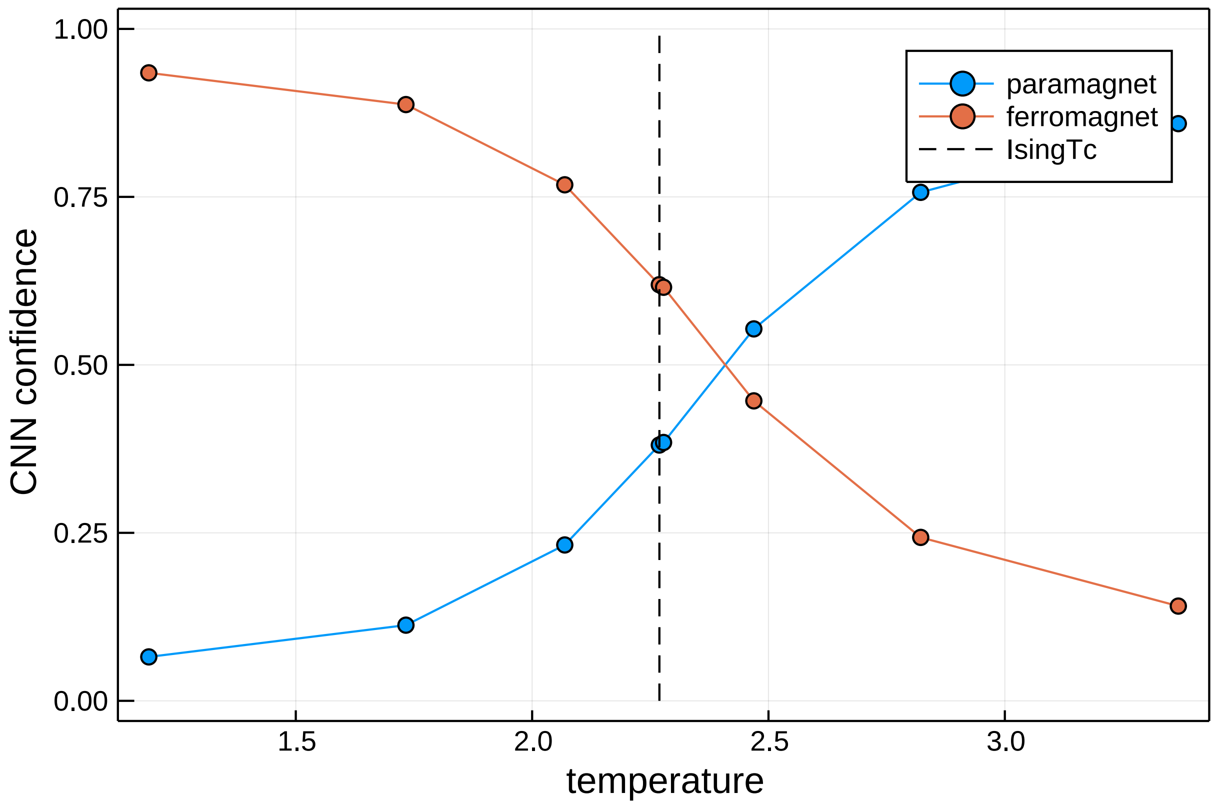
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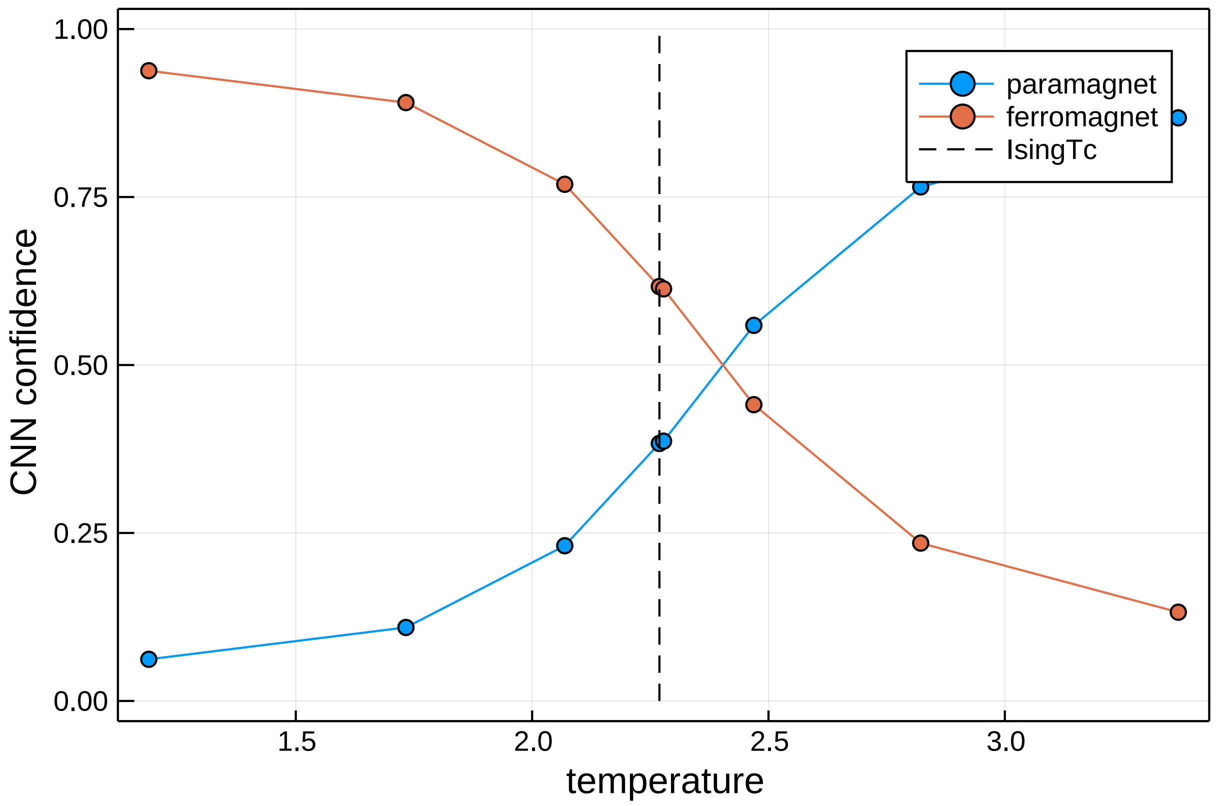
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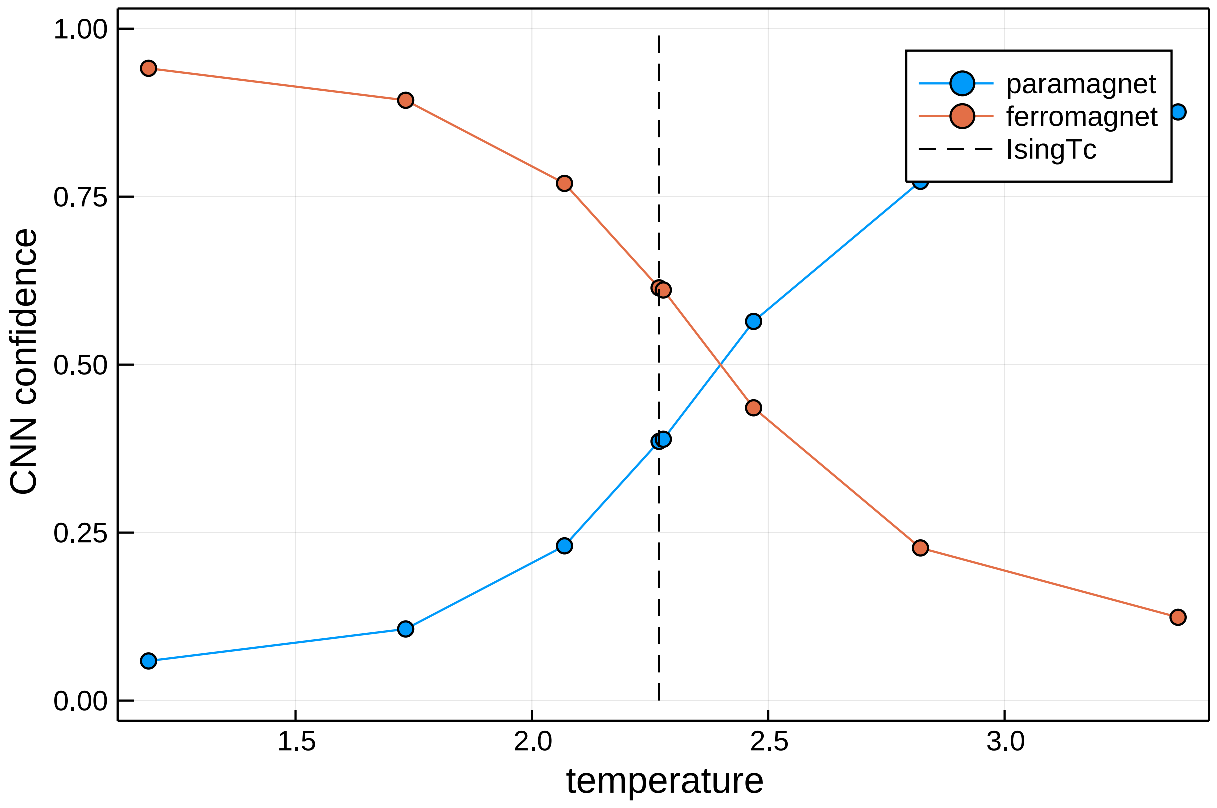

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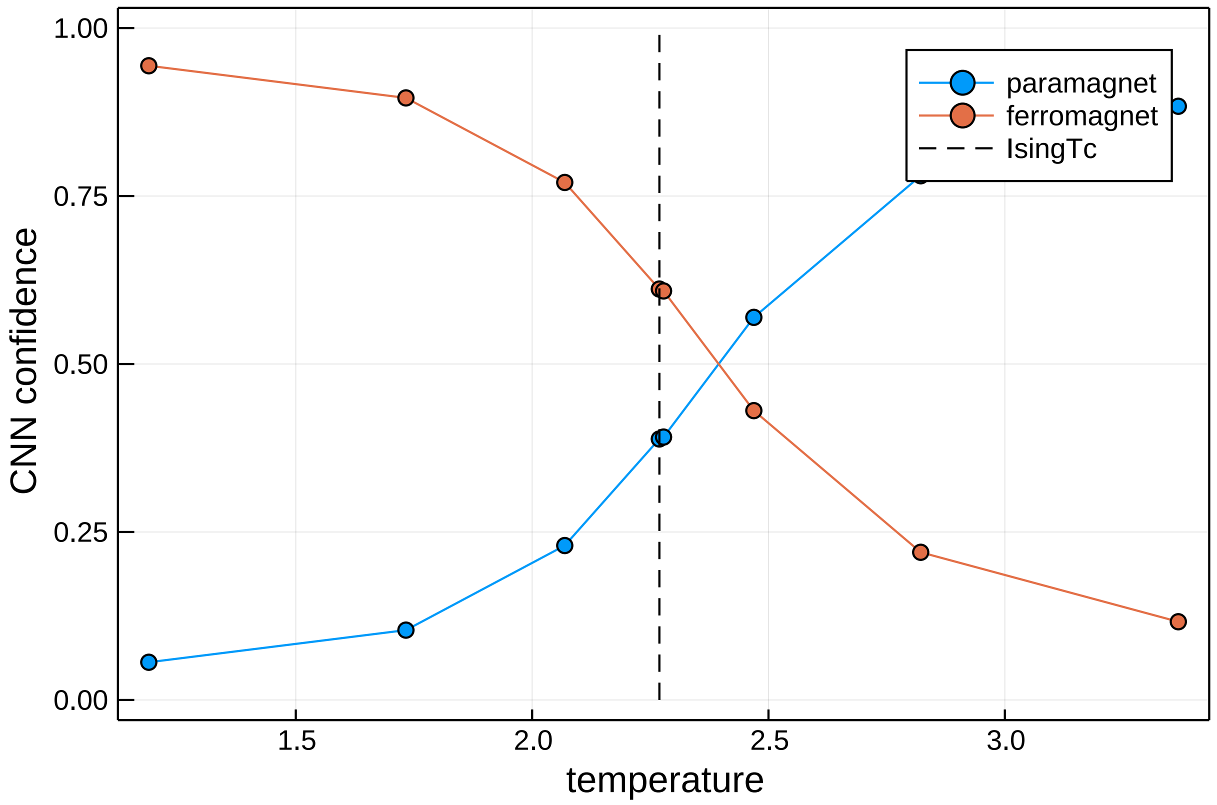

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CNN confidence
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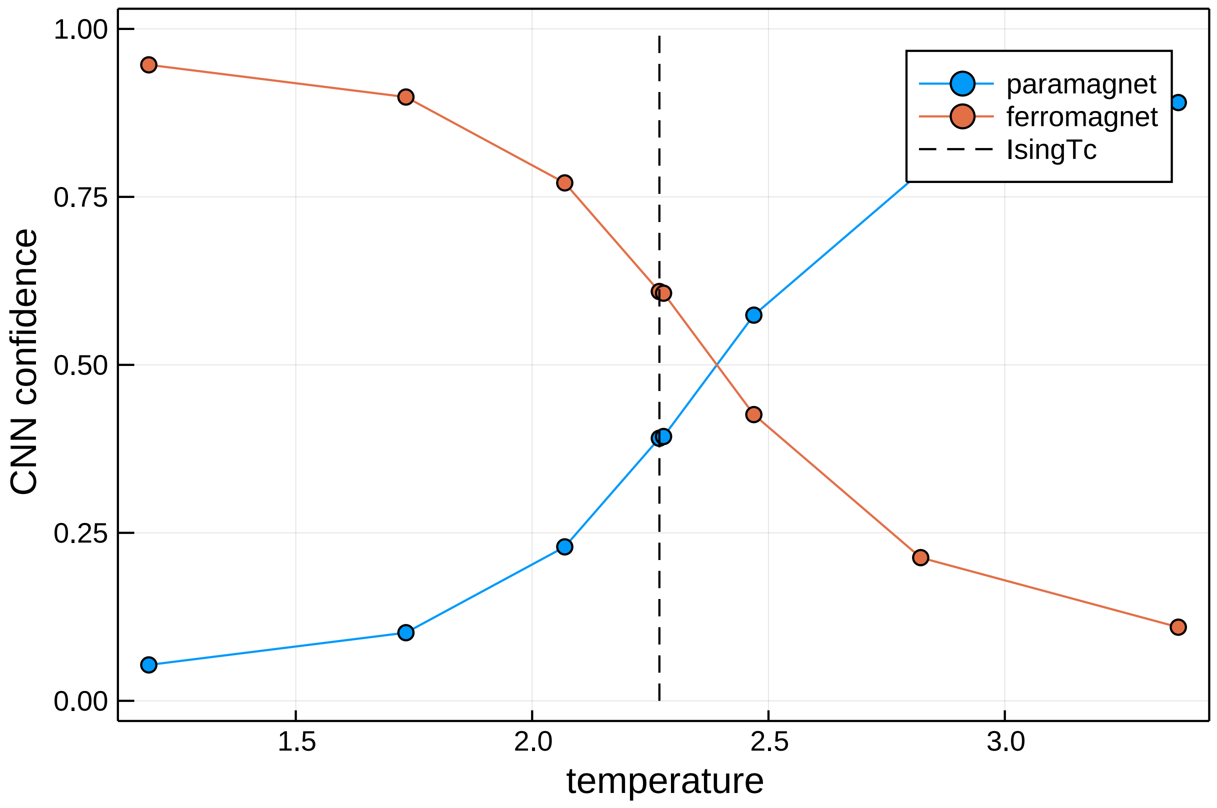
CNN confidence
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IsingTc
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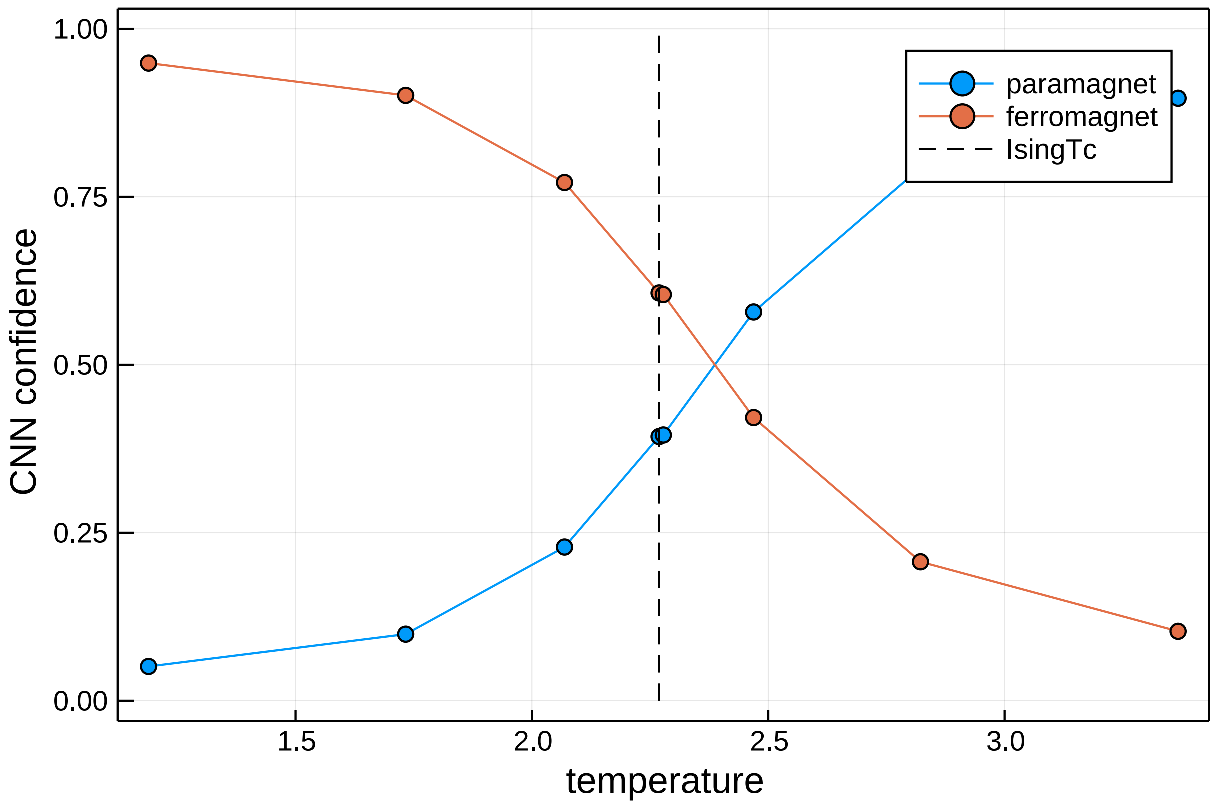
2.5
3.0


CNN confidence
temperature
paramagnet
ferromagnet
IsingTc
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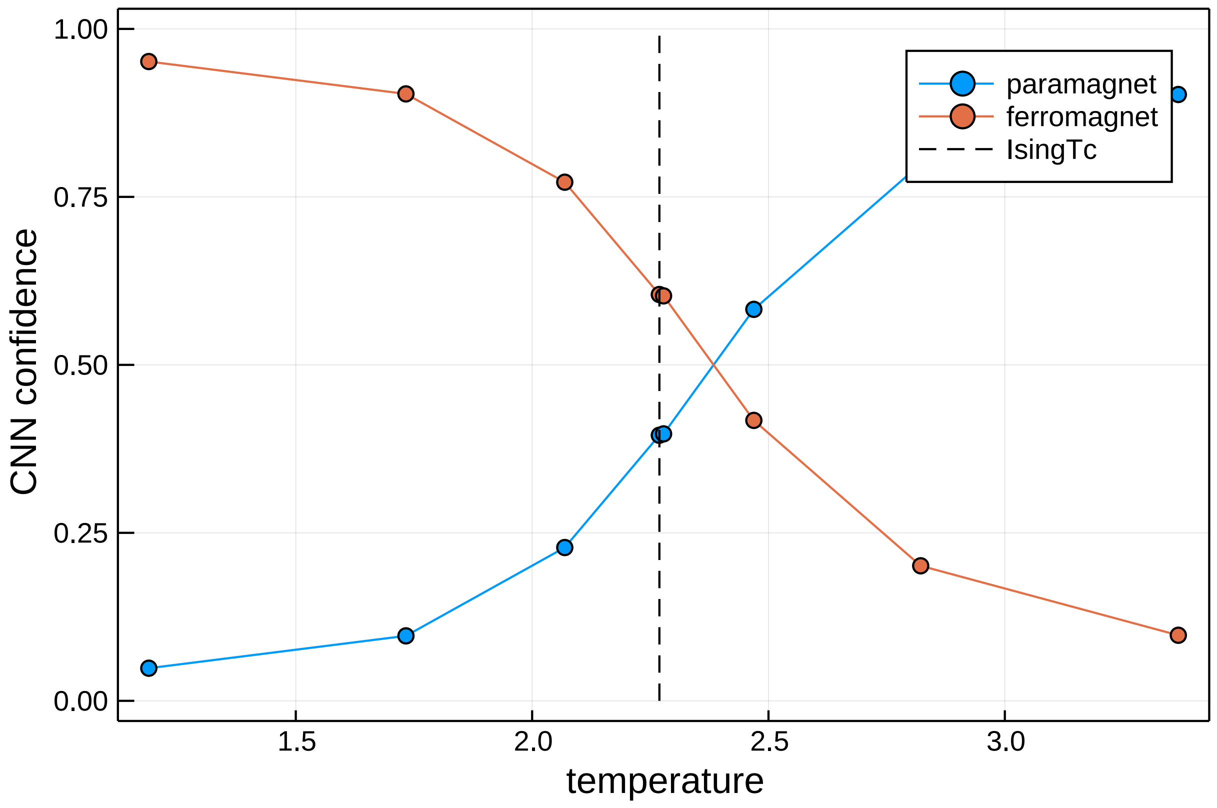
2.5
3.0


CNN confidence
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paramagnet
ferromagnet
IsingTc
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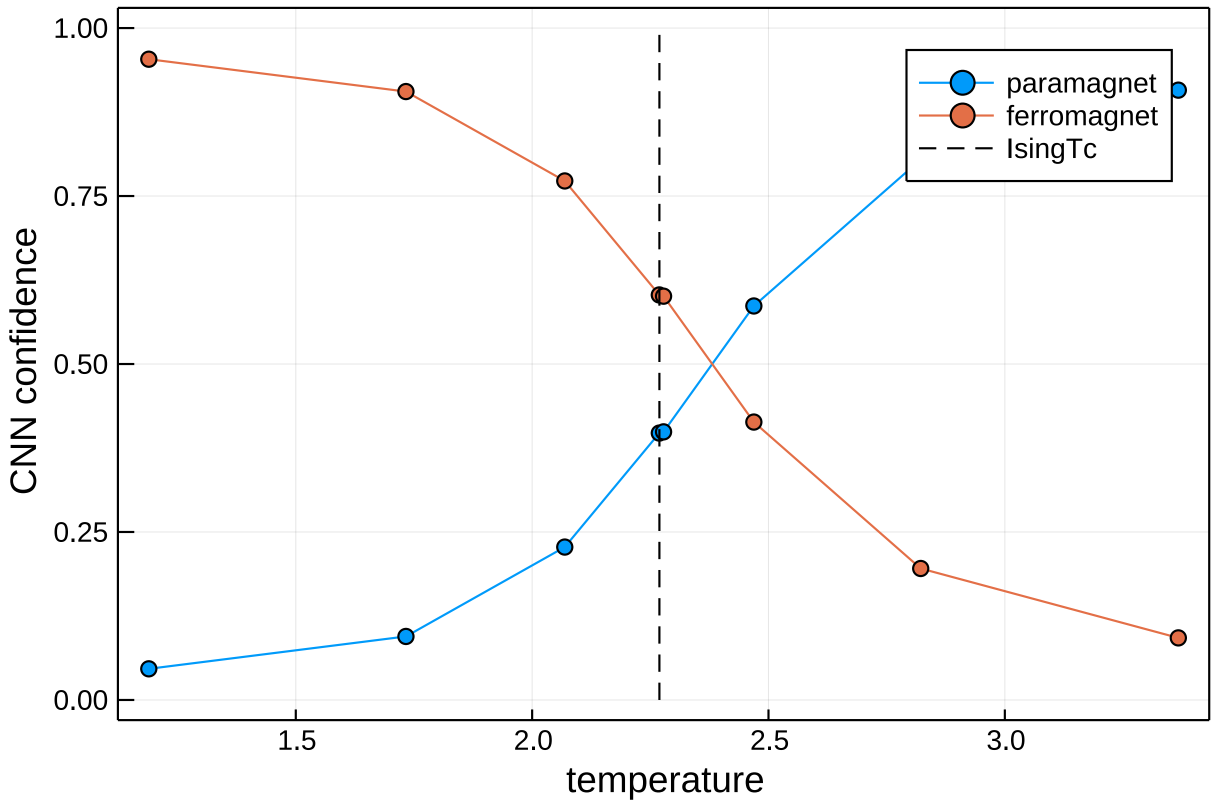
2.5
3.0


CNN confidence
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ferromagnet
IsingTc
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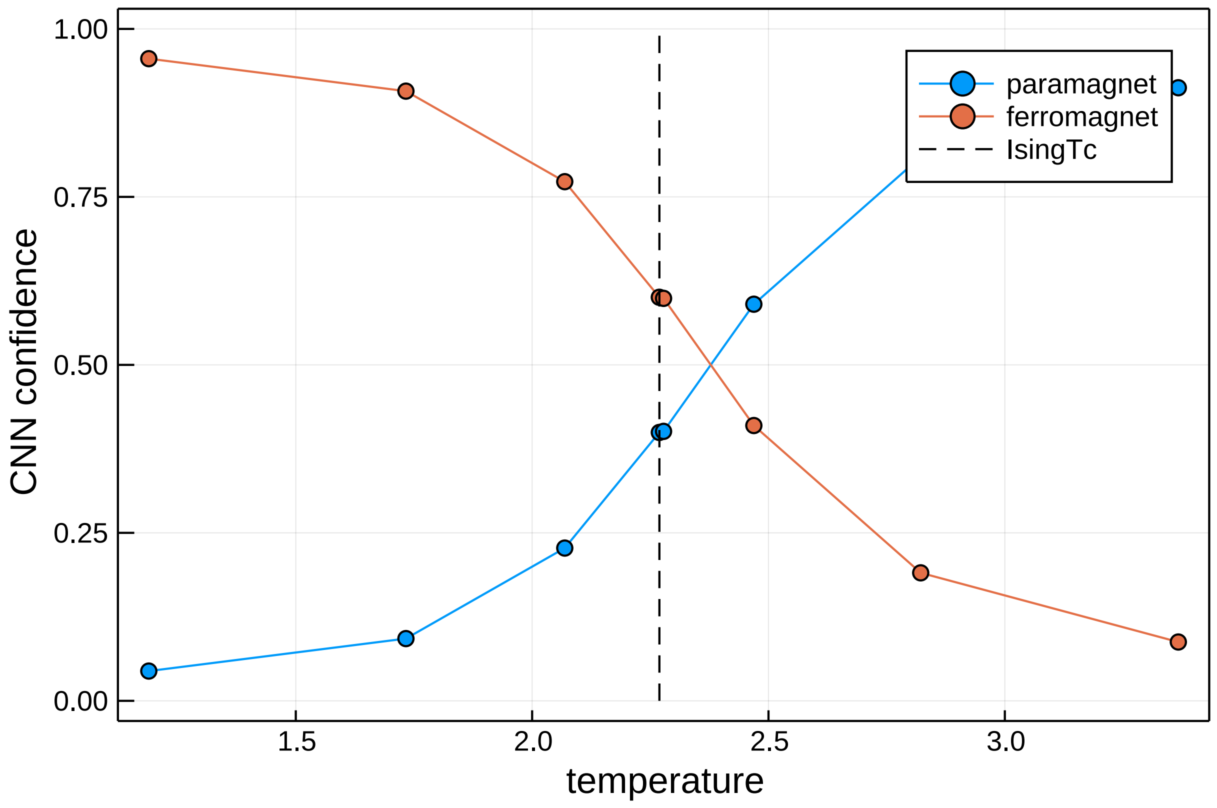
2.5
3.0



CNN confidence
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0.00
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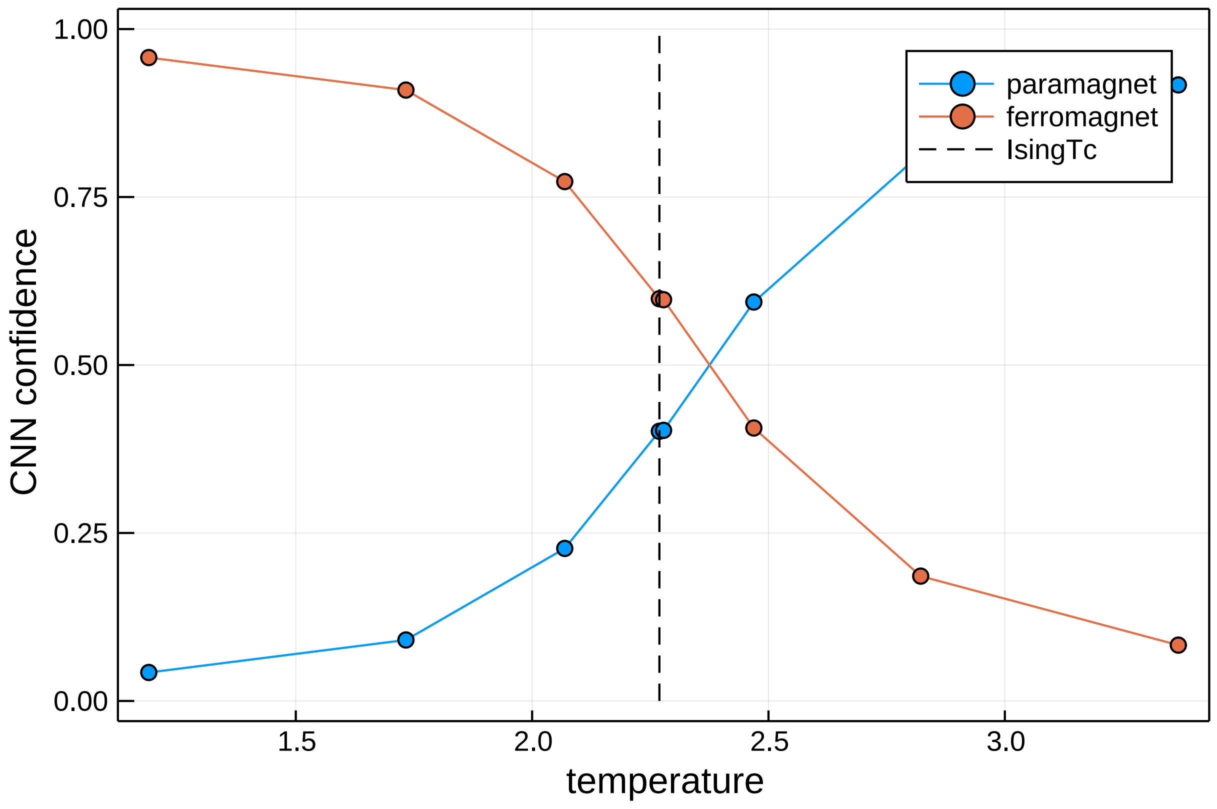
3.0
paramagnet
ferromagnet
IsingTc



CNN confidence
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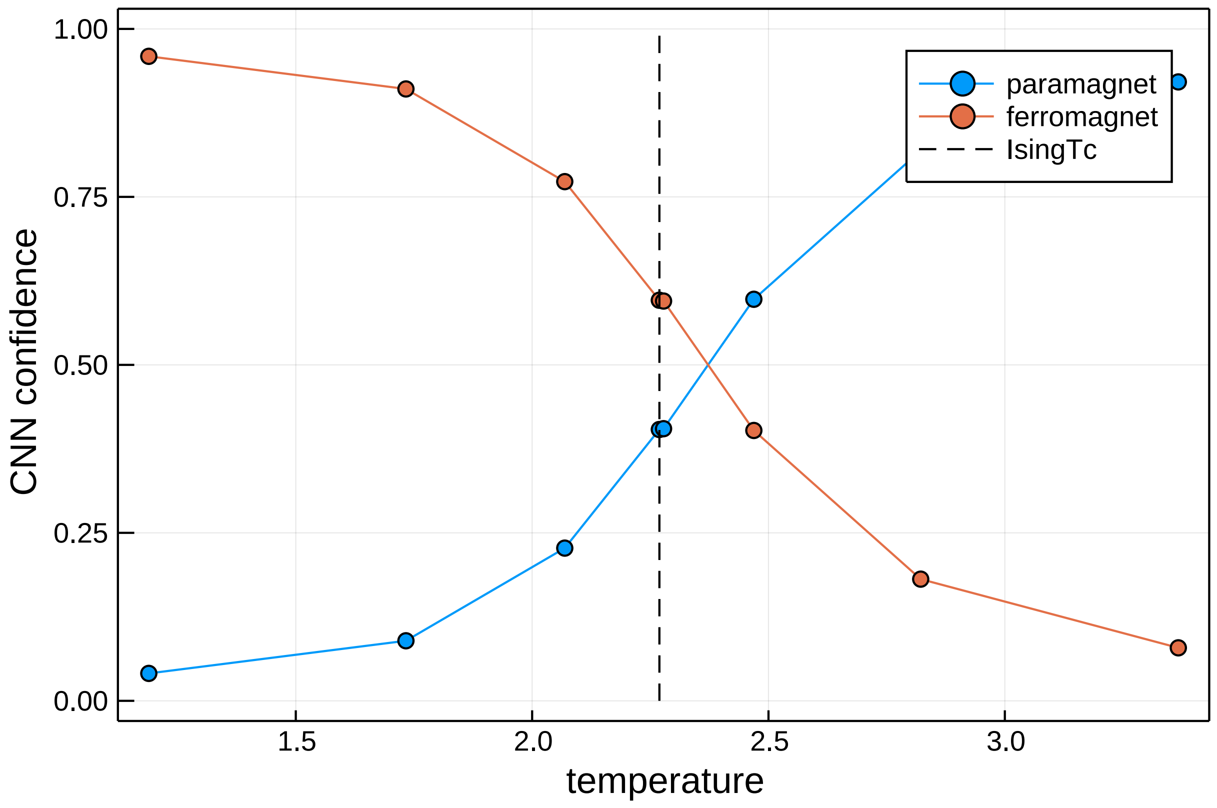
paramagnet
ferromagnet
IsingTc


CNN confidence
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ferromagnet
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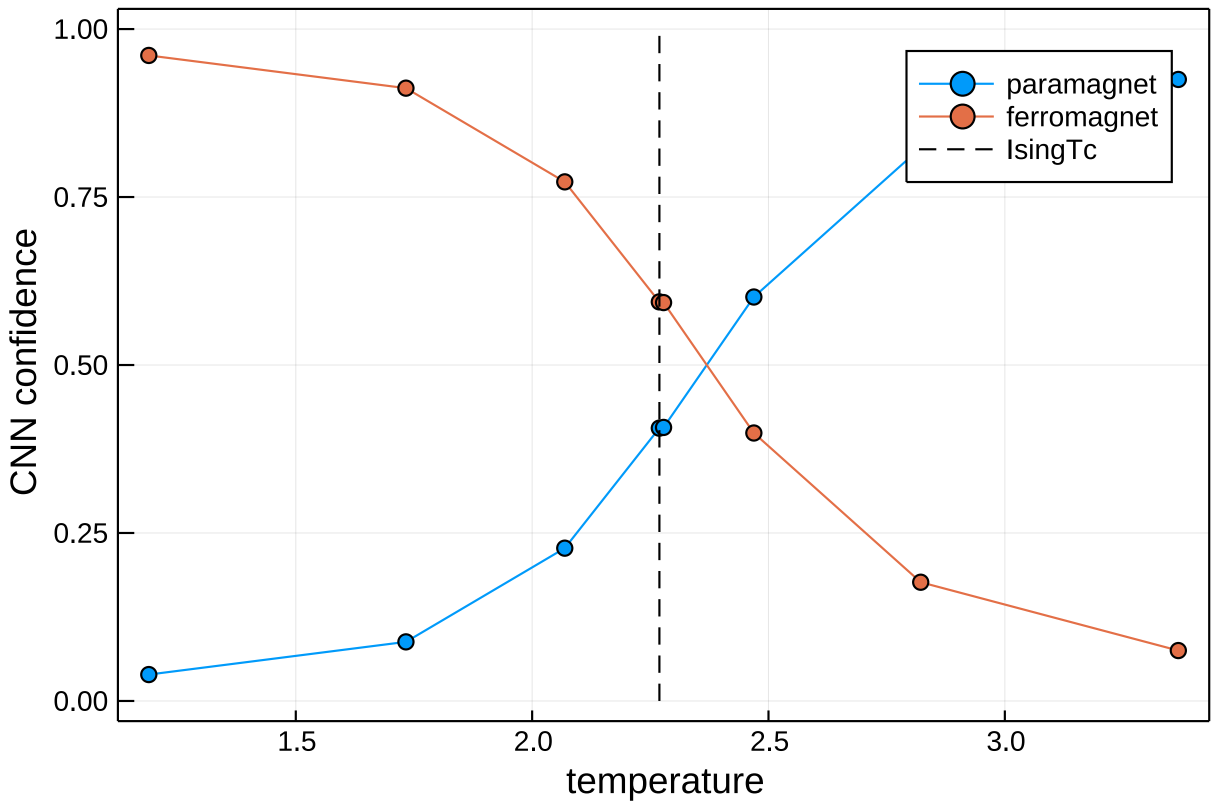
3.0


CNN confidence
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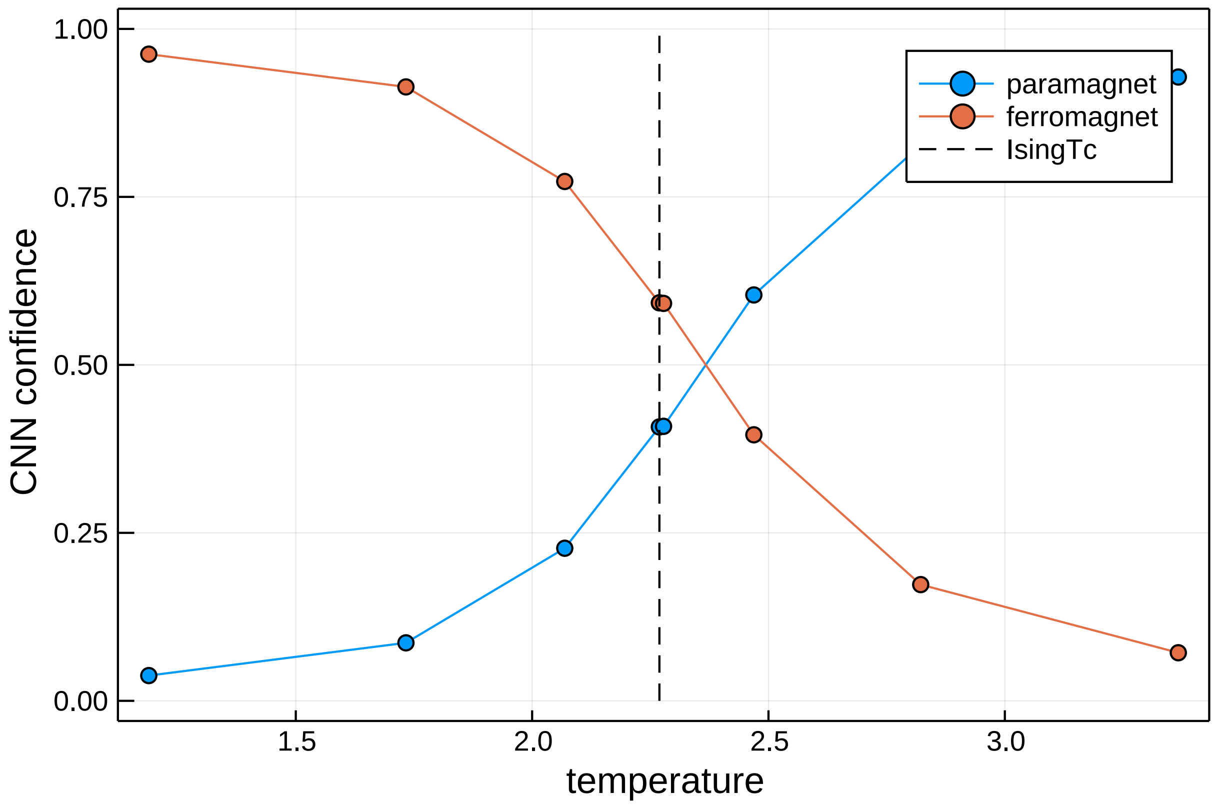
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CNN confidence
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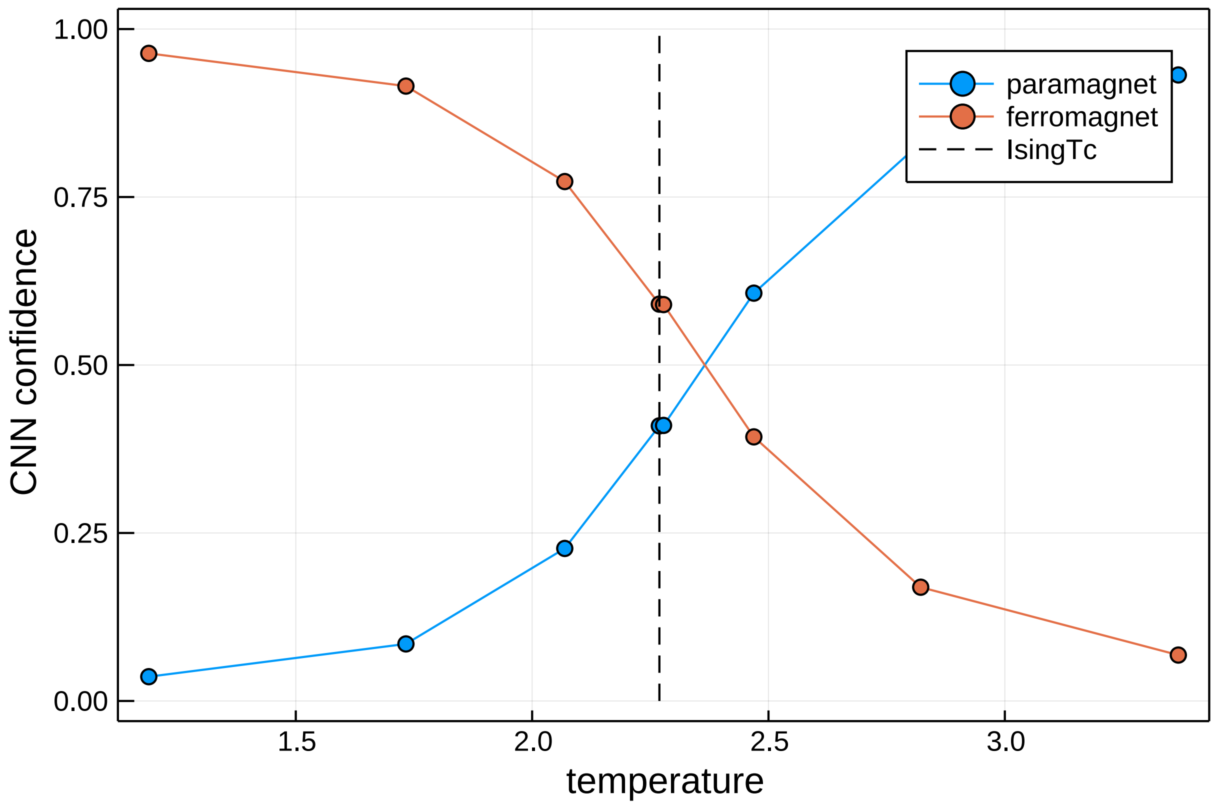
paramagnet
ferromagnet
IsingTc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CNN confidence
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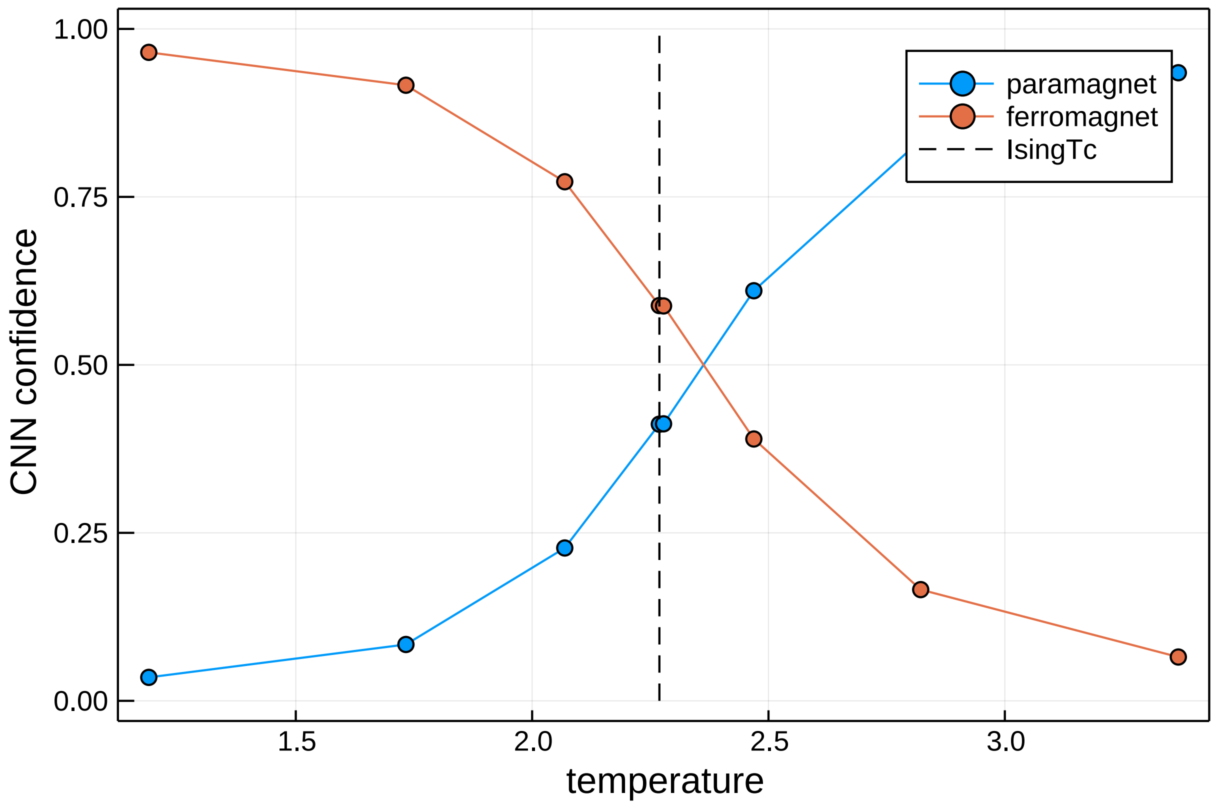
ferromagnet
IsingTc



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CNN confidence
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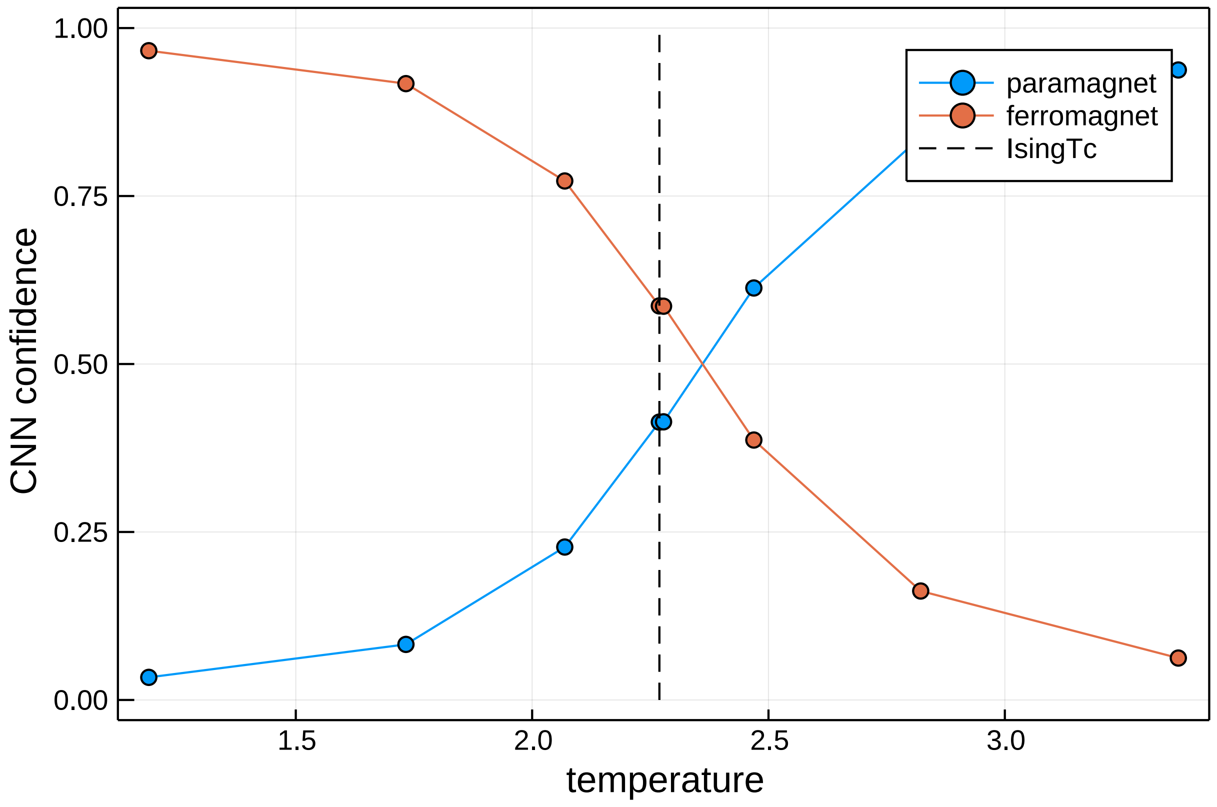
paramagnet
ferromagnet
IsingTc



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CNN confidence
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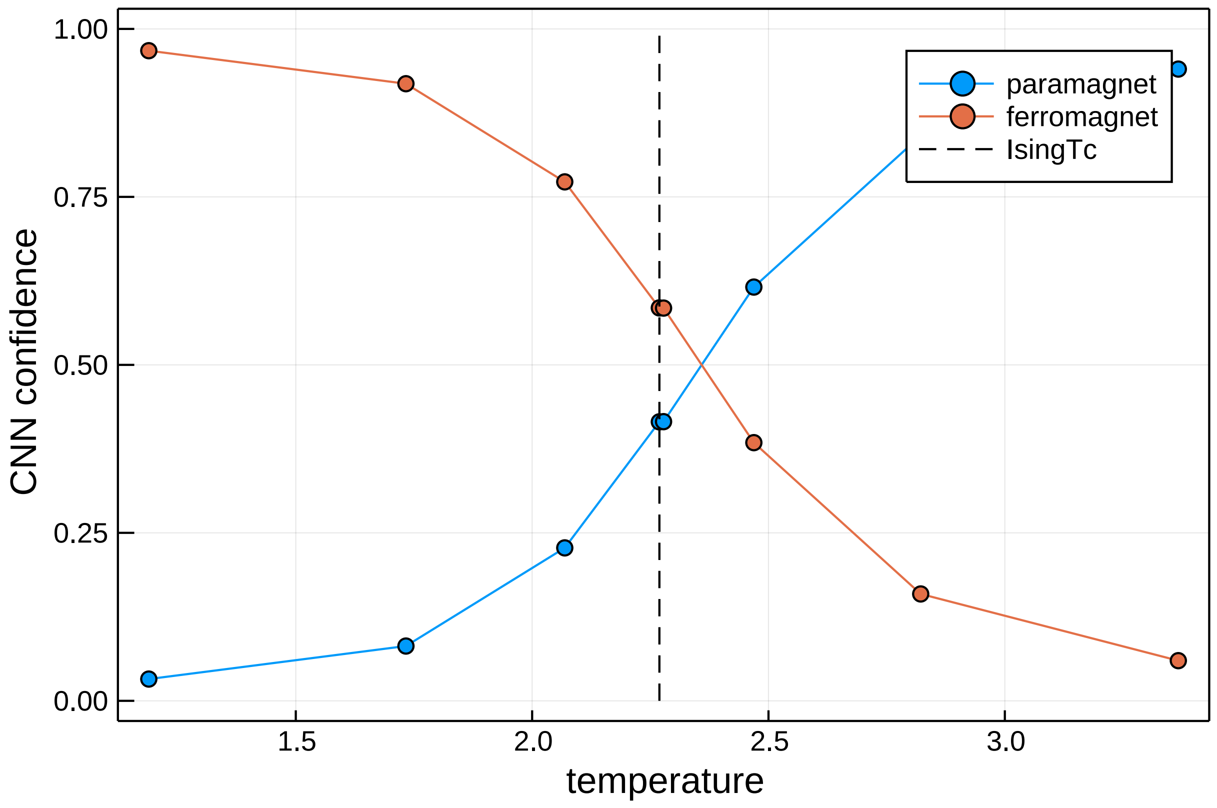
IsingTc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CNN confidence
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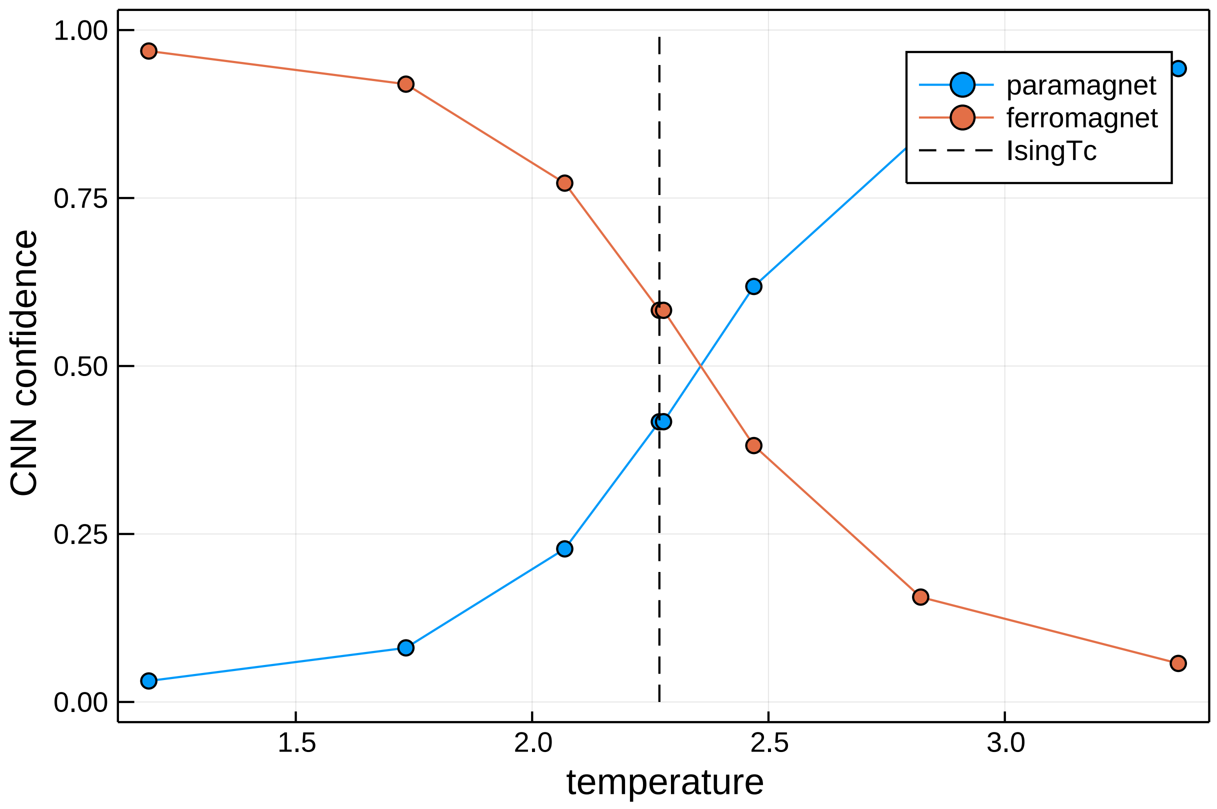
ferromagnet
IsingTc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CNN confidence
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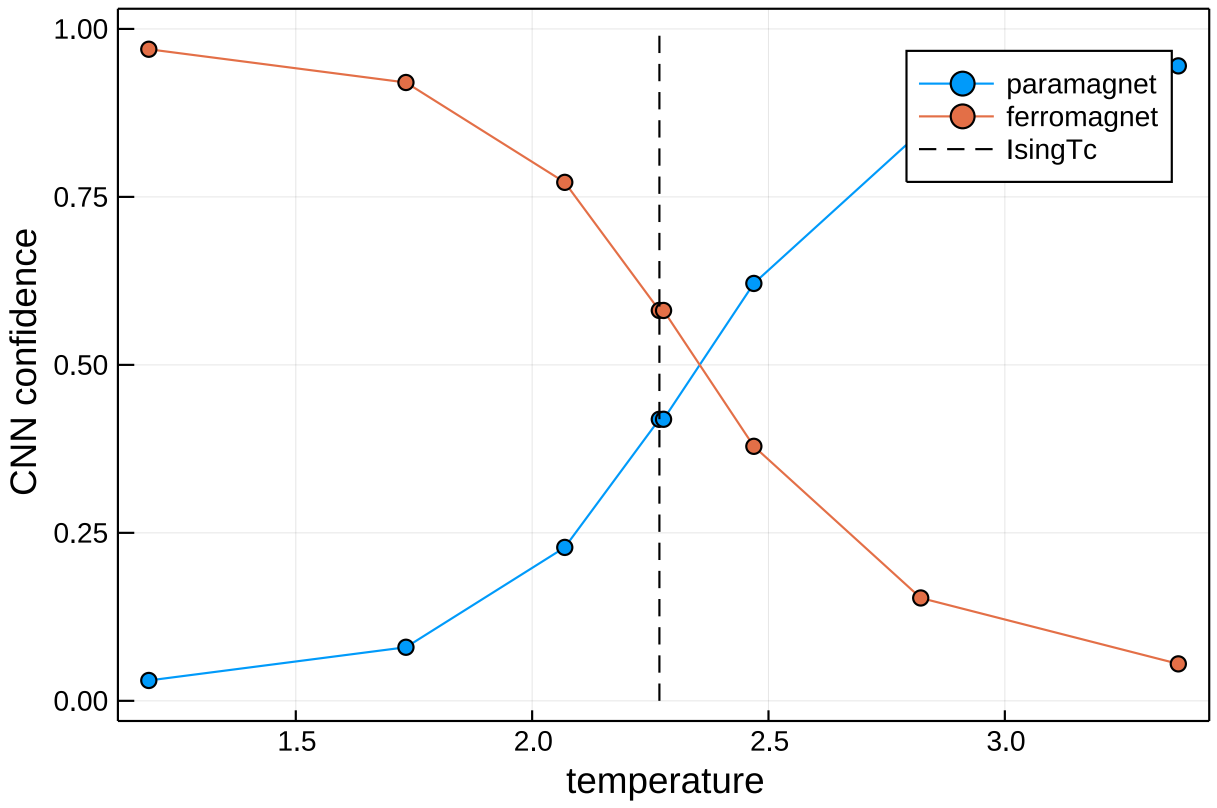
temperature
paramagnet
ferromagnet
IsingTc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CNN confidence
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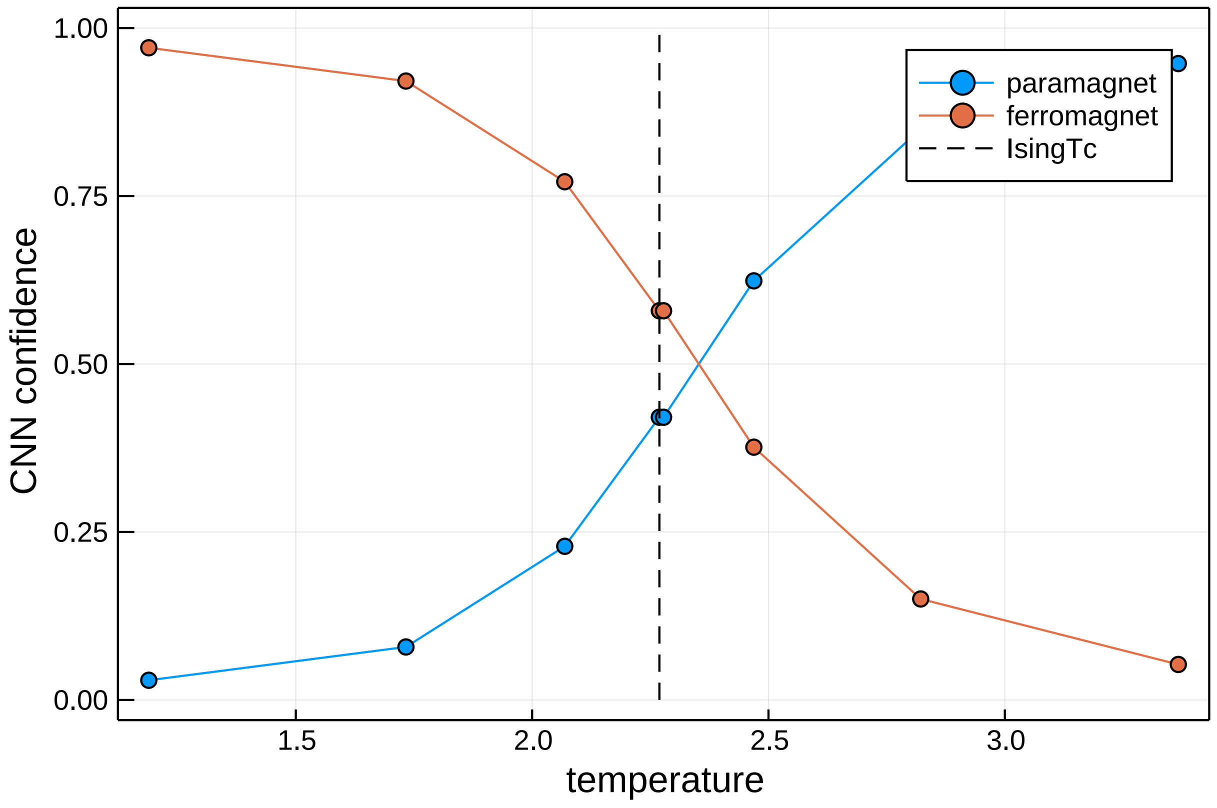
temperature
paramagnet
ferromagnet
IsingTc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CNN confidence
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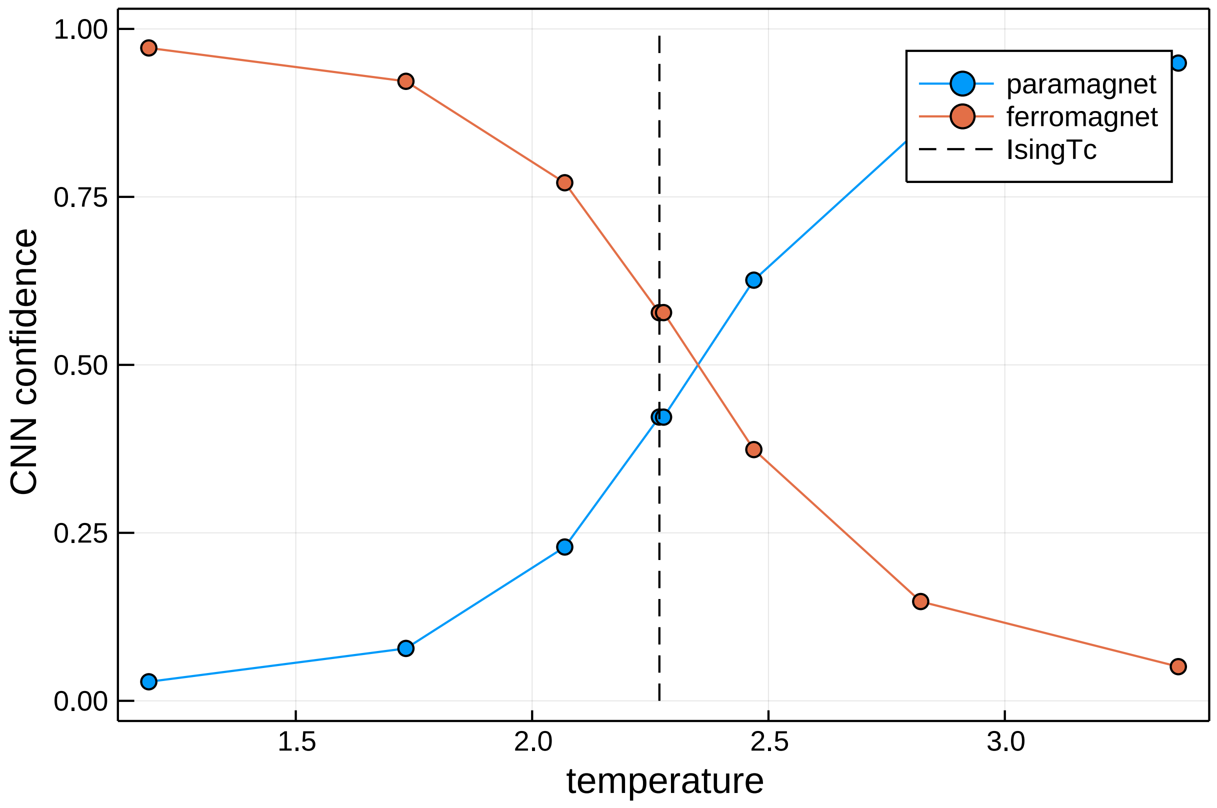
ferromagnet
IsingTc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CNN confidence
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temperature
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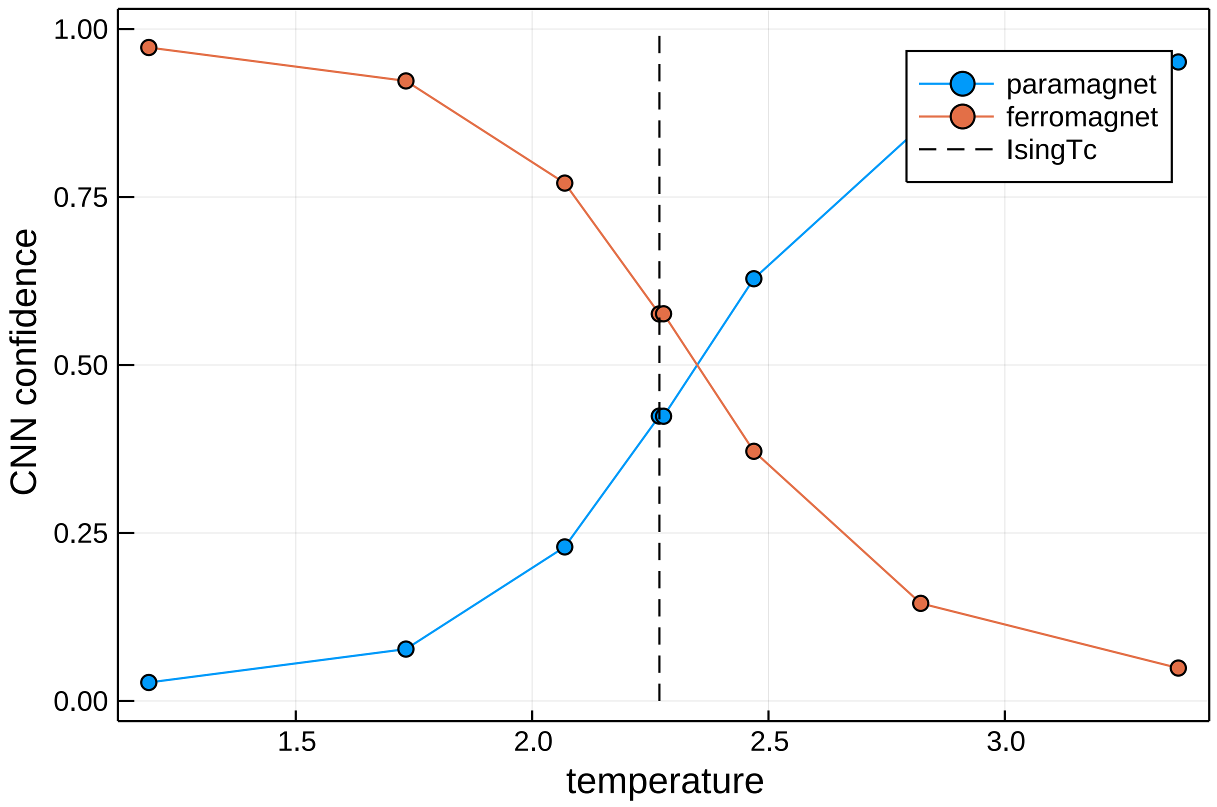
ferromagnet
IsingTc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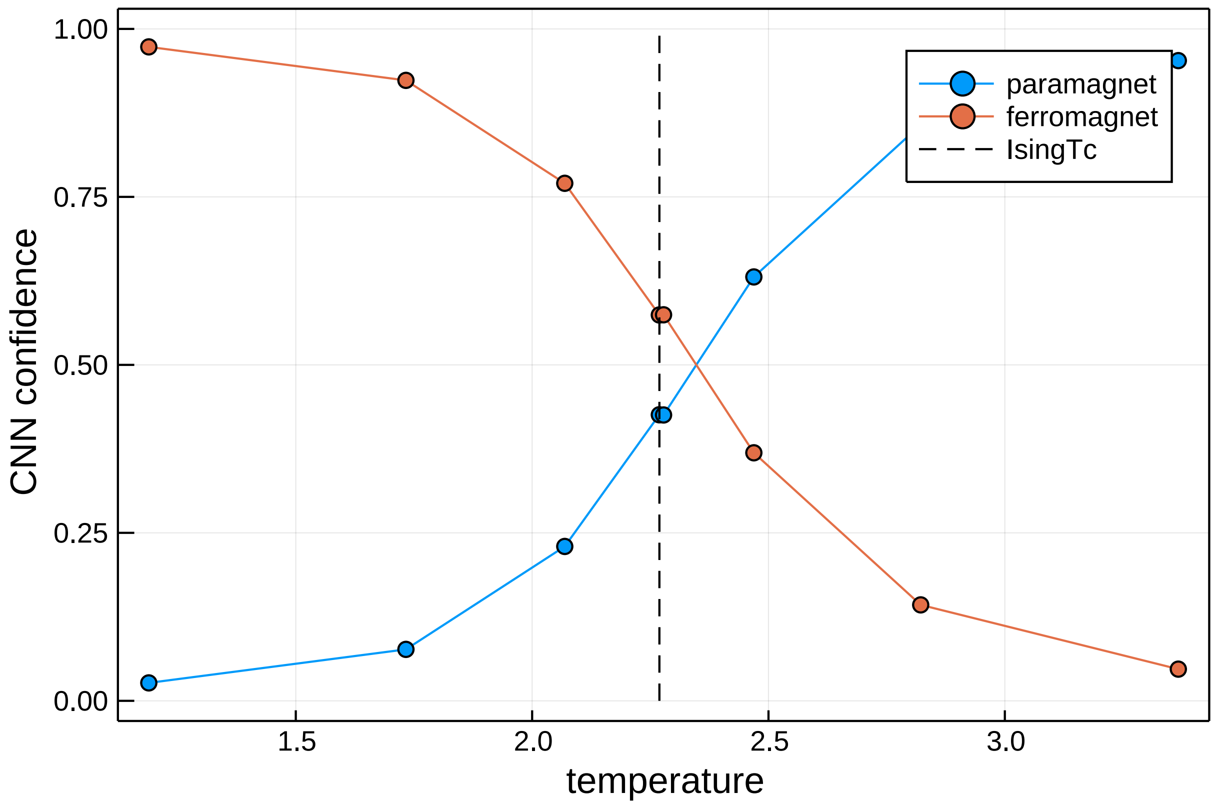
ferromagnet
IsingTc



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CNN confidence
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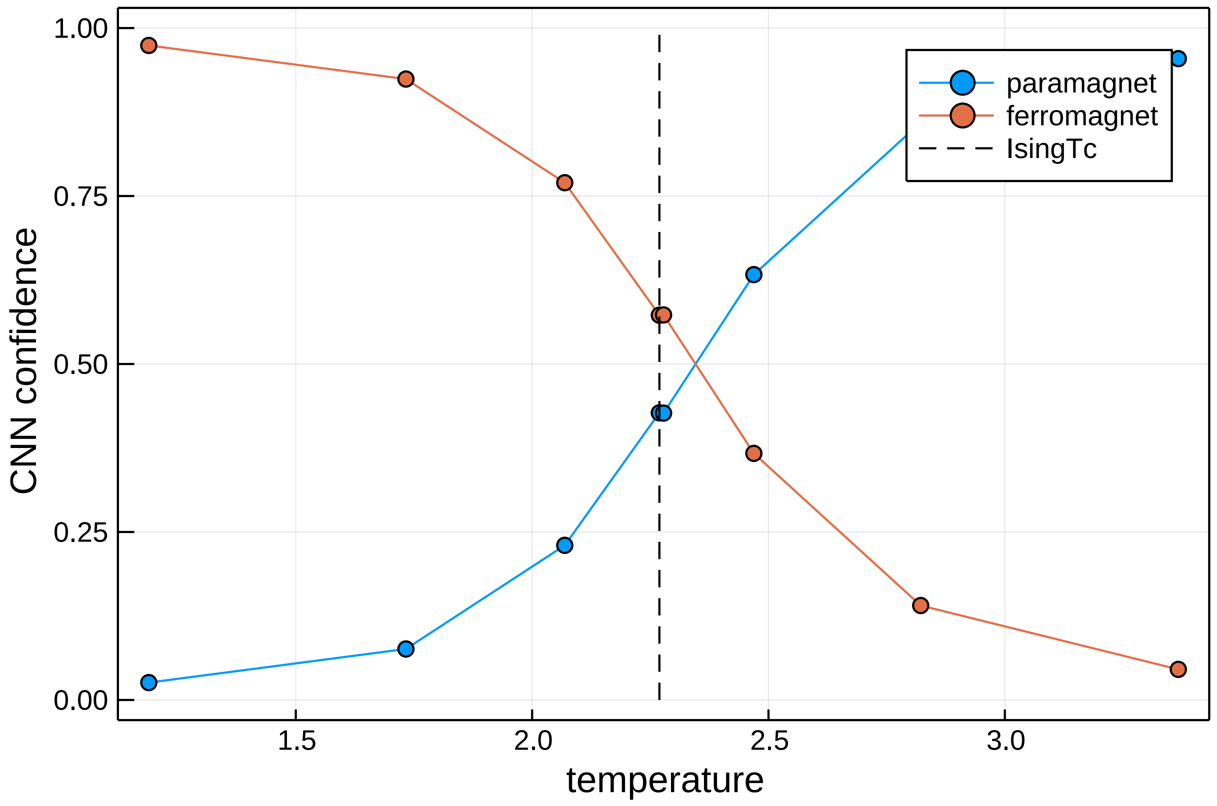
temperature
paramagnet
ferromagnet
IsingTc



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CNN confidence
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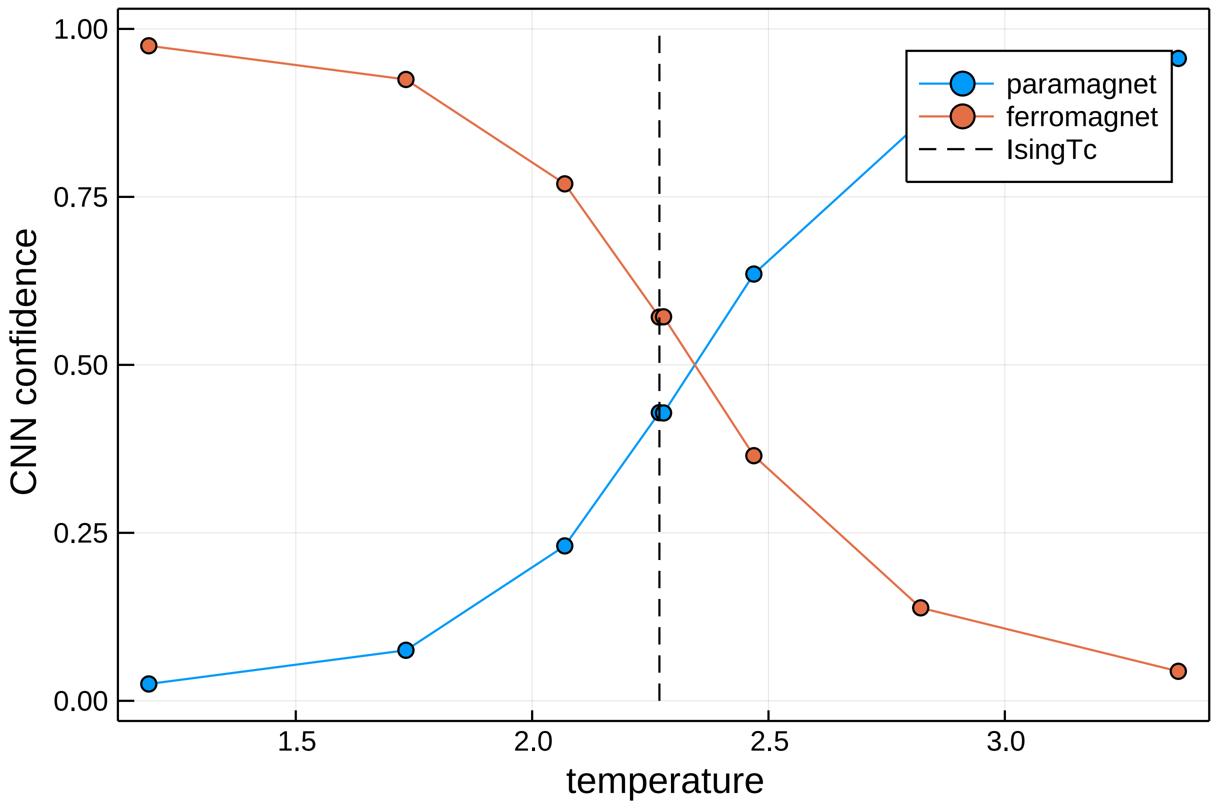
ferromagnet
IsingTc



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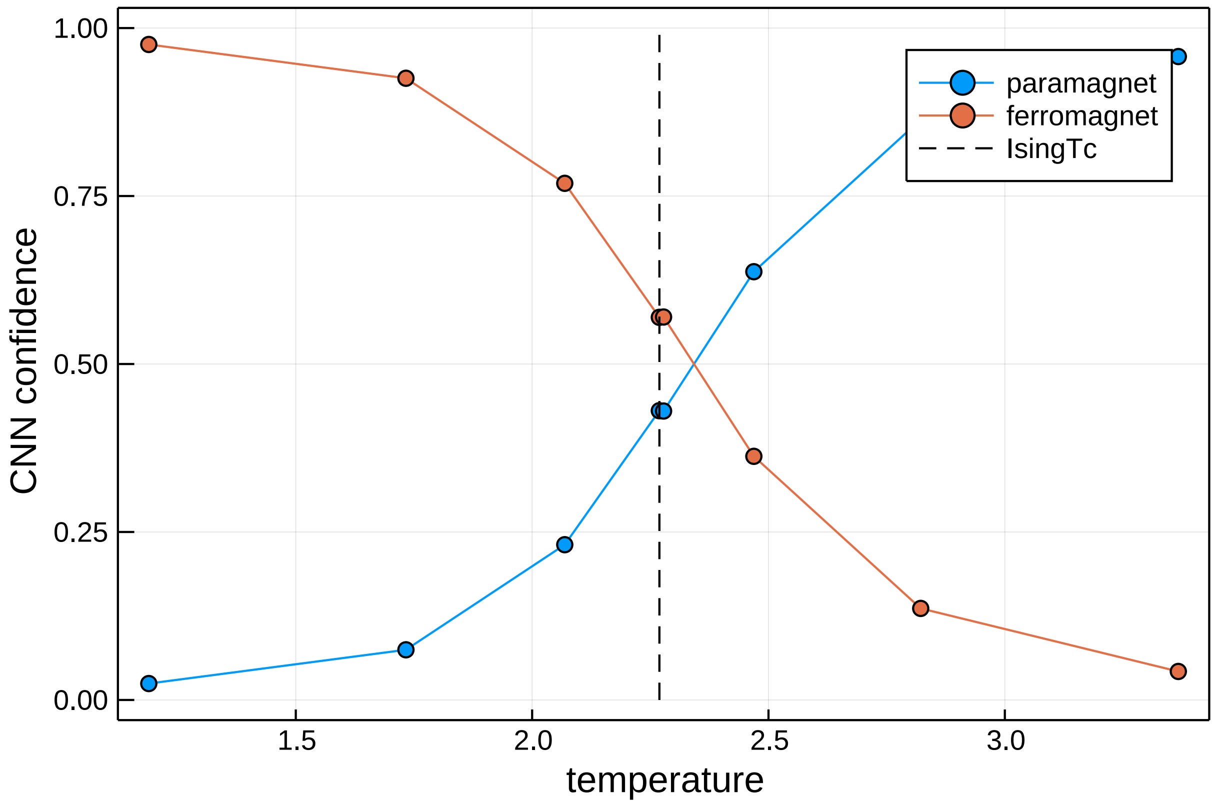
IsingTc



CNN confidence
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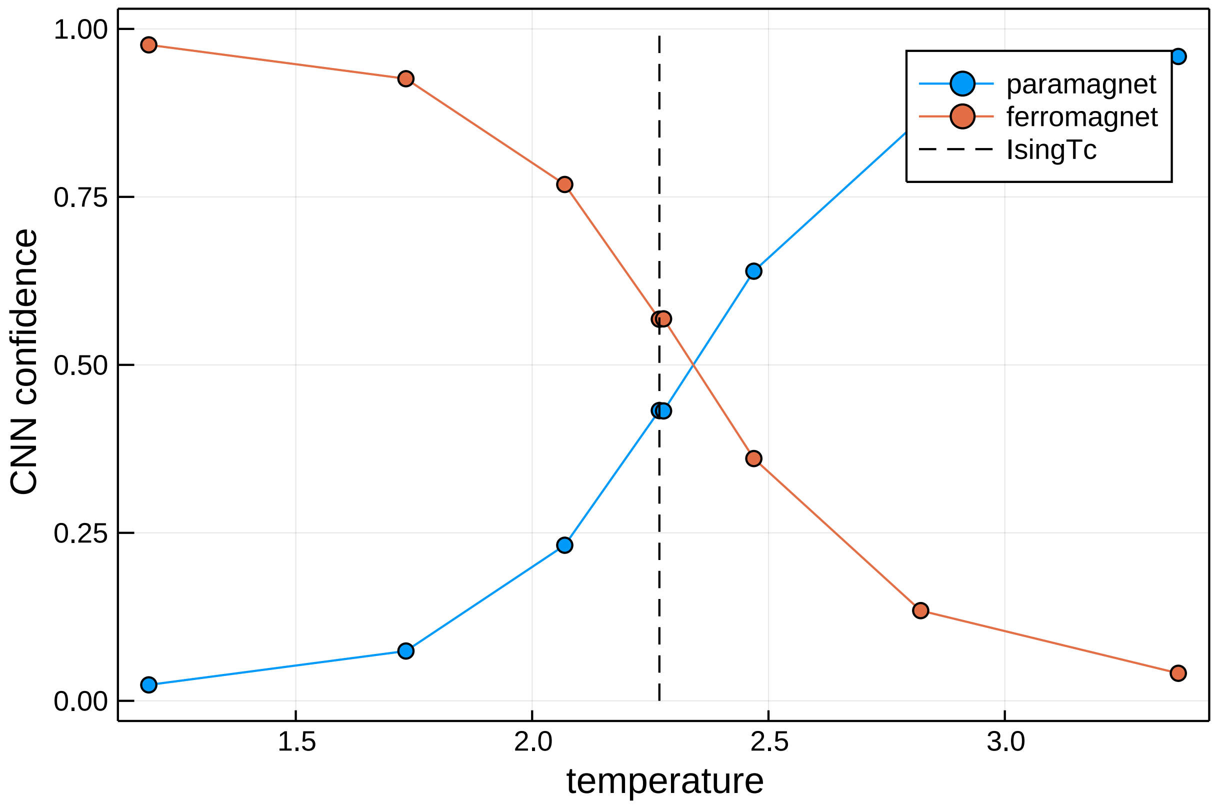
ferromagnet
IsingTc



CNN confidence
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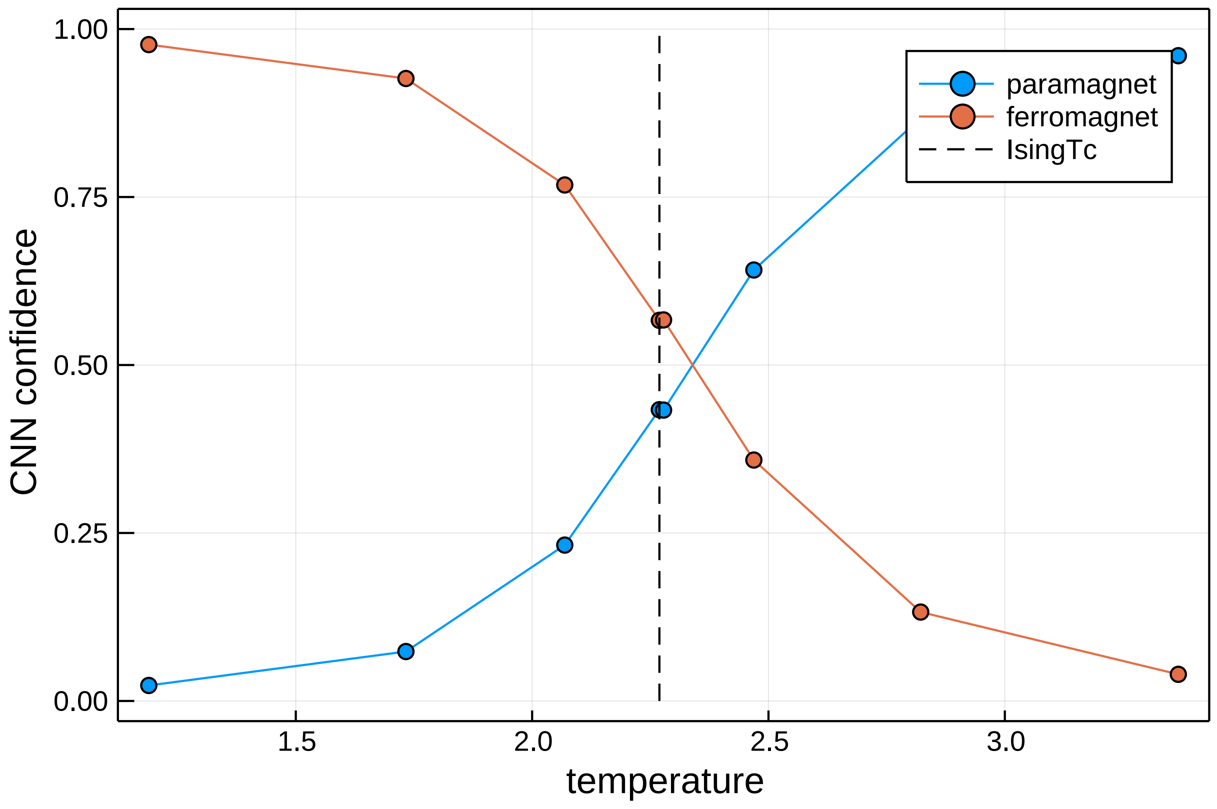
IsingTc



CNN confidence
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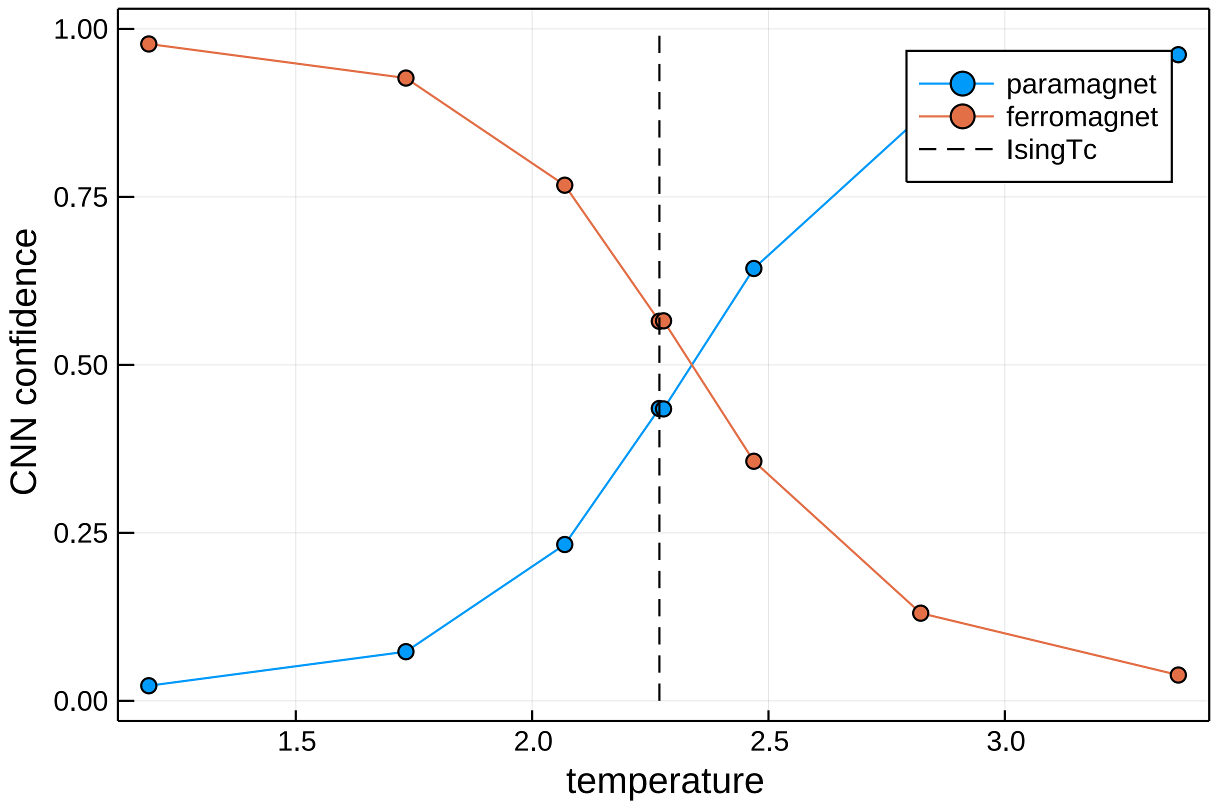
IsingTc


CNN confidence
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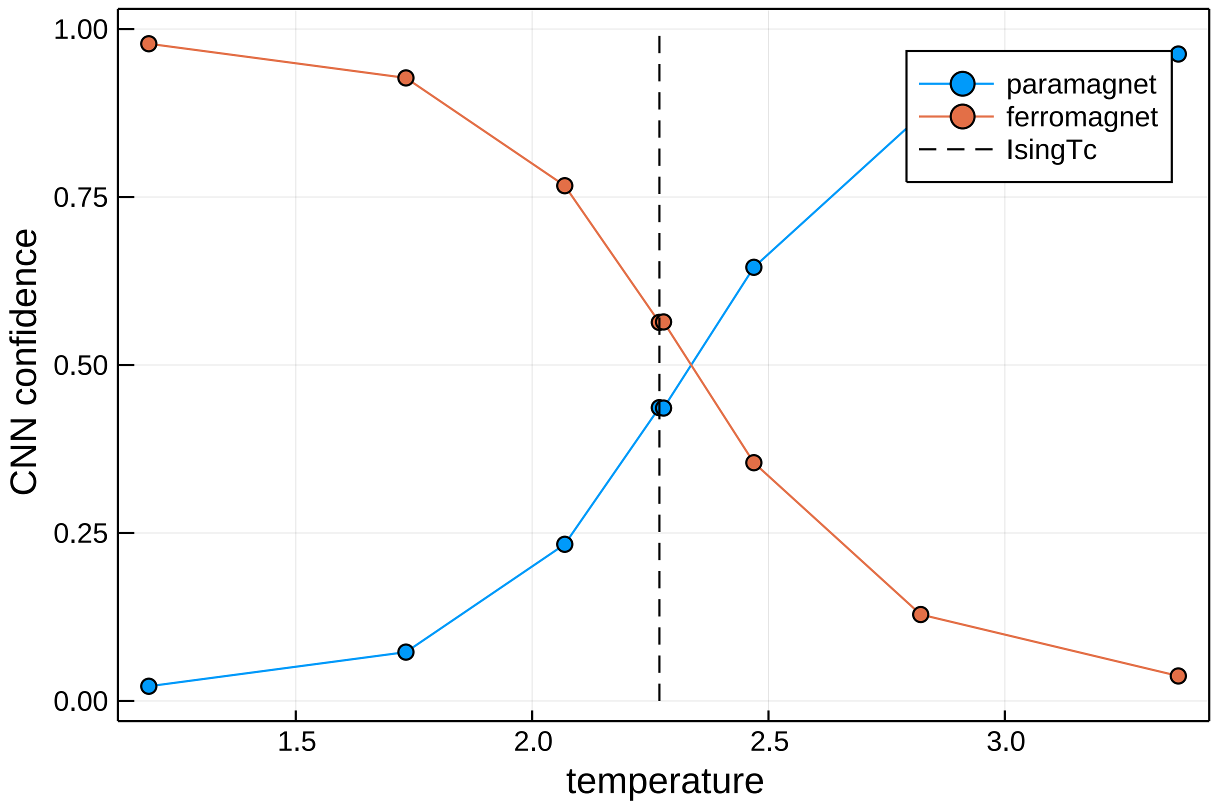
IsingTc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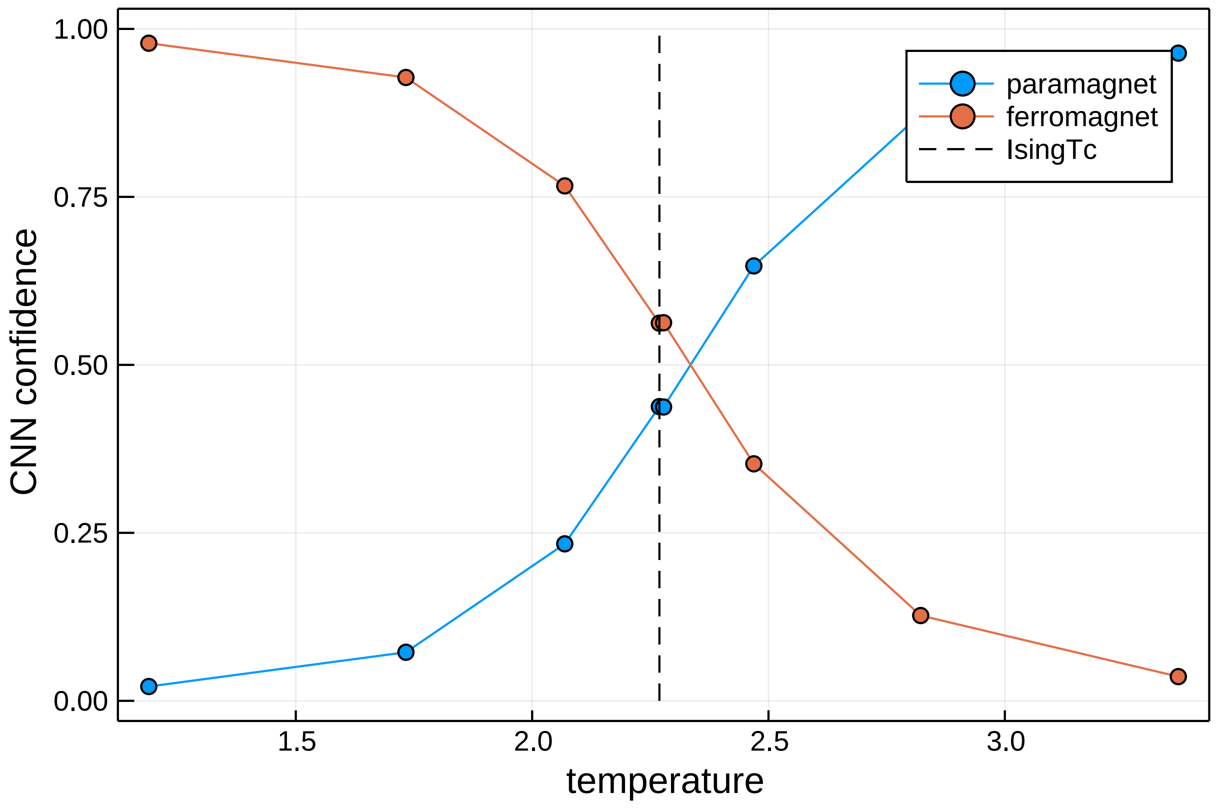
IsingTc



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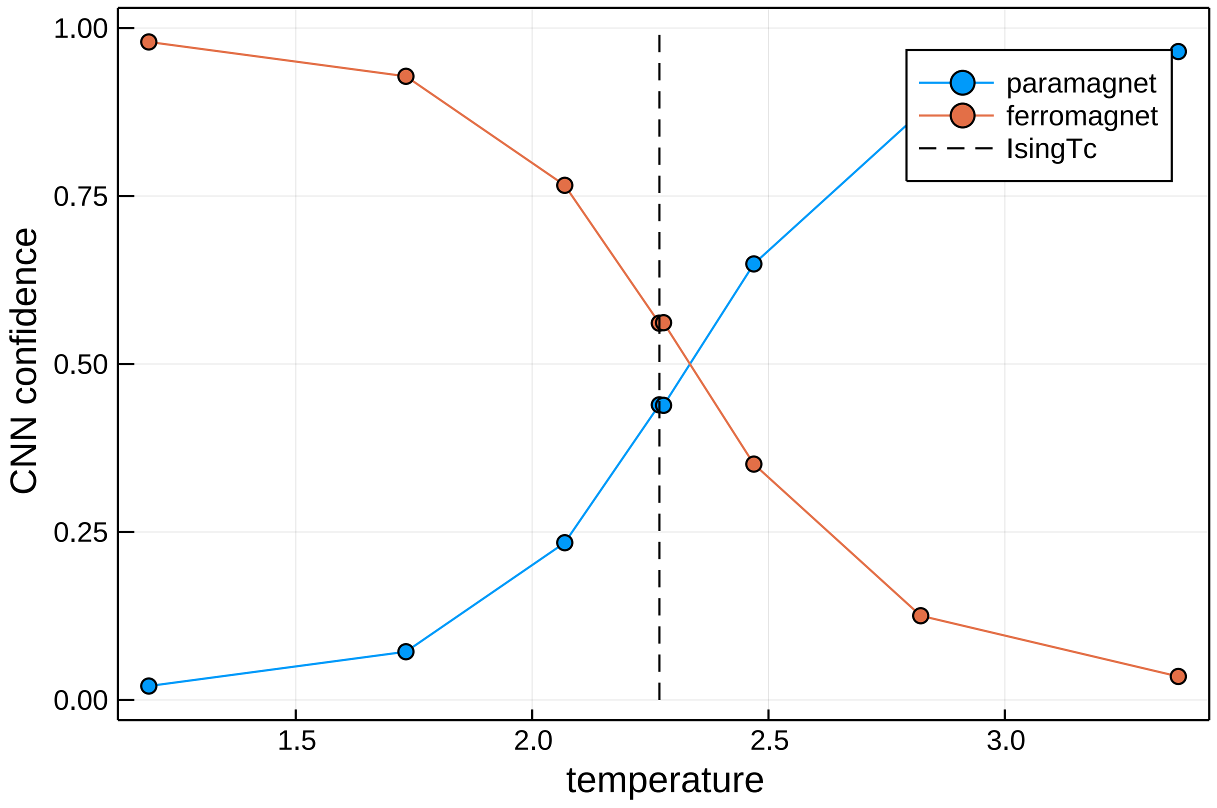
IsingTc



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CNN confidence
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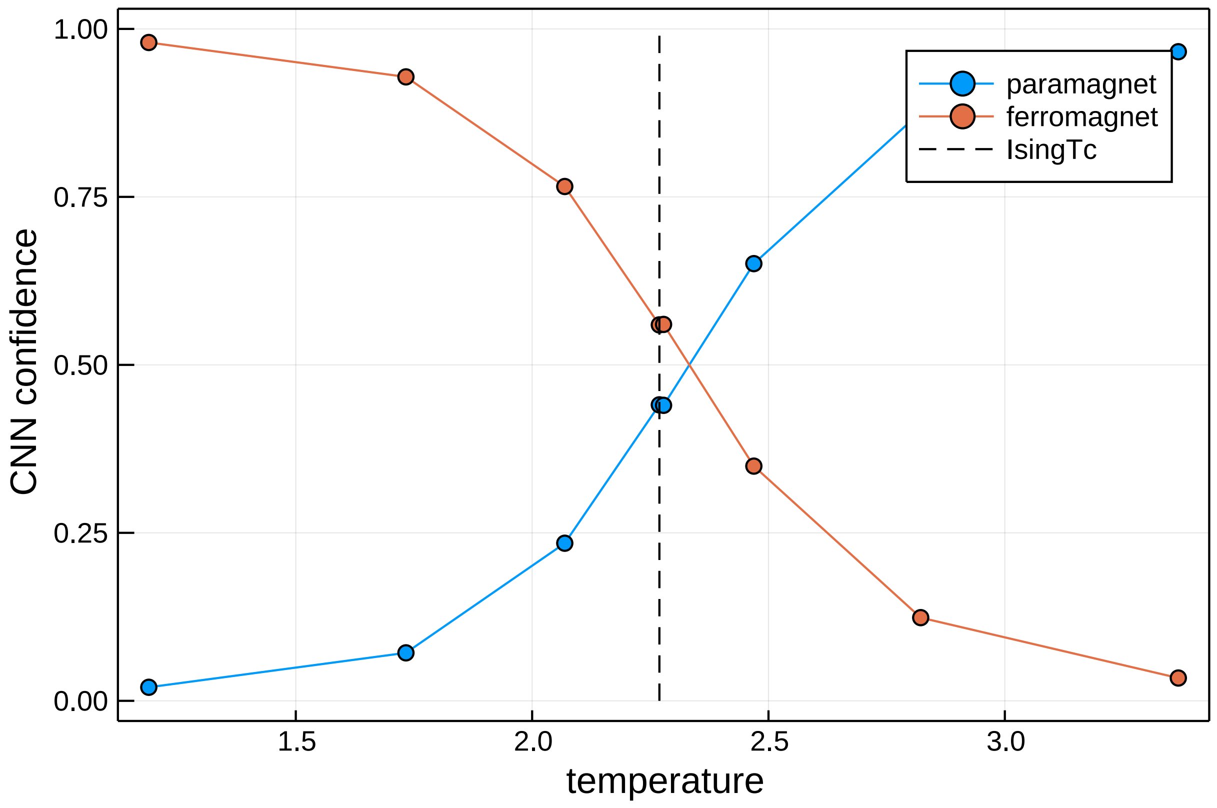
ferromagnet
IsingTc



paramagnet
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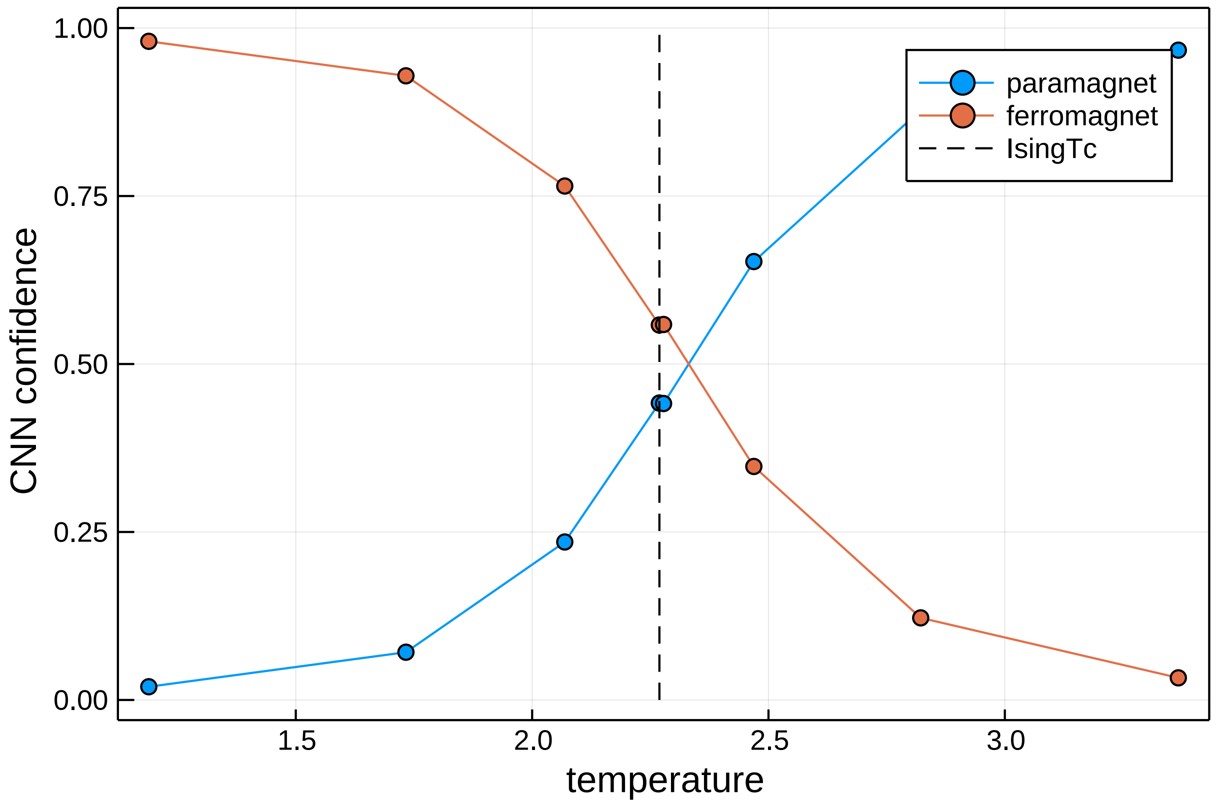

paramagnet
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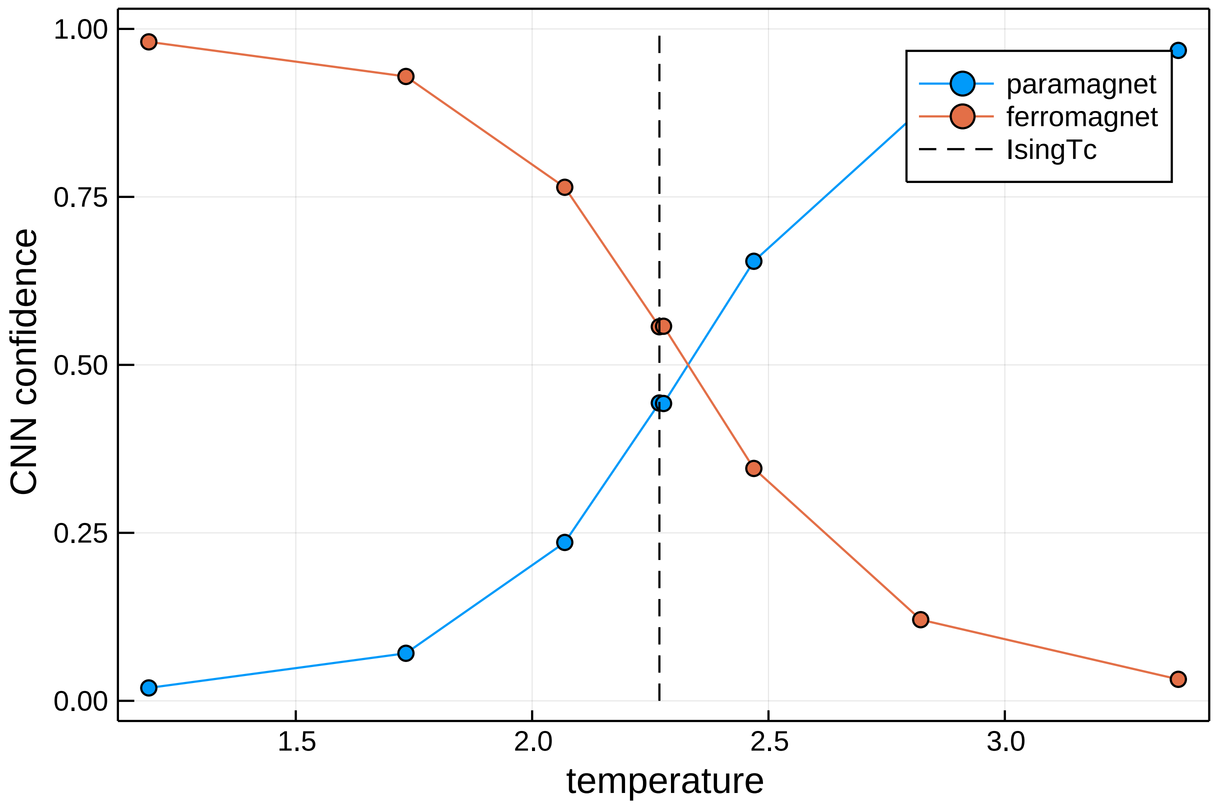

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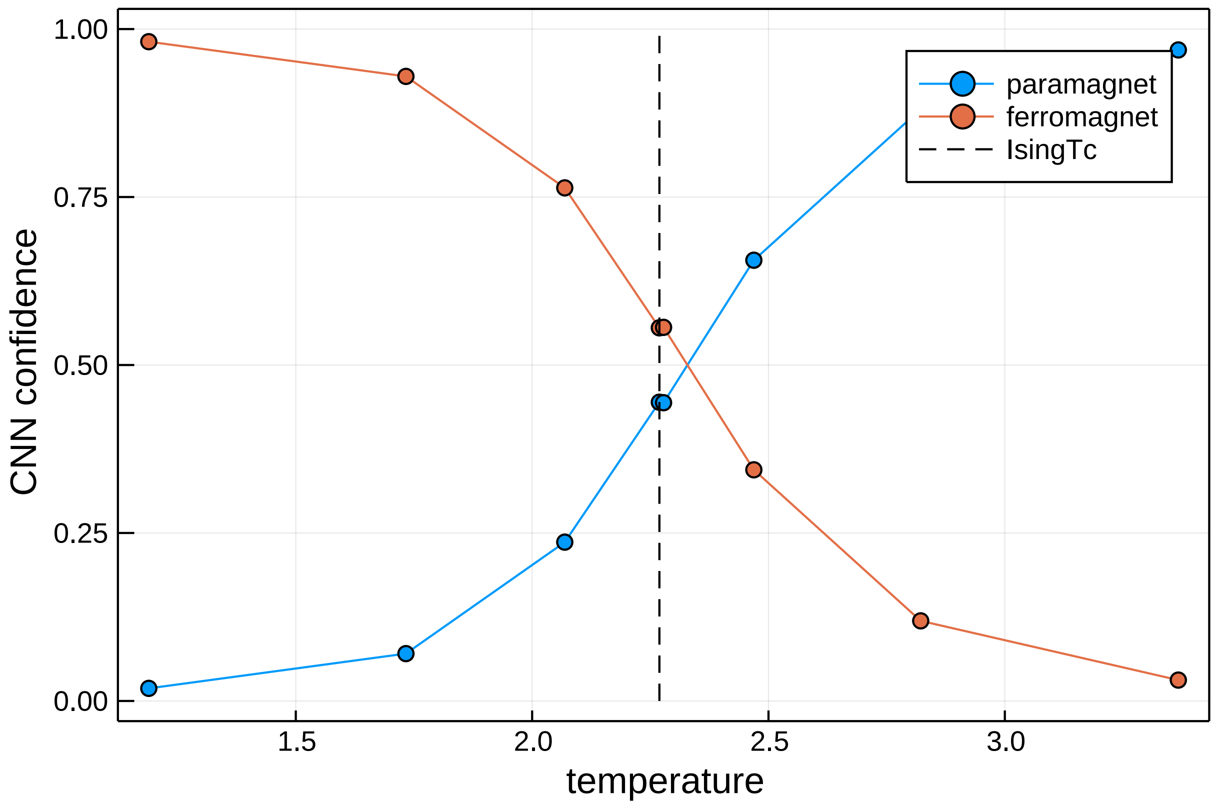
ferromagnet
IsingTc



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CNN confidence
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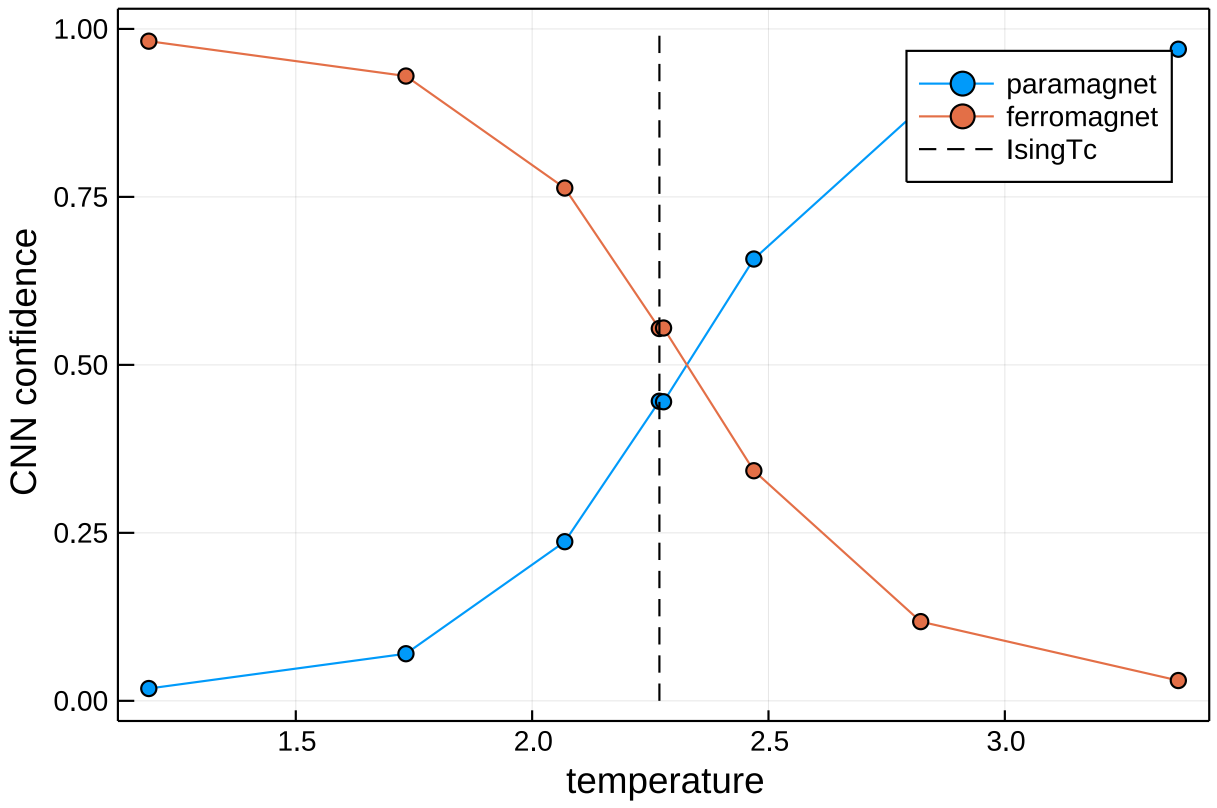
IsingTc



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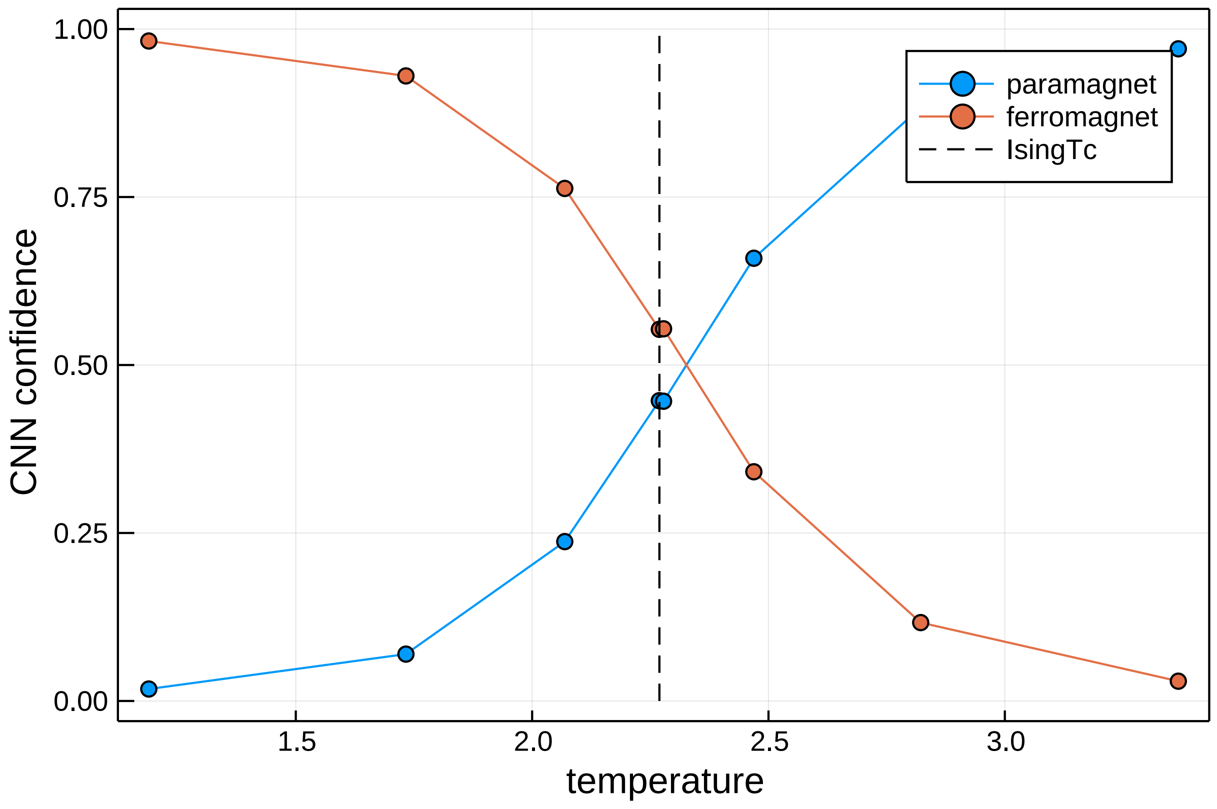
ferromagnet
IsingTc



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CNN confidence
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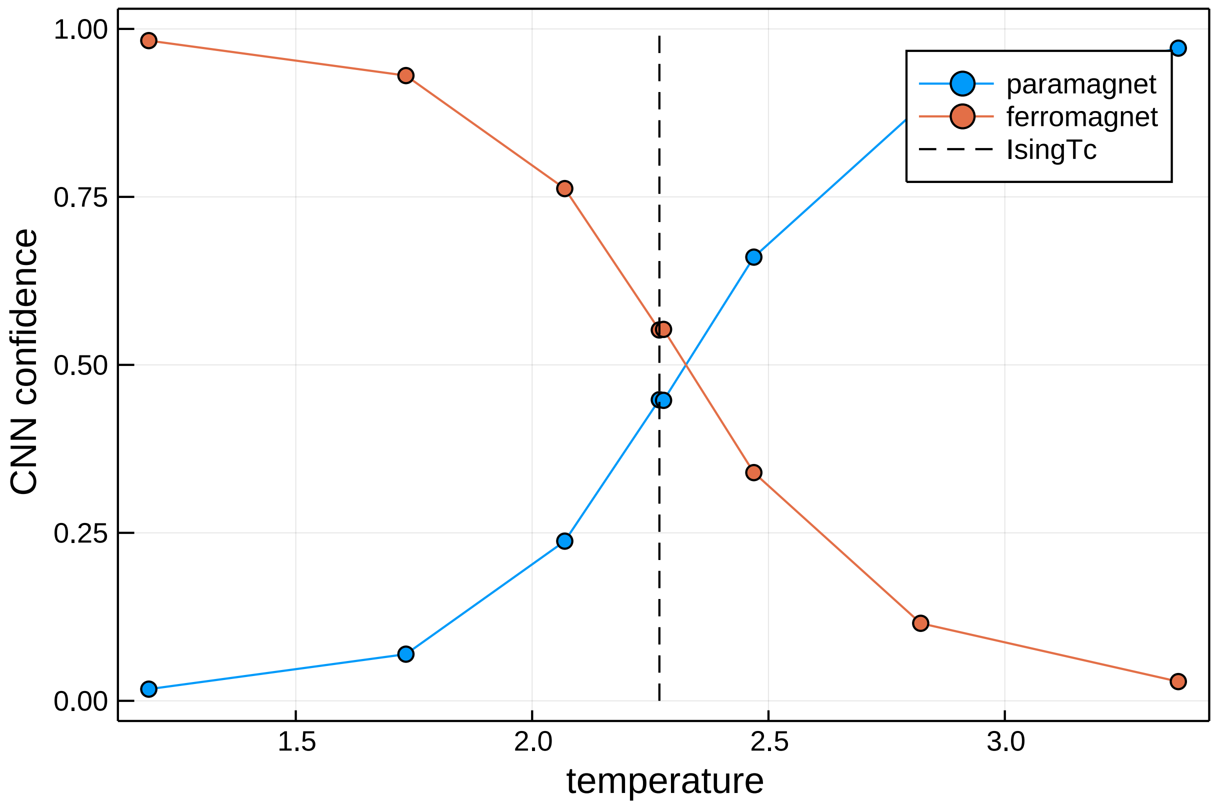
IsingTc



CNN confidence
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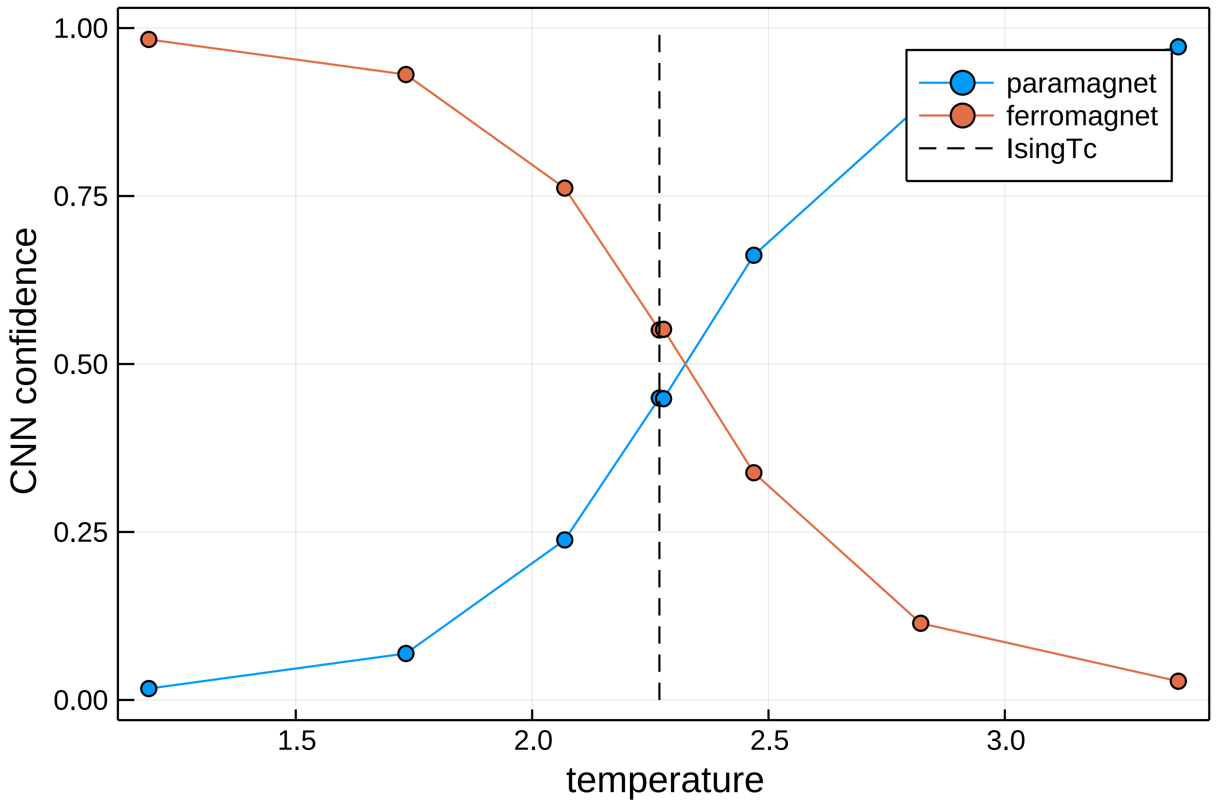
IsingTc



CNN confidence
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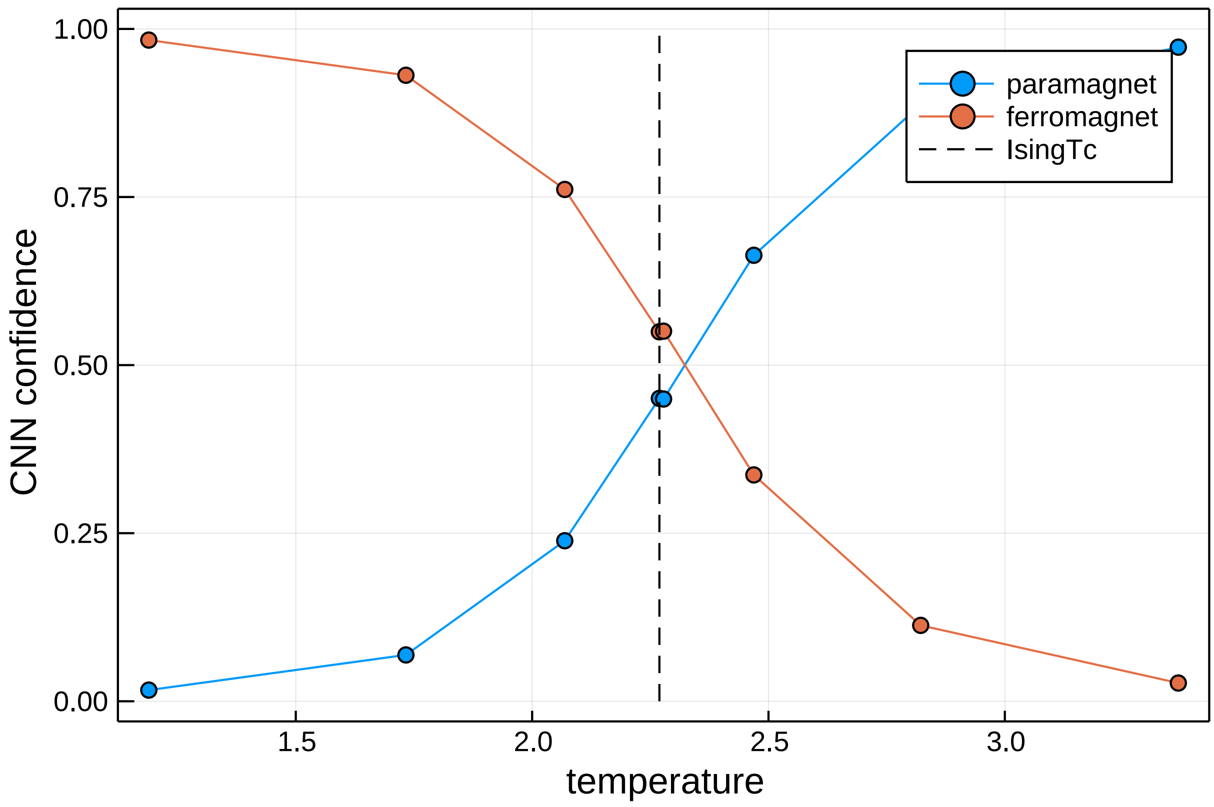
ferromagnet
IsingTc



CNN confidence
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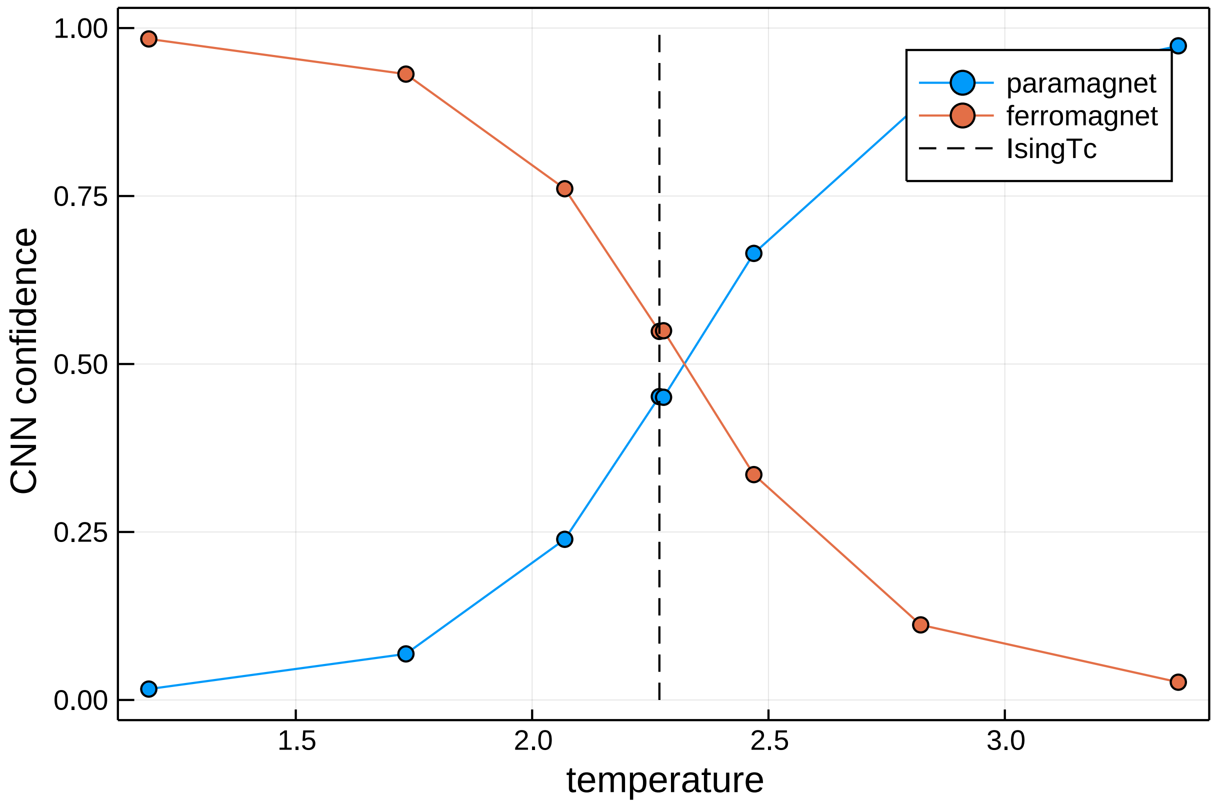
IsingTc



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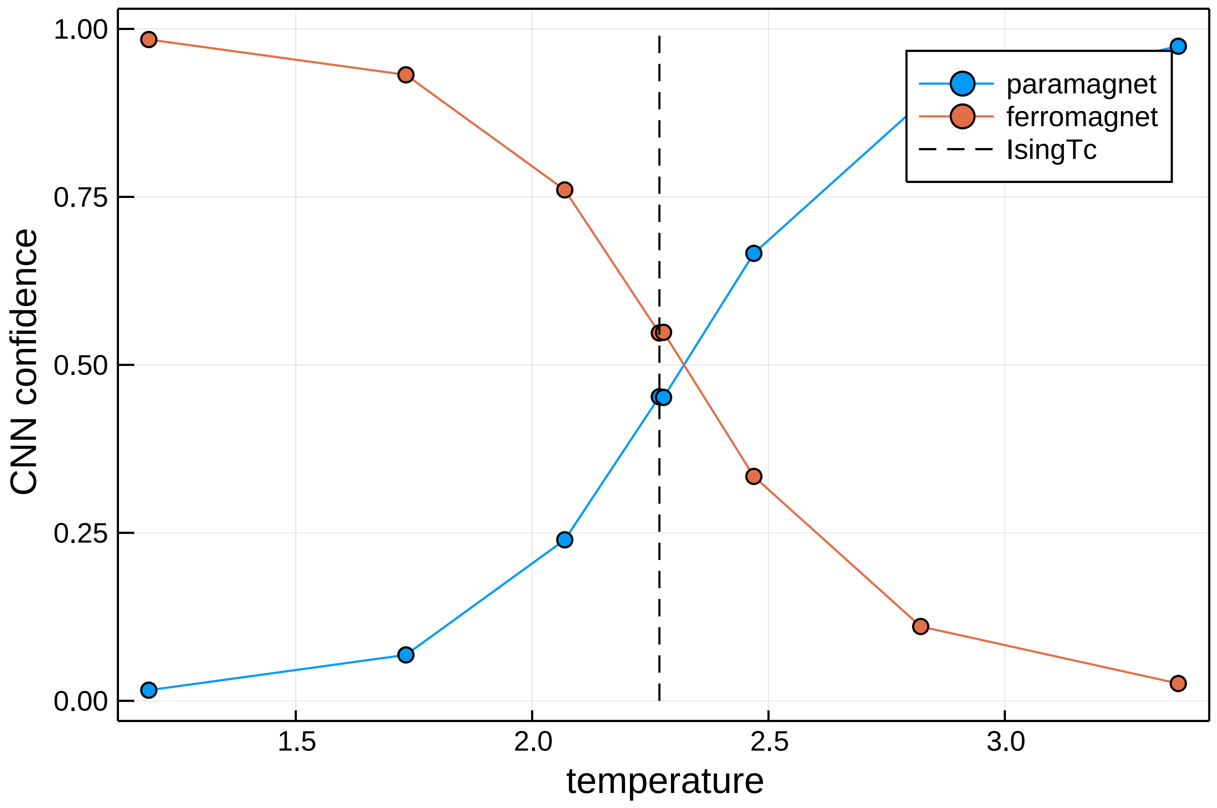
IsingTc



CNN confidence
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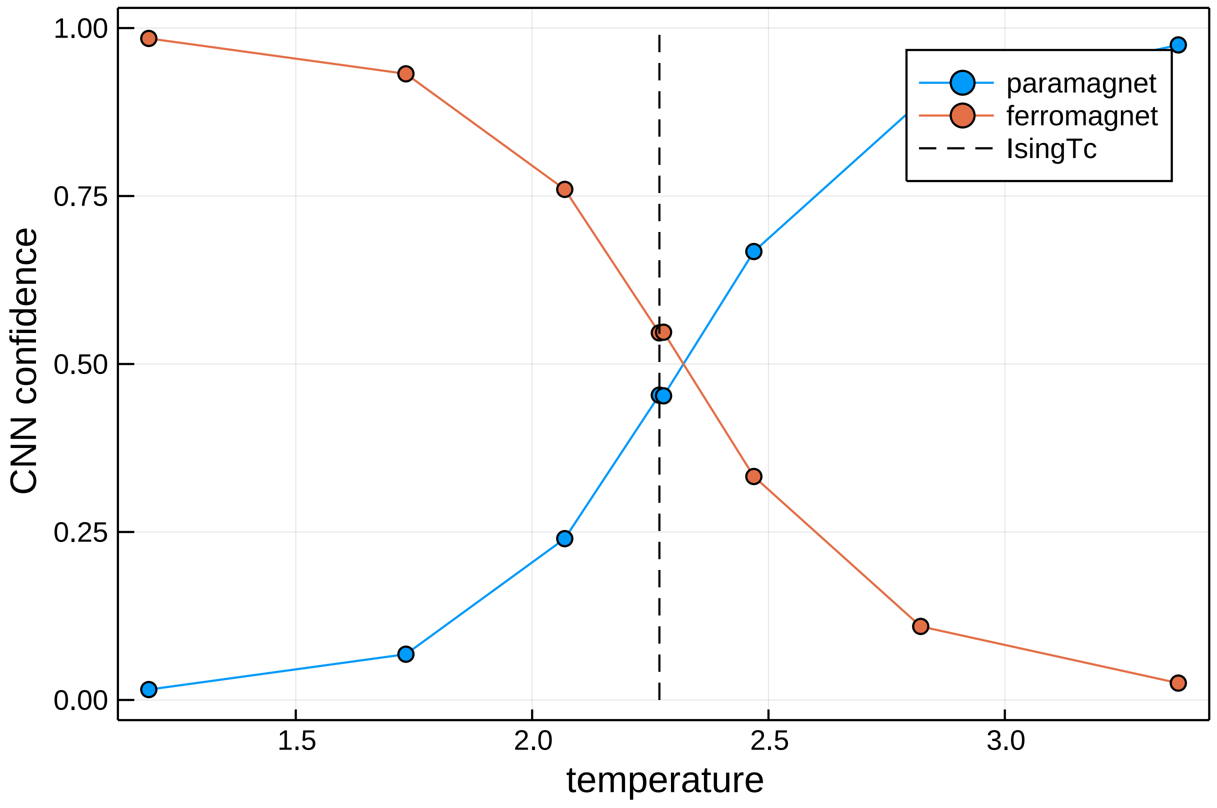
IsingTc



CNN confidence
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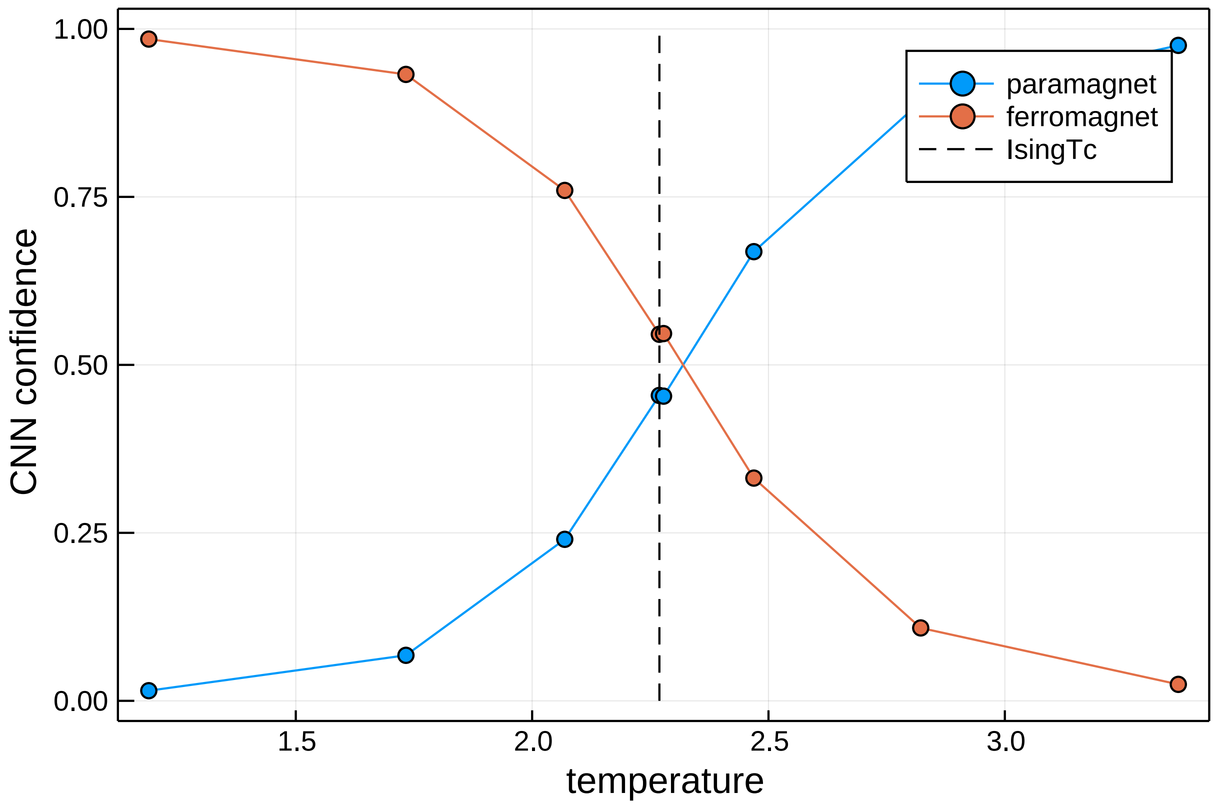
IsingTc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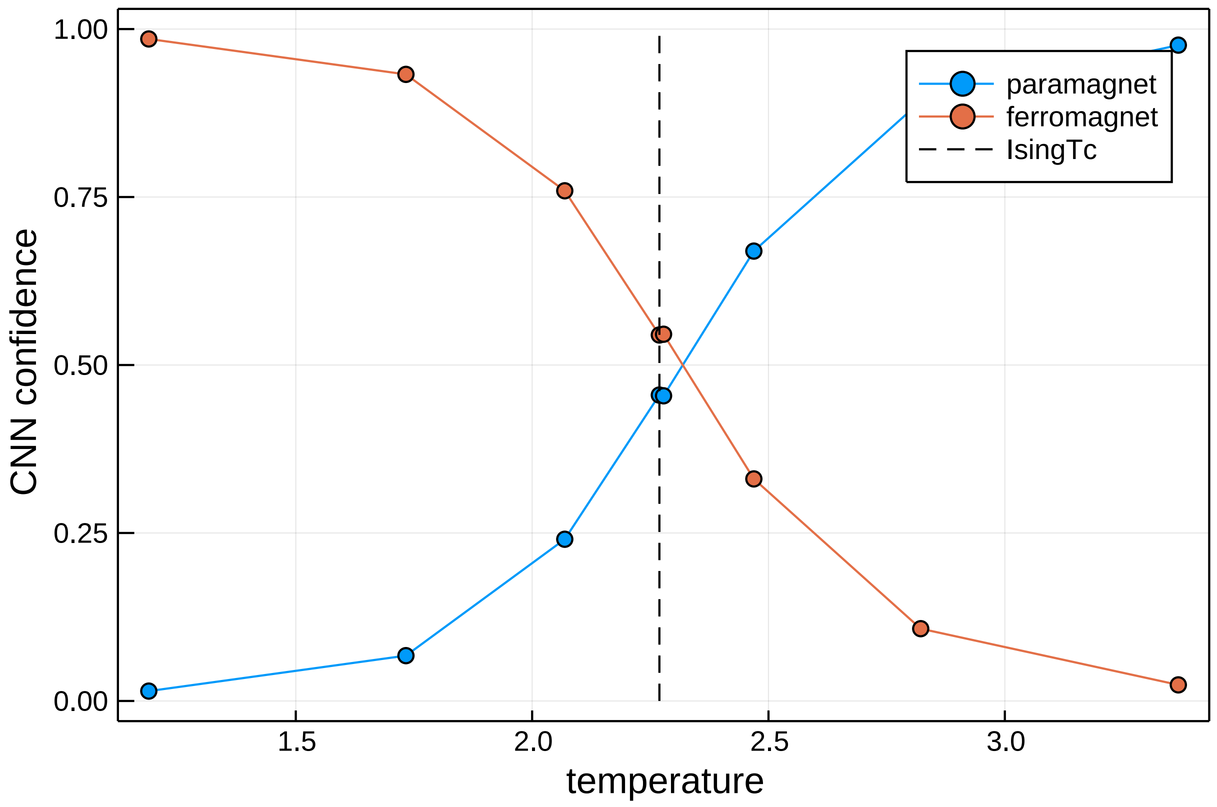
IsingTc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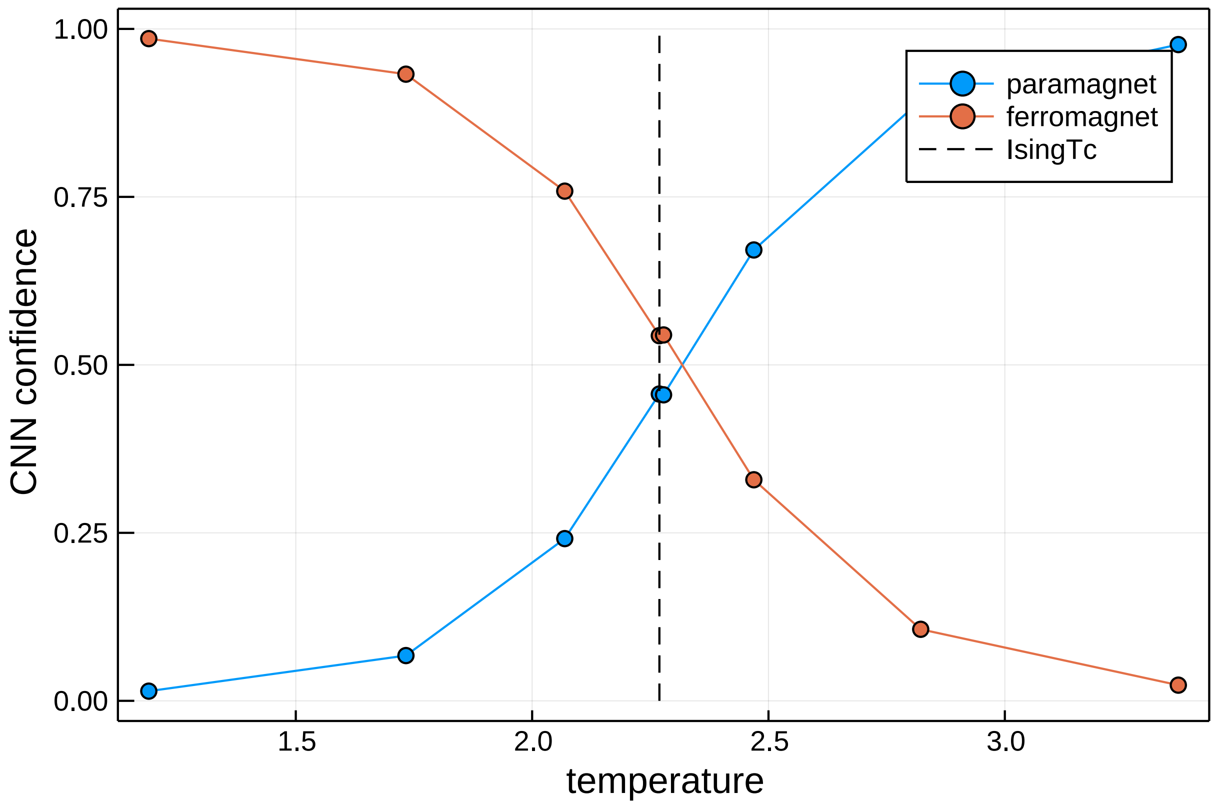
IsingTc



CNN confidence
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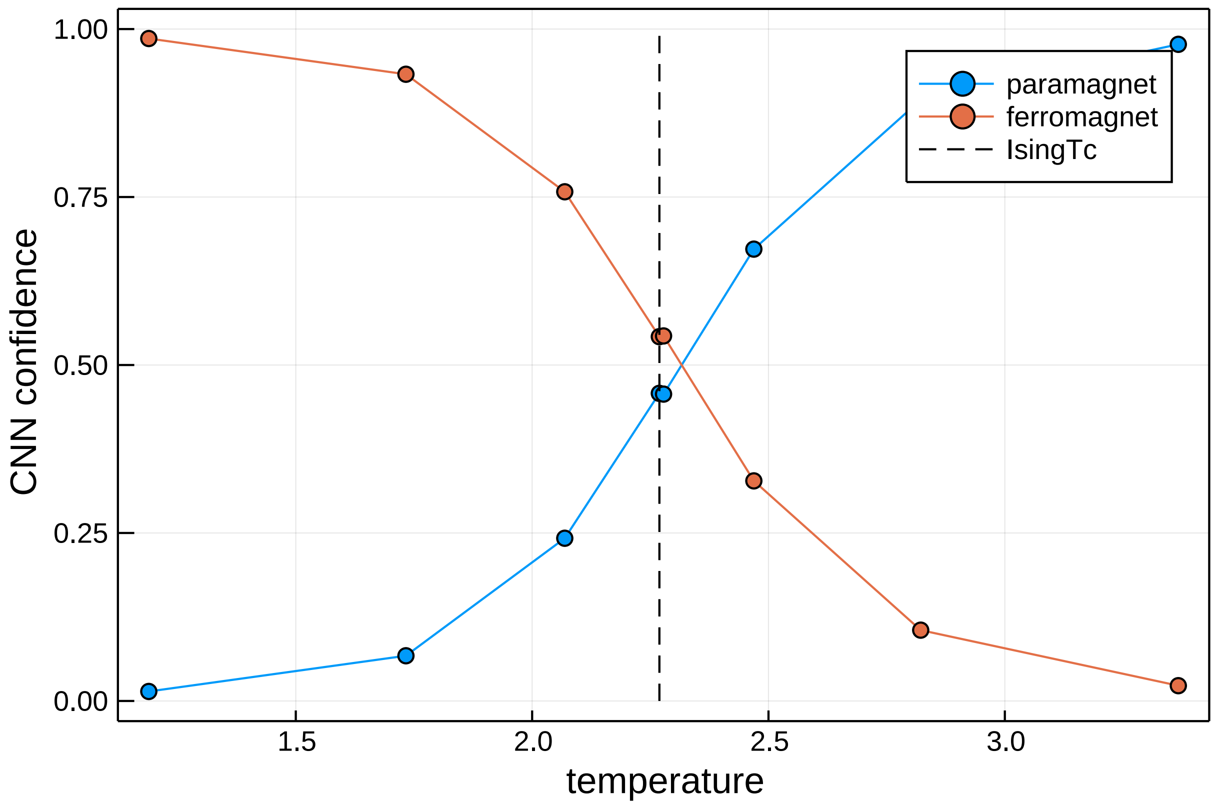

CNN confidence
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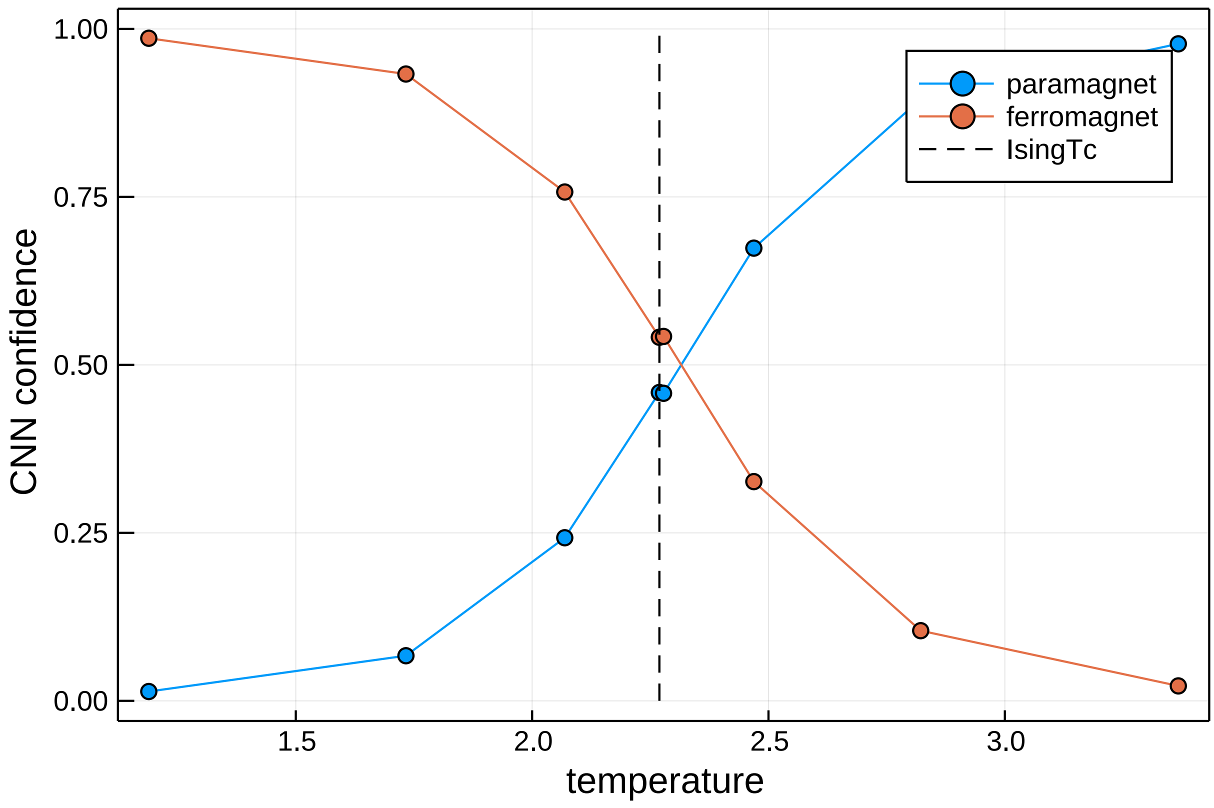
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CNN confidence
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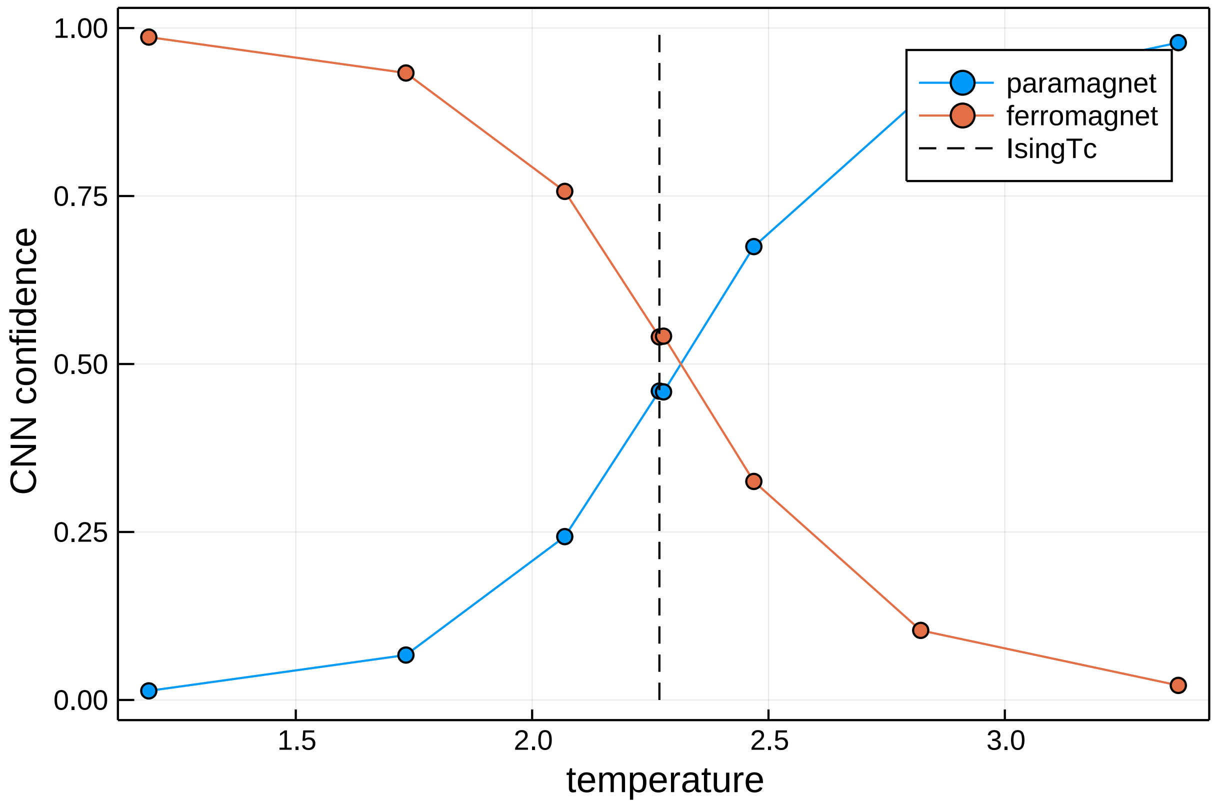
IsingTc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CNN confidence
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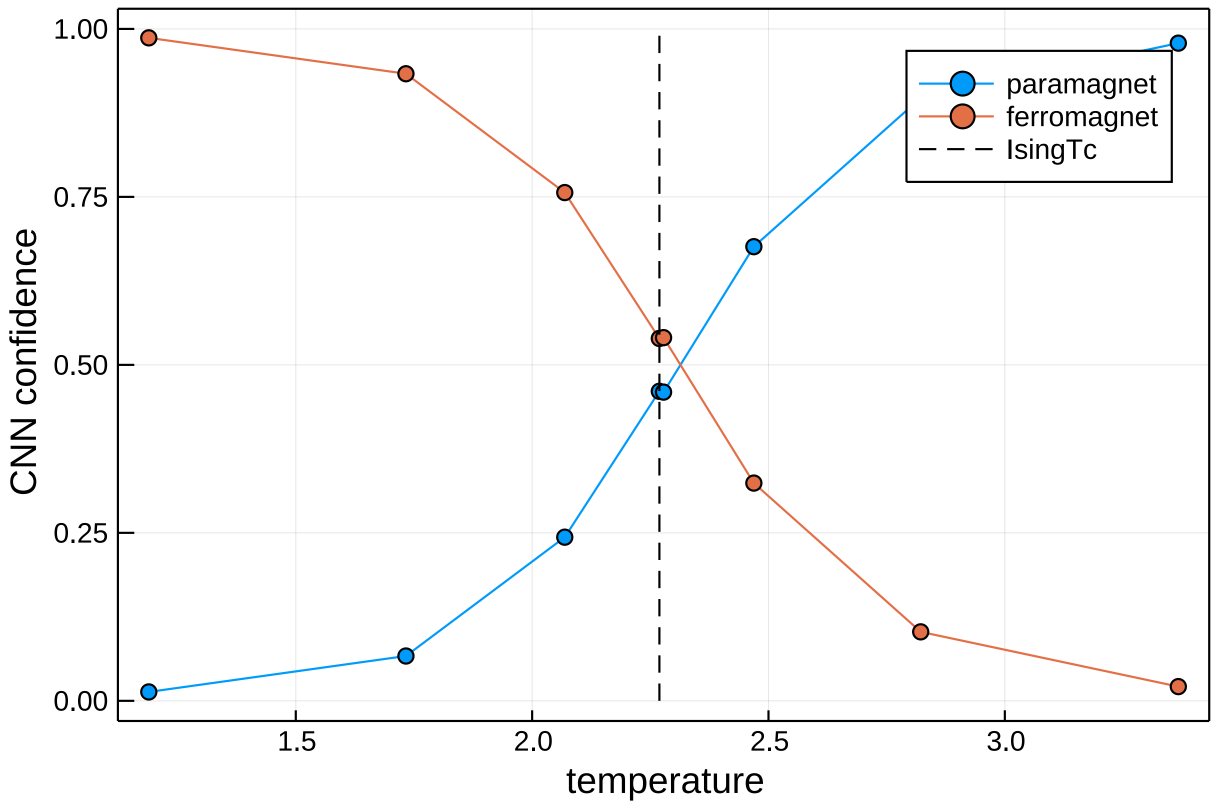
IsingTc


CNN confidence
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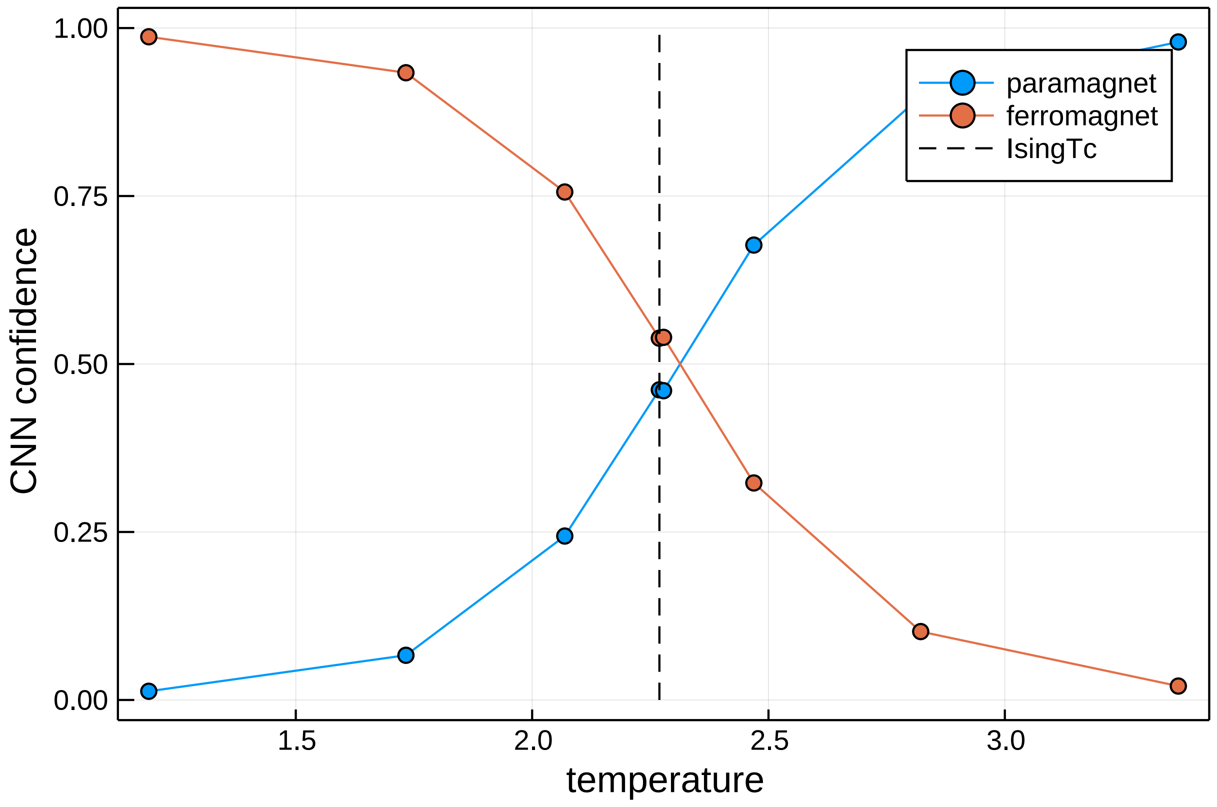
CNN confidence
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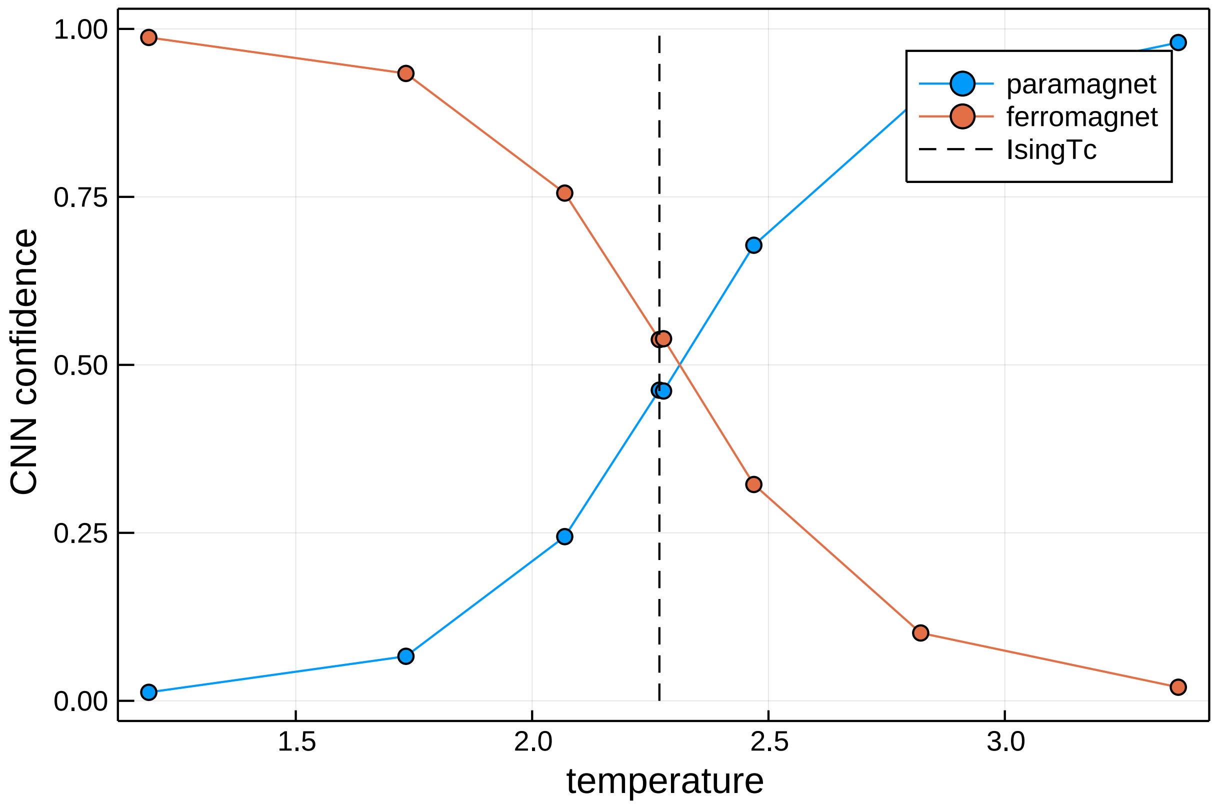

1.00
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CNN confidence
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temperature
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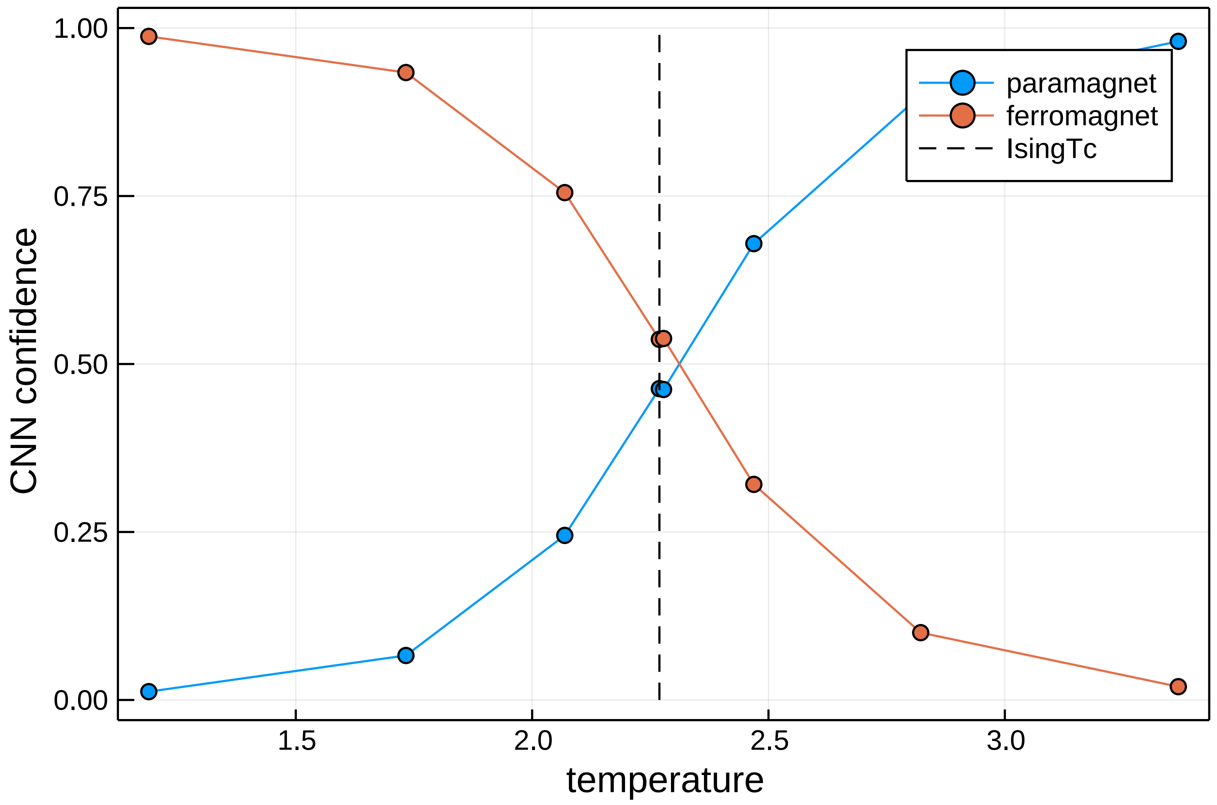
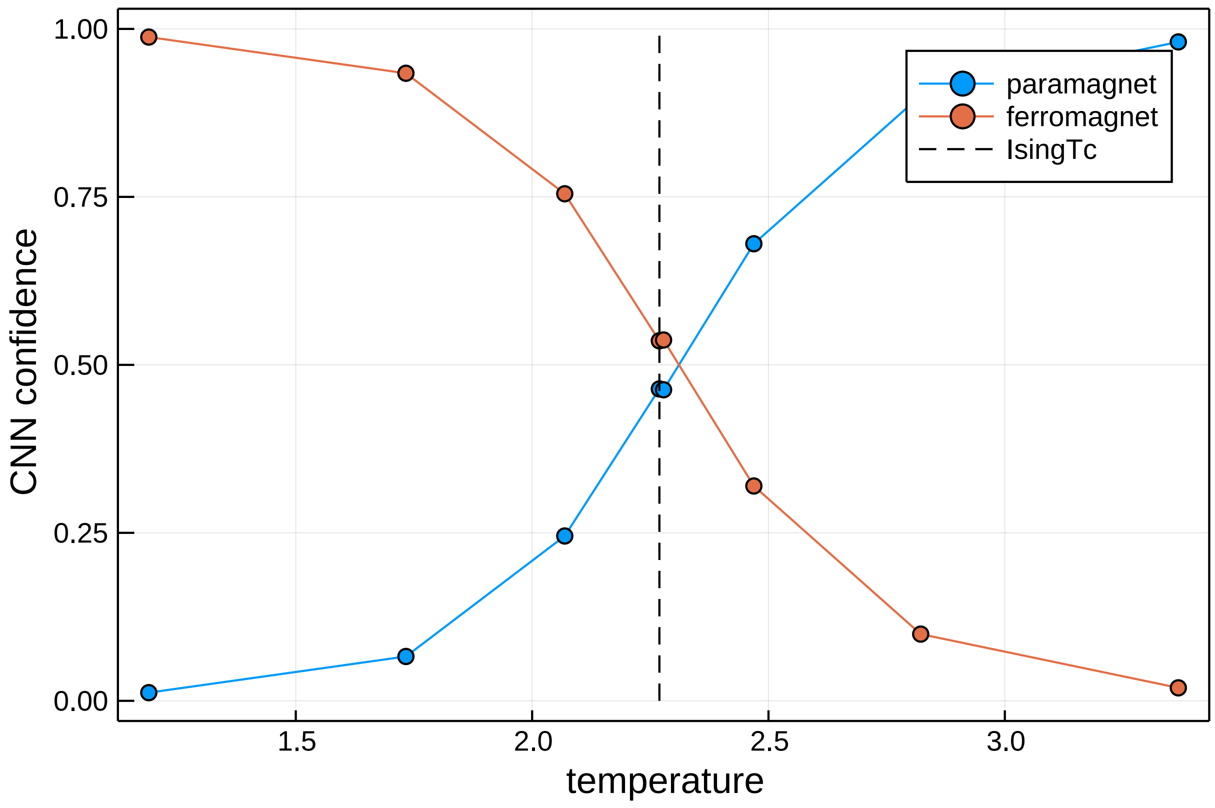
ferromagnet
IsingTc



1.00
0.75
0.50
0.25
0.00
CNN confidence
1.5
2.0
2.5
3.0
temperature
paramagnet
ferromagnet
IsingTc


CNN confidence
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0.75
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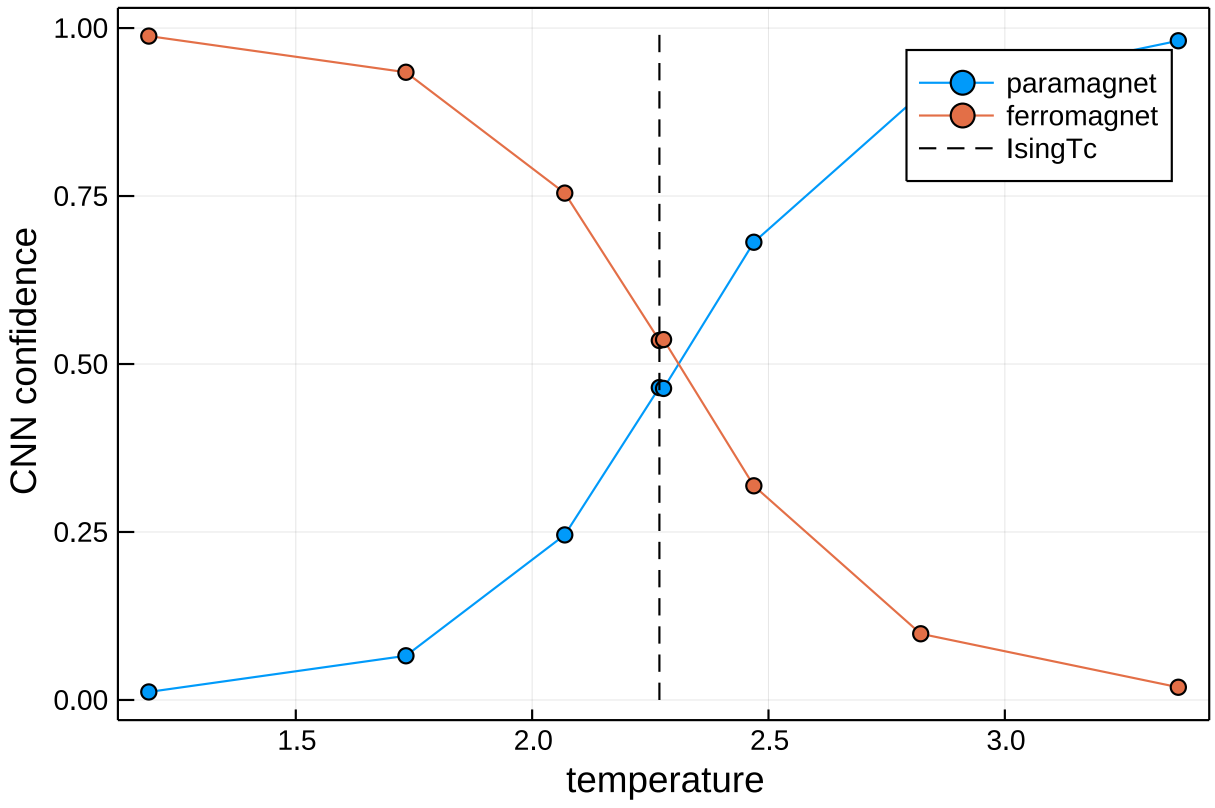
0.25
0.00
1.5
2.0
2.5
3.0
temperature
paramagnet
ferromagnet
IsingTc


CNN confidence
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0.25
0.00
1.5
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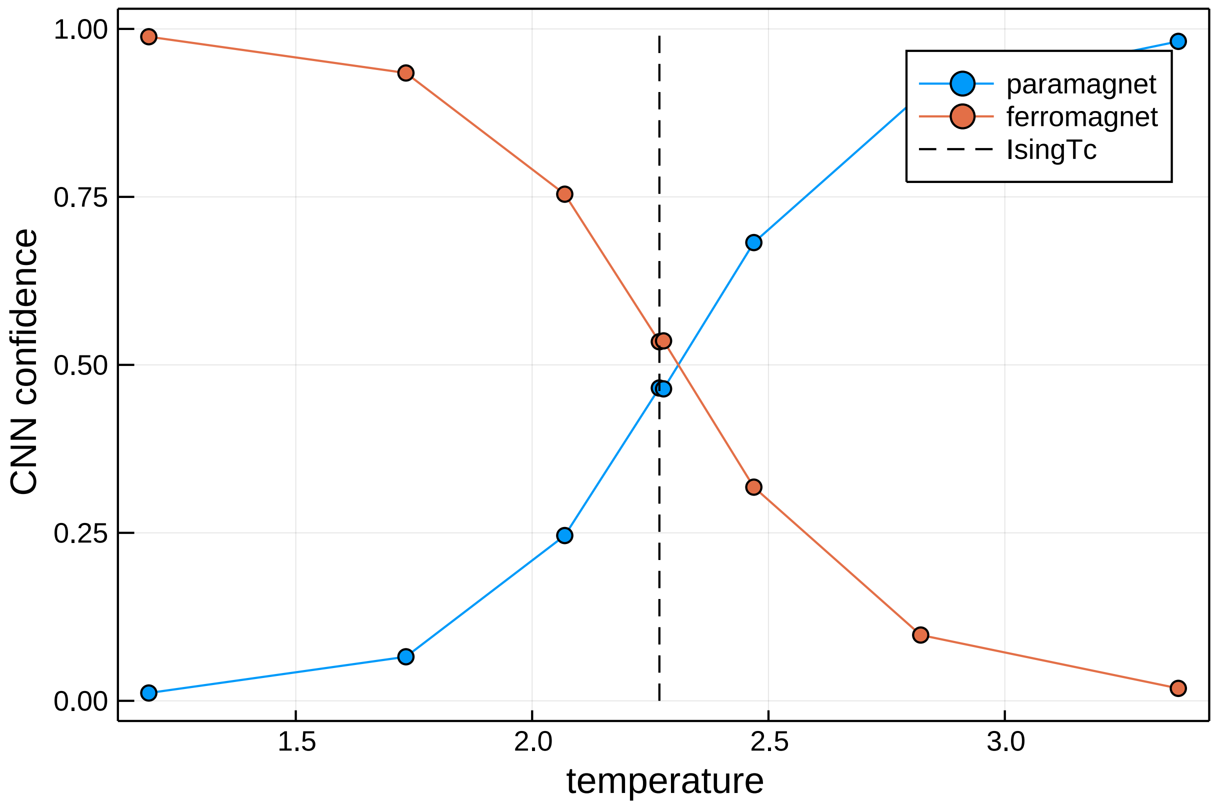
3.0
temperature
paramagnet
ferromagnet
IsingTc



paramagnet
ferromagnet
IsingTc
CNN confidence
temperature
0.00
0.25
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0.75
1.00
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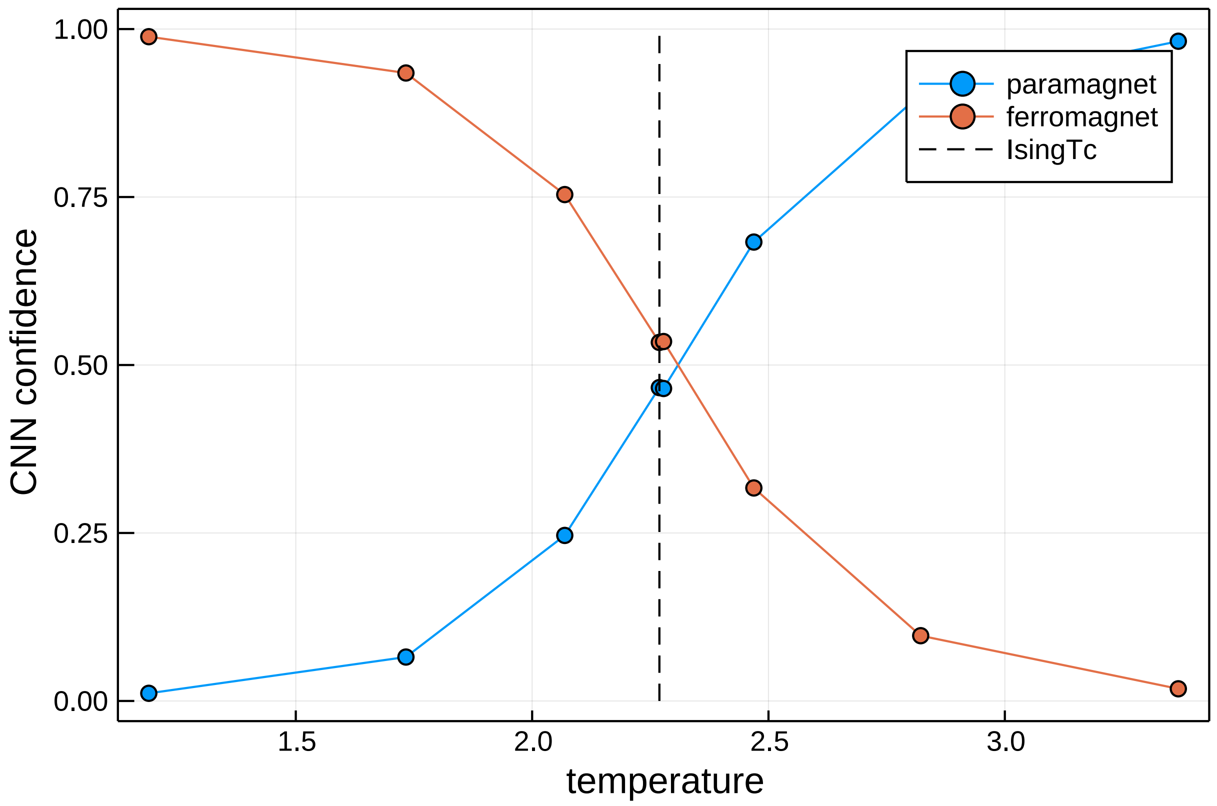
2.0
2.5
3.0



paramagnet
ferromagnet
IsingTc
CNN confidence
temperature
0.00
0.25
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0.75
1.00
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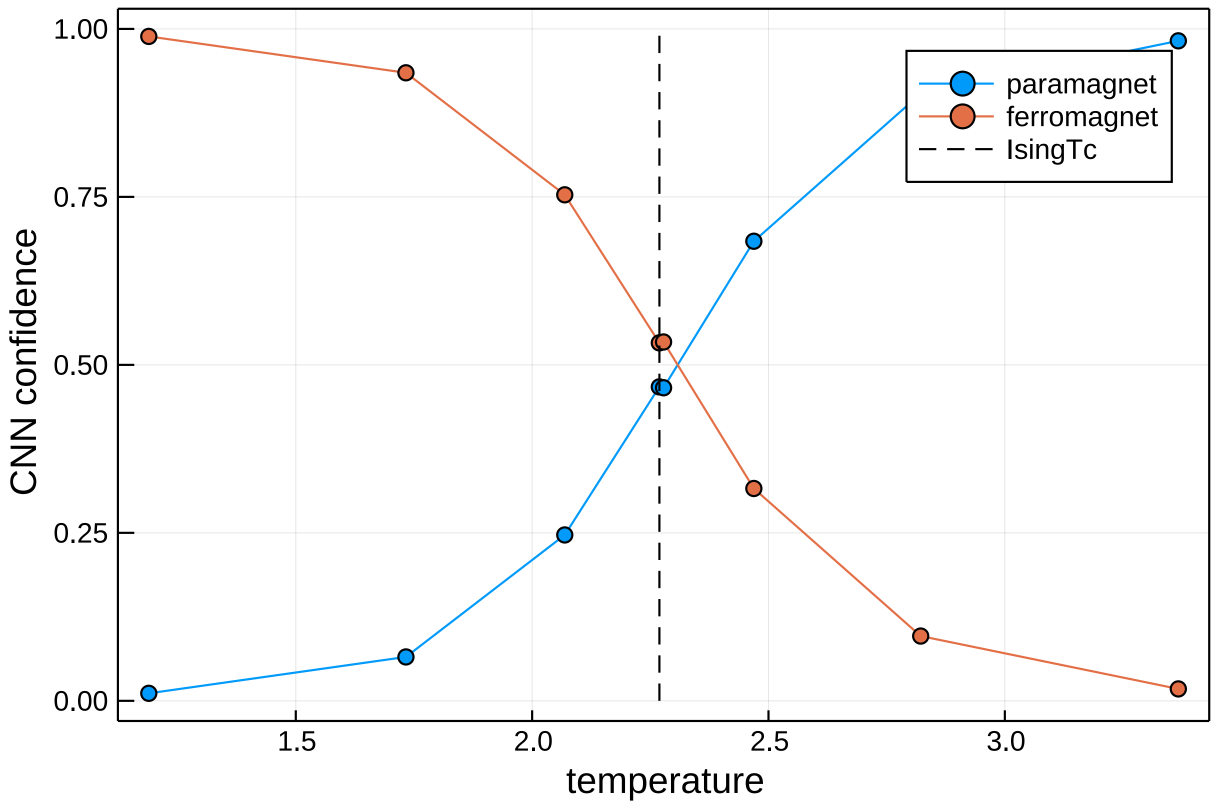
2.0
2.5
3.0



CNN confidence
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paramagnet
ferromagnet
IsingTc
1.00
0.75
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0.00
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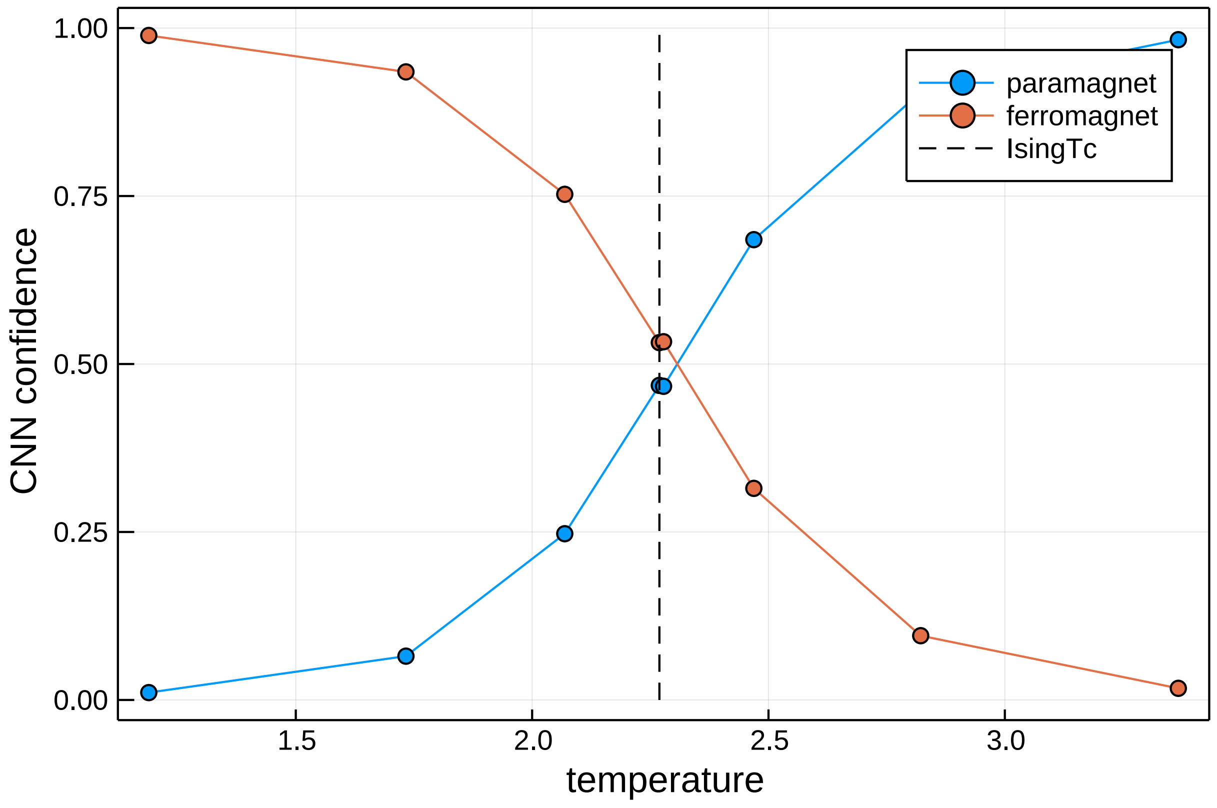
2.0
2.5
3.0



CNN confidence
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paramagnet
ferromagnet
IsingTc
1.00
0.75
0.50
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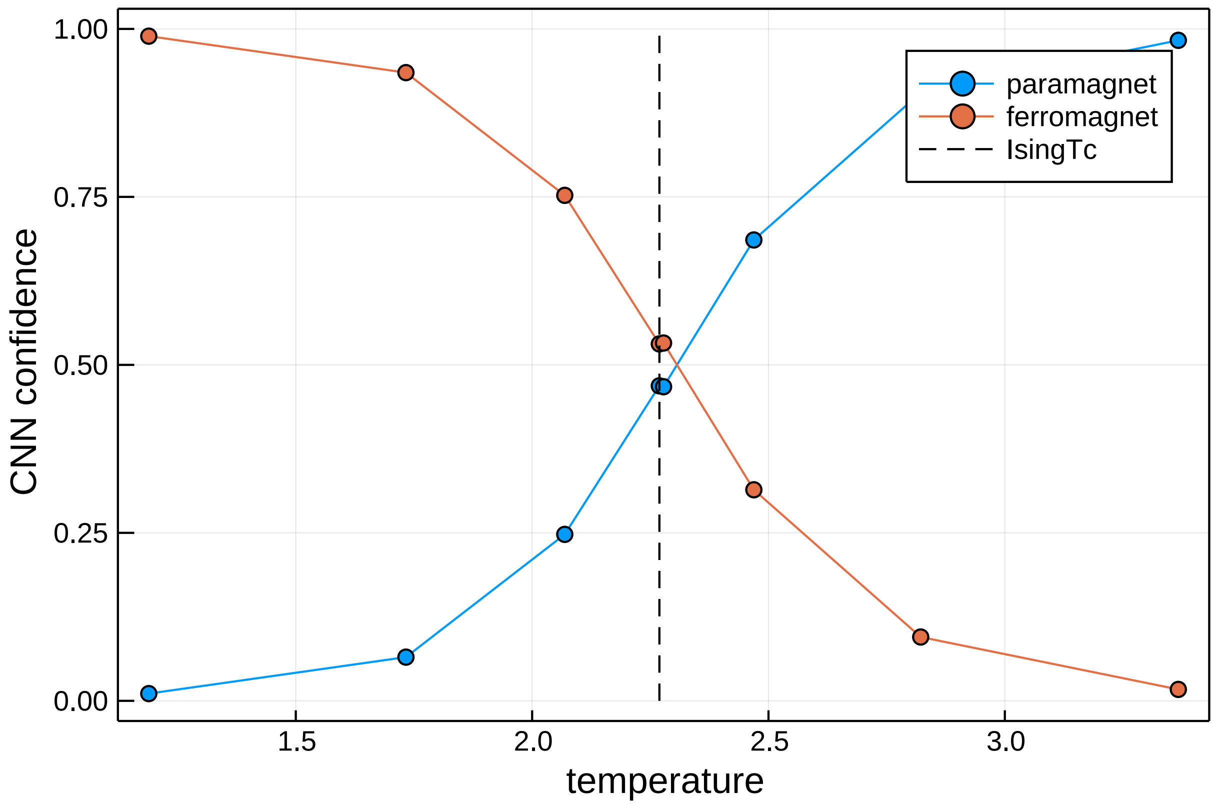
0.00
1.5
2.0
2.5
3.0


CNN confidence
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ferromagnet
IsingTc
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1.5
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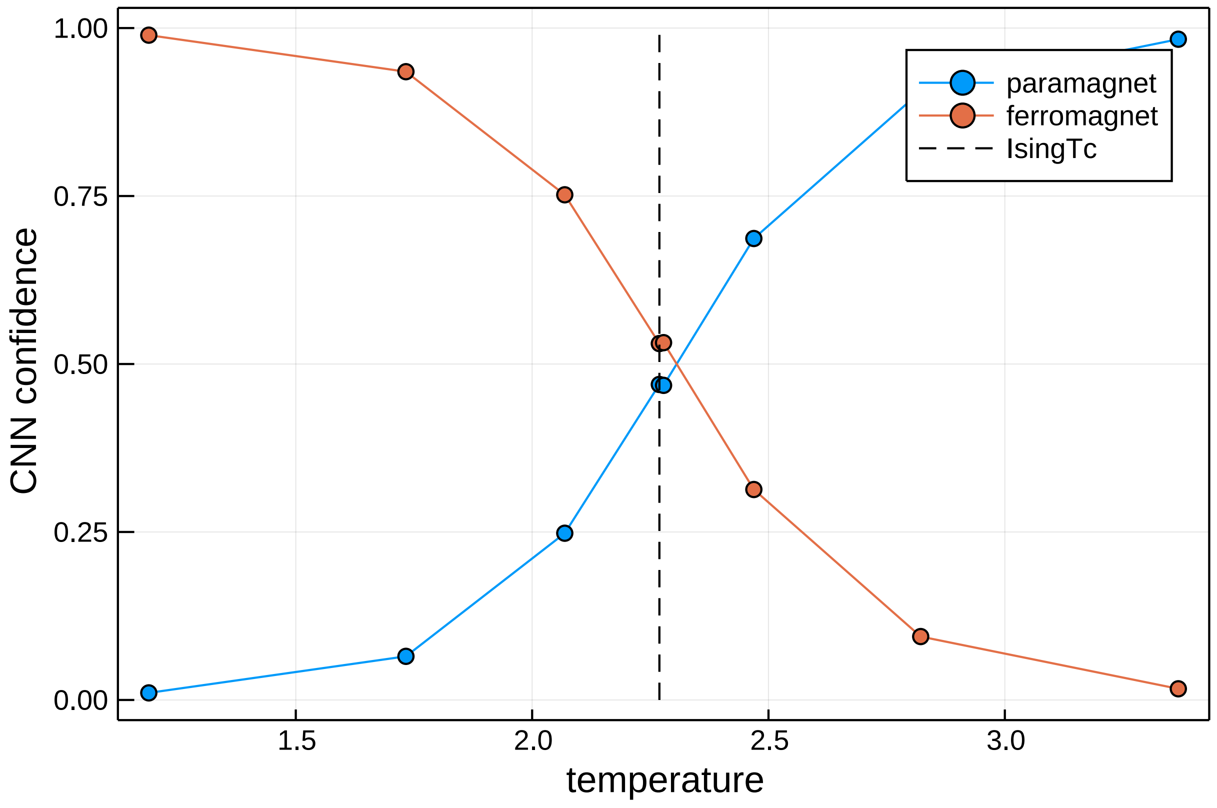
2.5
3.0


CNN confidence
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ferromagnet
IsingTc
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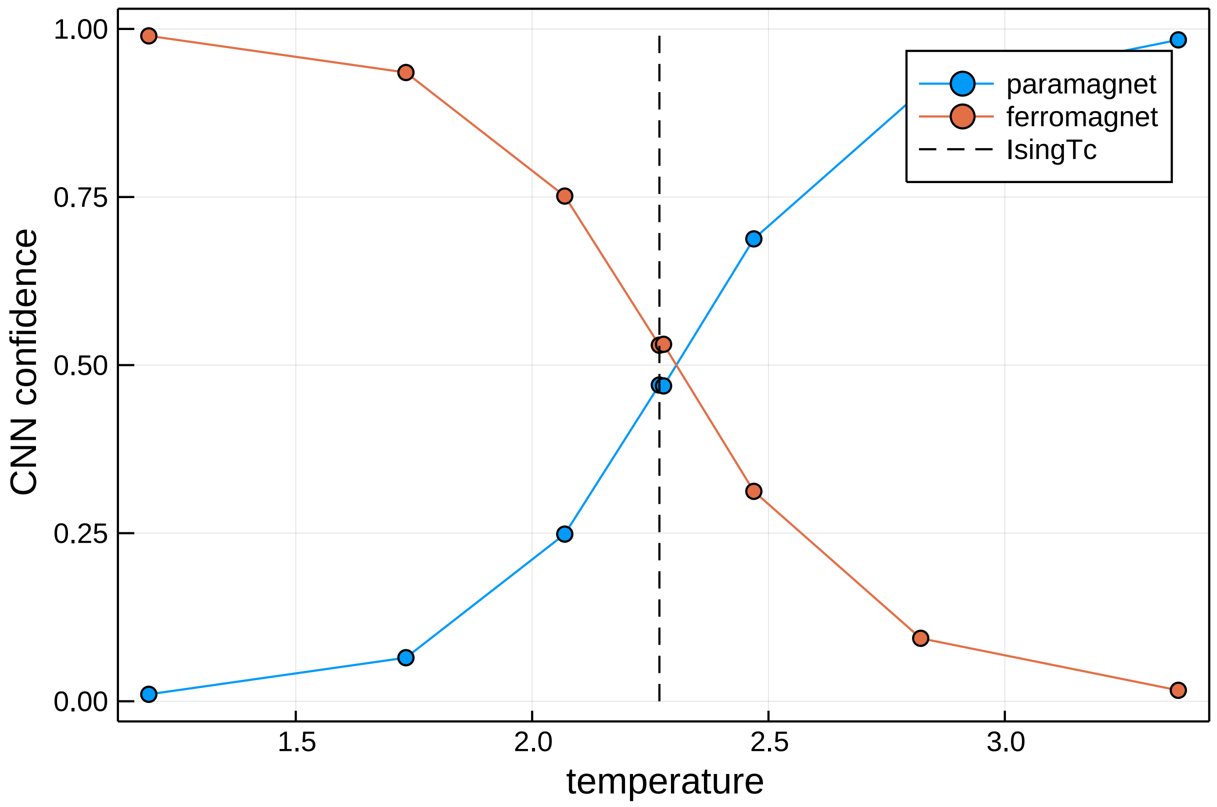
3.0



CNN confidence
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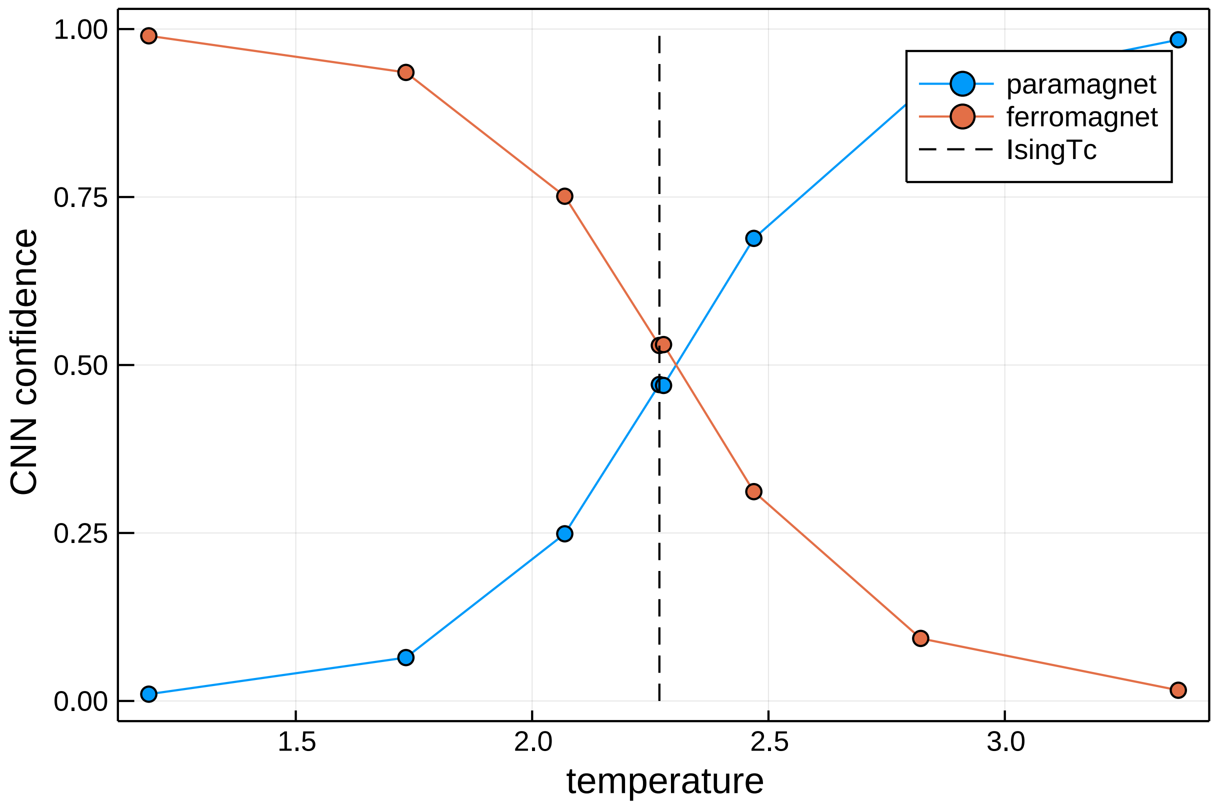
3.0
temperature
paramagnet
ferromagnet
IsingTc



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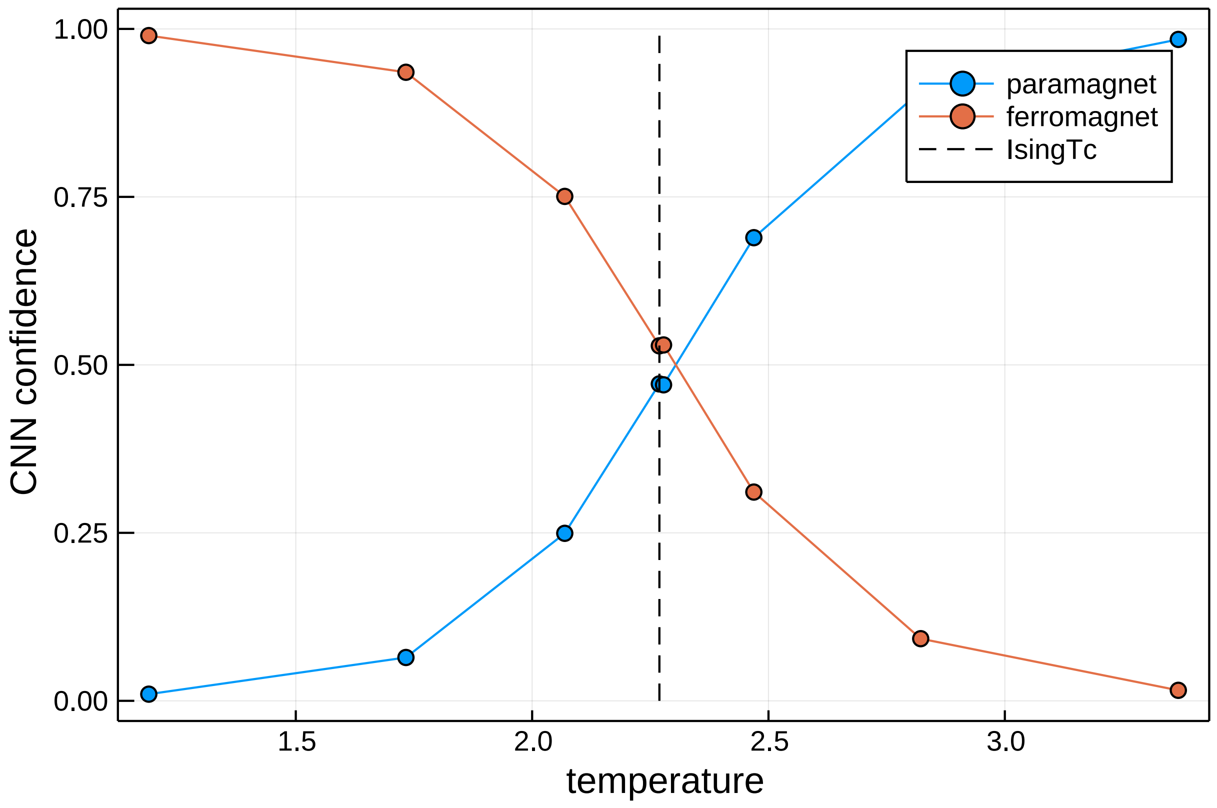
3.0
temperature
paramagnet
ferromagnet
IsingTc



1.00
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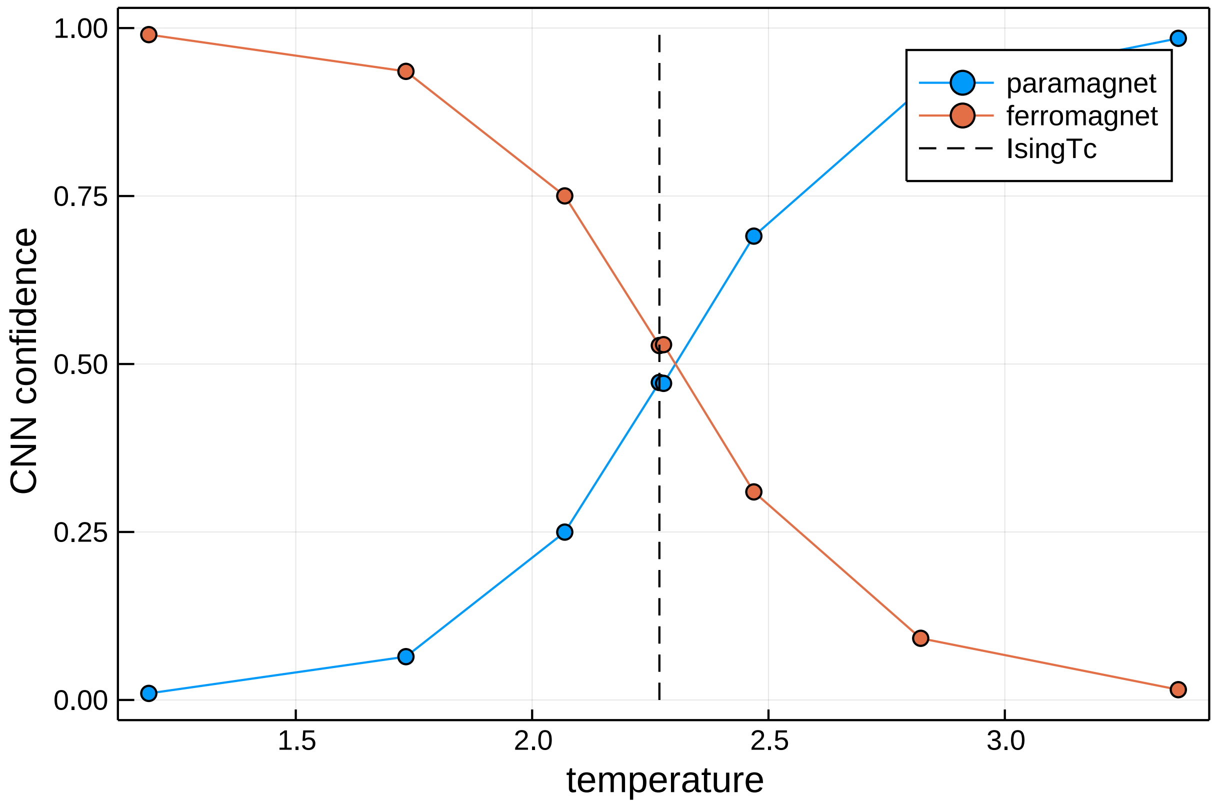
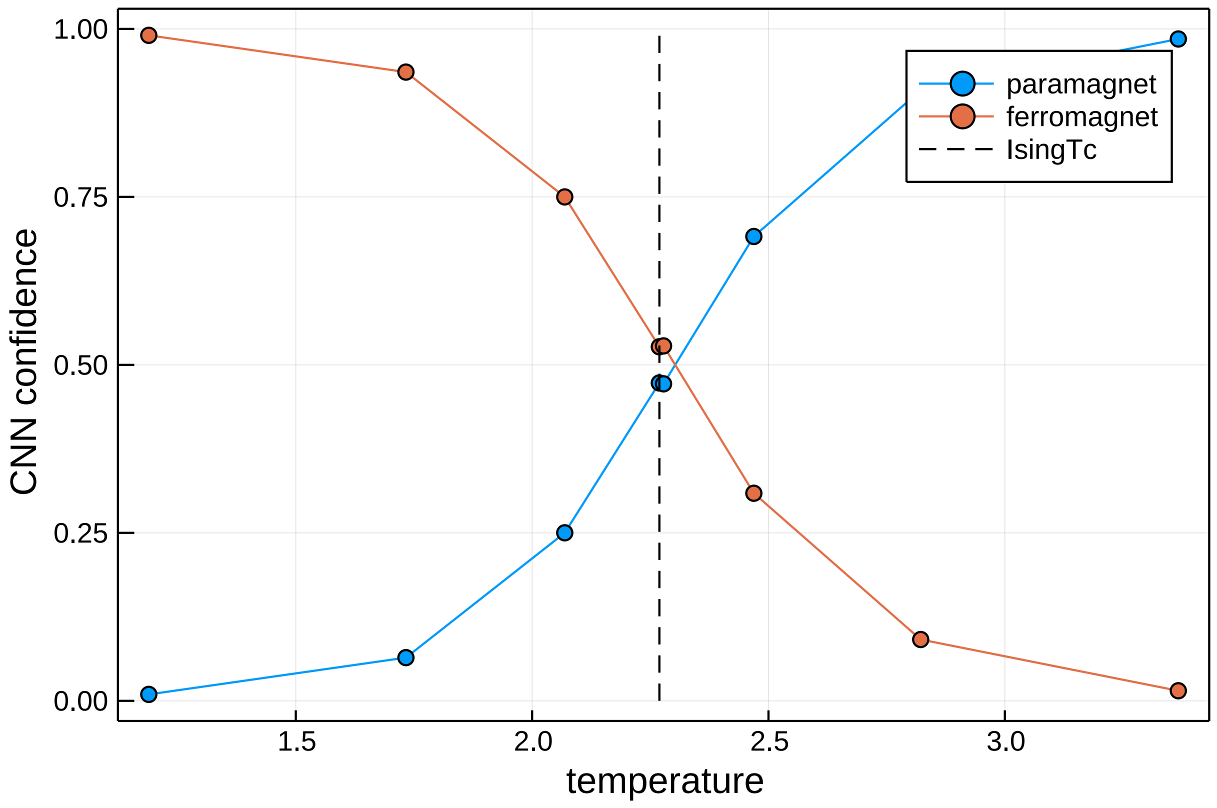
0.00
CNN confidence
1.5
2.0
2.5
3.0
temperature
paramagnet
ferromagnet
IsingTc



1.00
0.75
0.50
0.25
0.00
CNN confidence
1.5
2.0
2.5
3.0
temperature
paramagnet
ferromagnet
IsingTc



paramagnet
ferromagnet
IsingTc
CNN confidence
temperature
1.00
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0.50
0.25
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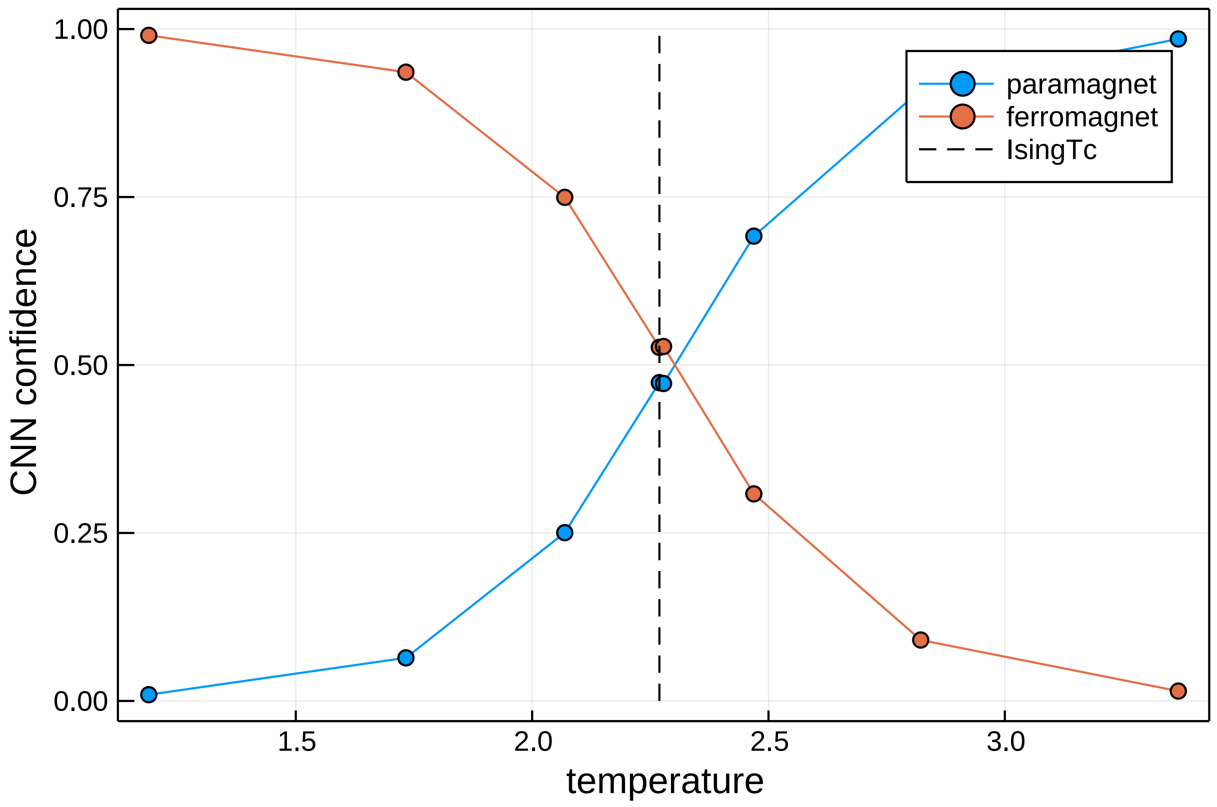
1.5
2.0
2.5
3.0



paramagnet
ferromagnet
IsingTc
CNN confidence
temperature
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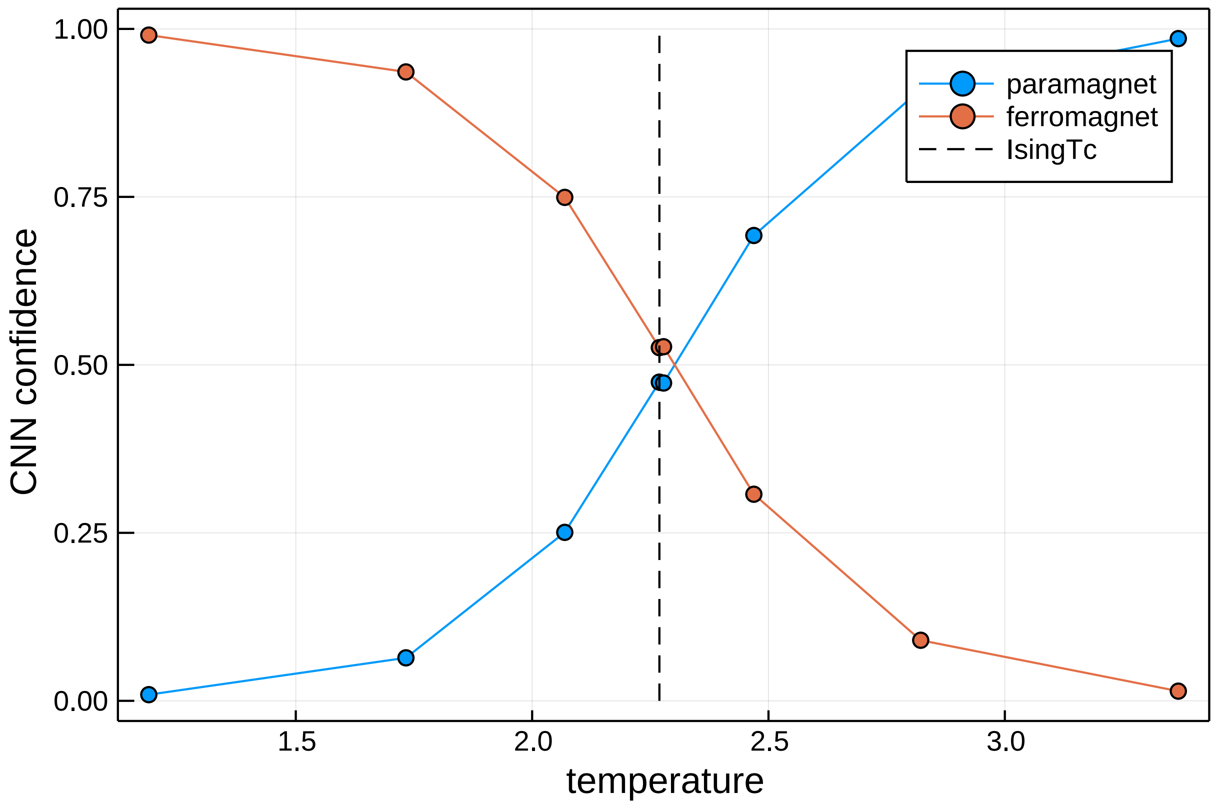
paramagnet
ferromagnet
IsingTc
CNN confidence
temperature
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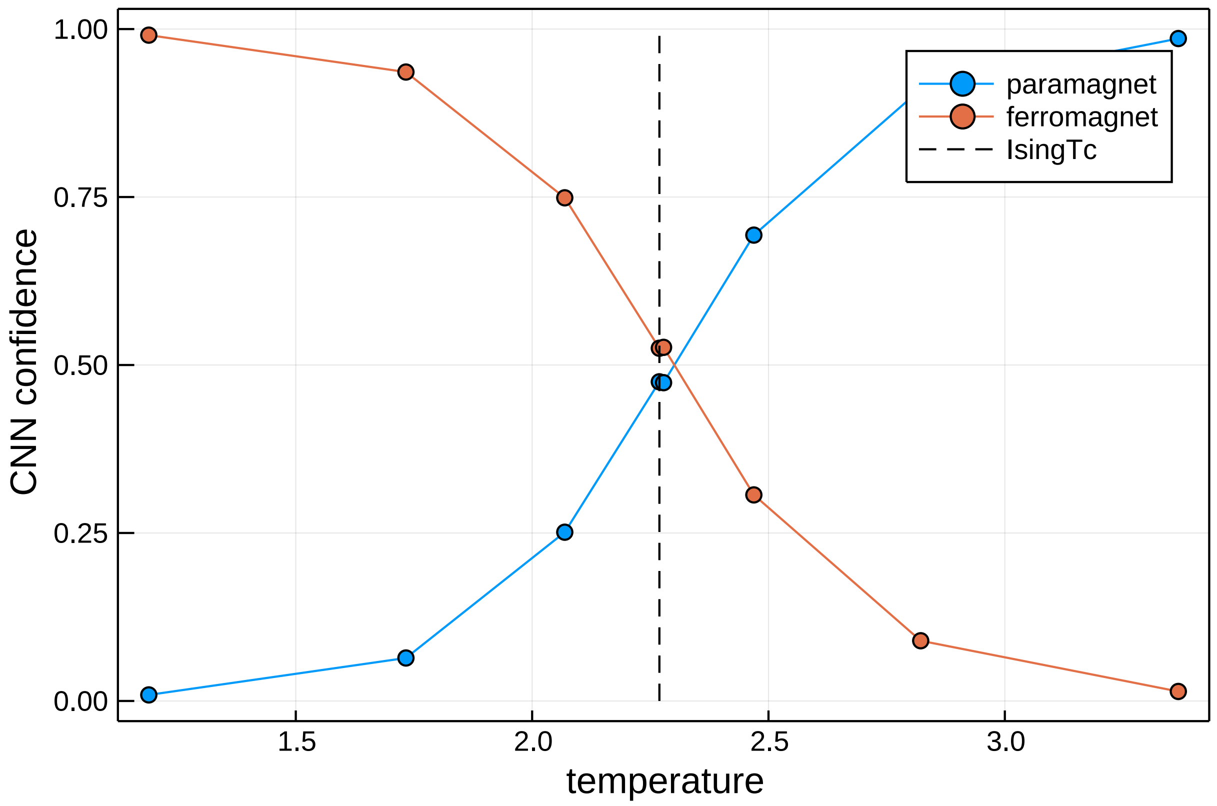
paramagnet
ferromagnet
IsingTc
CNN confidence
temperature
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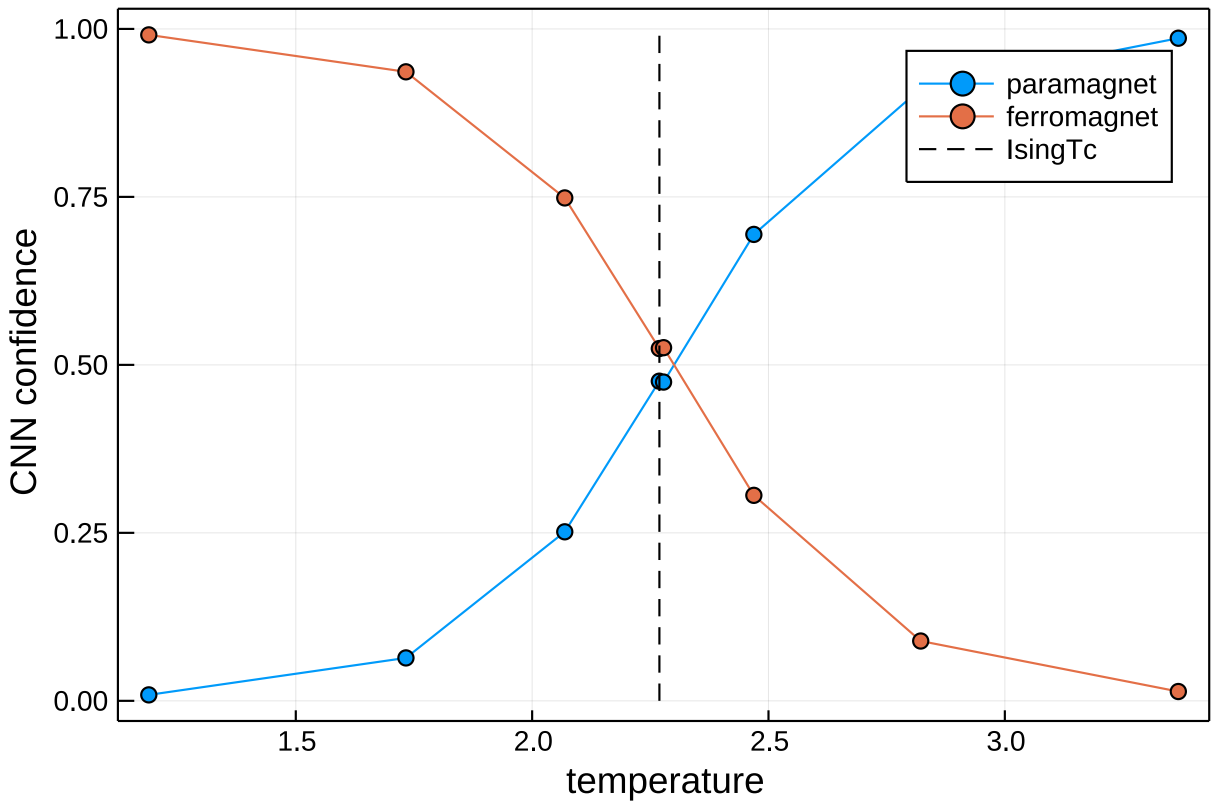

CNN confidence
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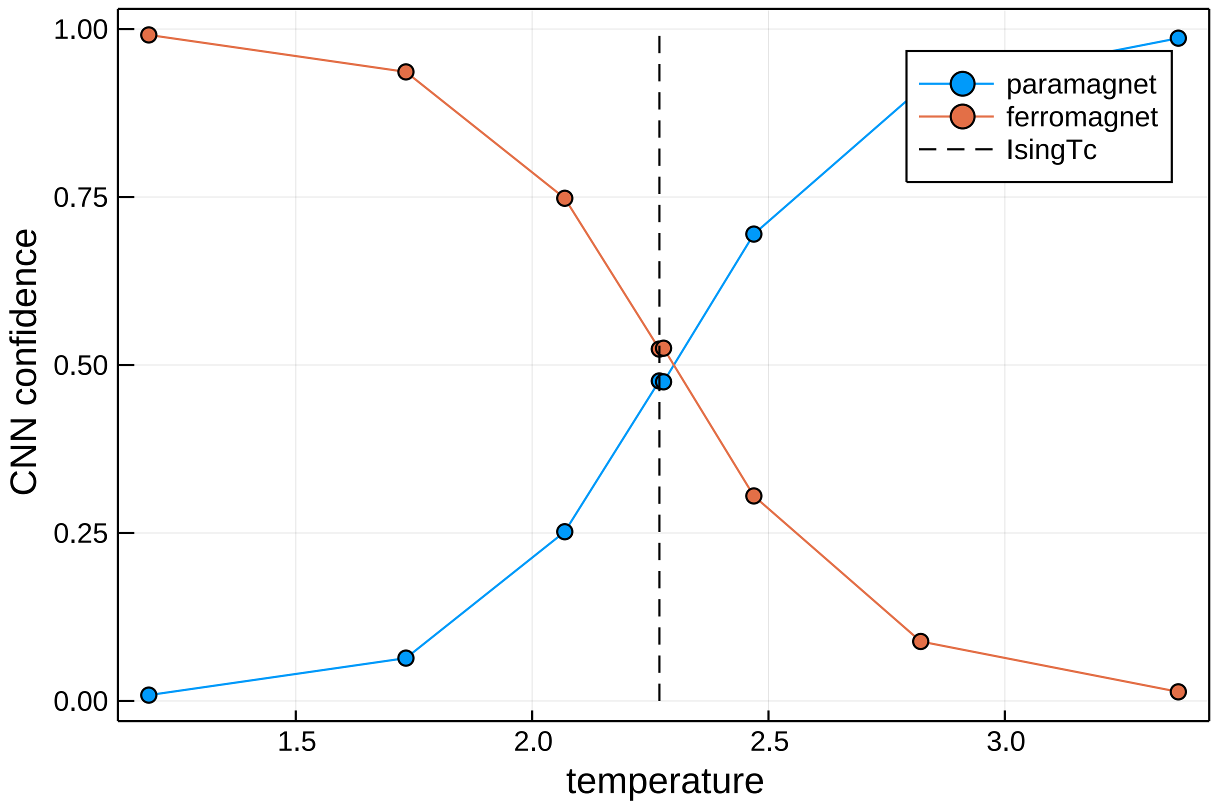
3.0
temperature
paramagnet
ferromagnet
IsingTc



CNN confidence
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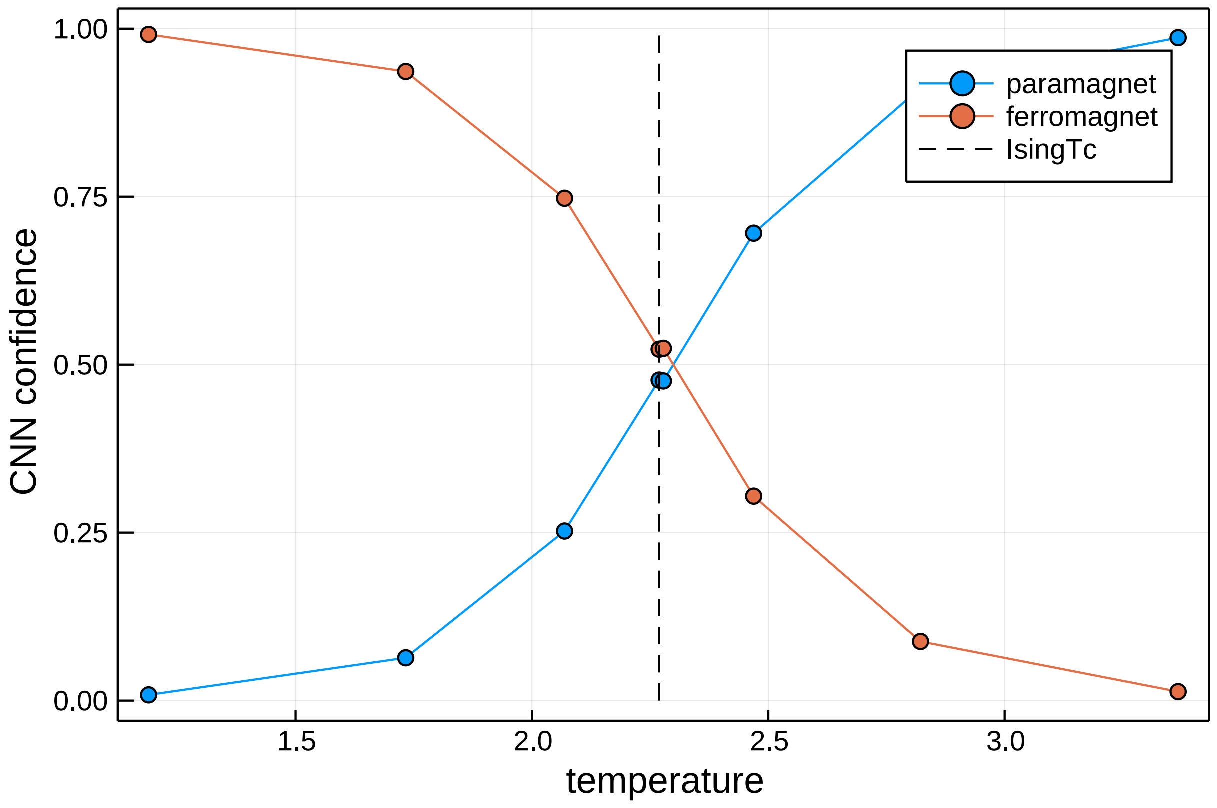
ferromagnet
IsingTc



1.00
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CNN confidence
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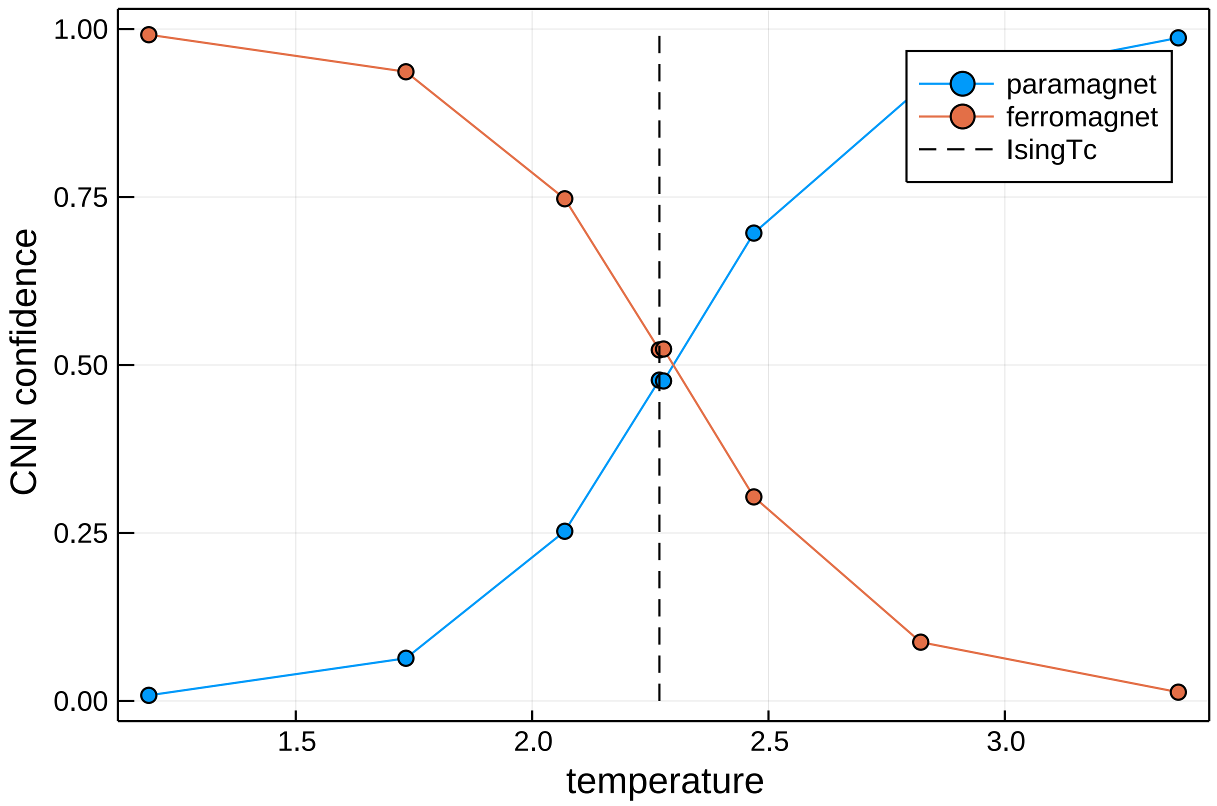
IsingTc



1.00
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CNN confidence
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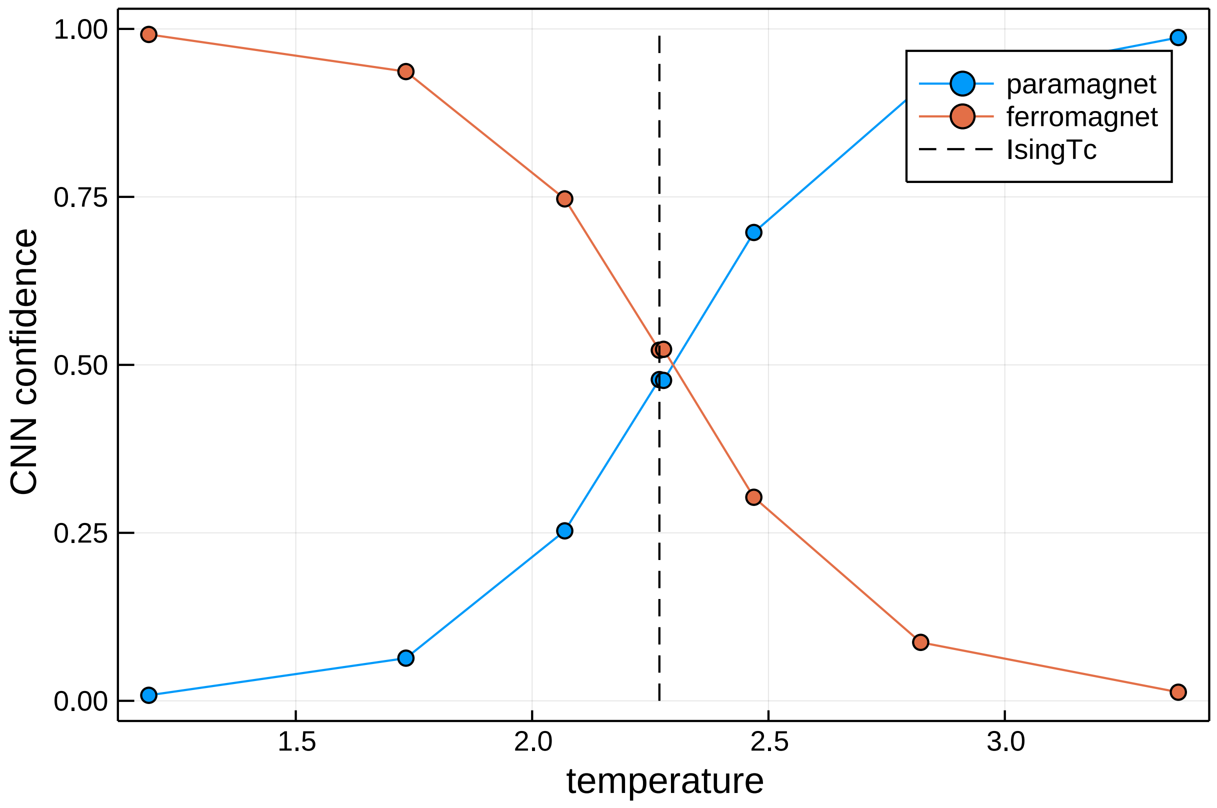
IsingTc



CNN confidence
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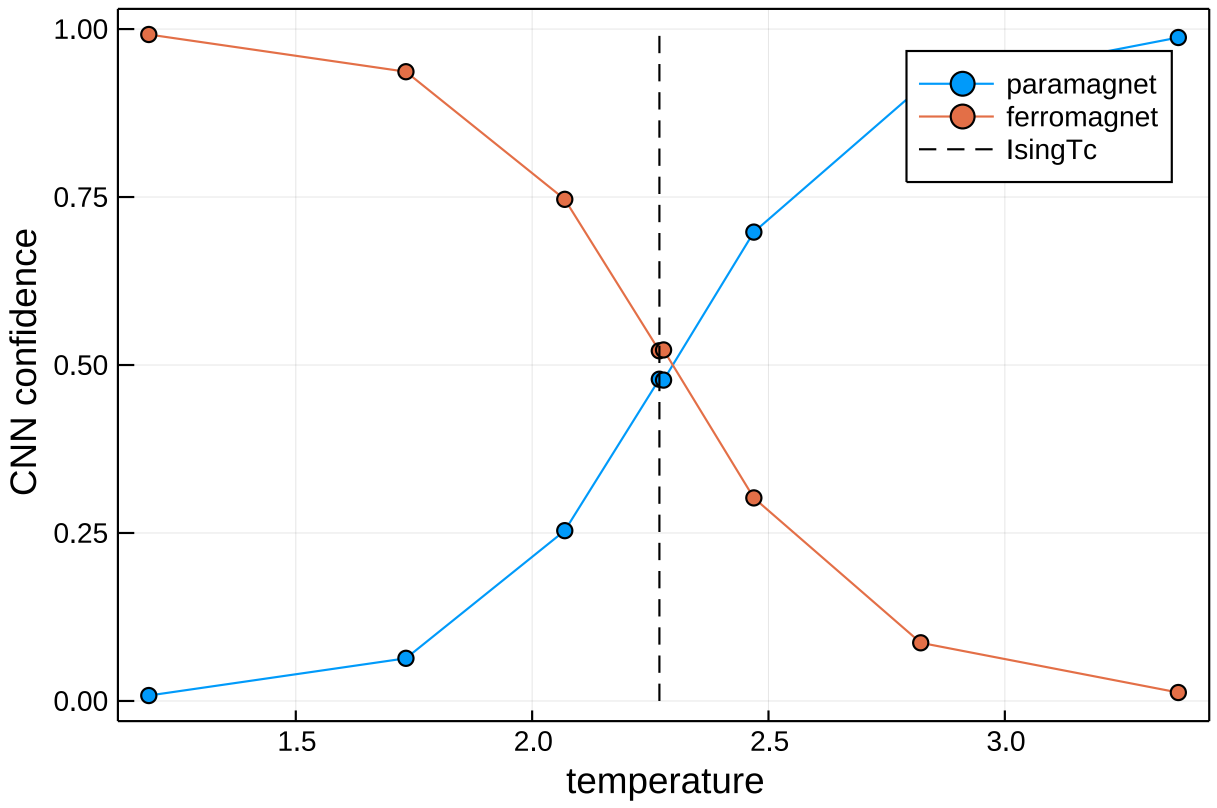
ferromagnet
IsingTc



CNN confidence
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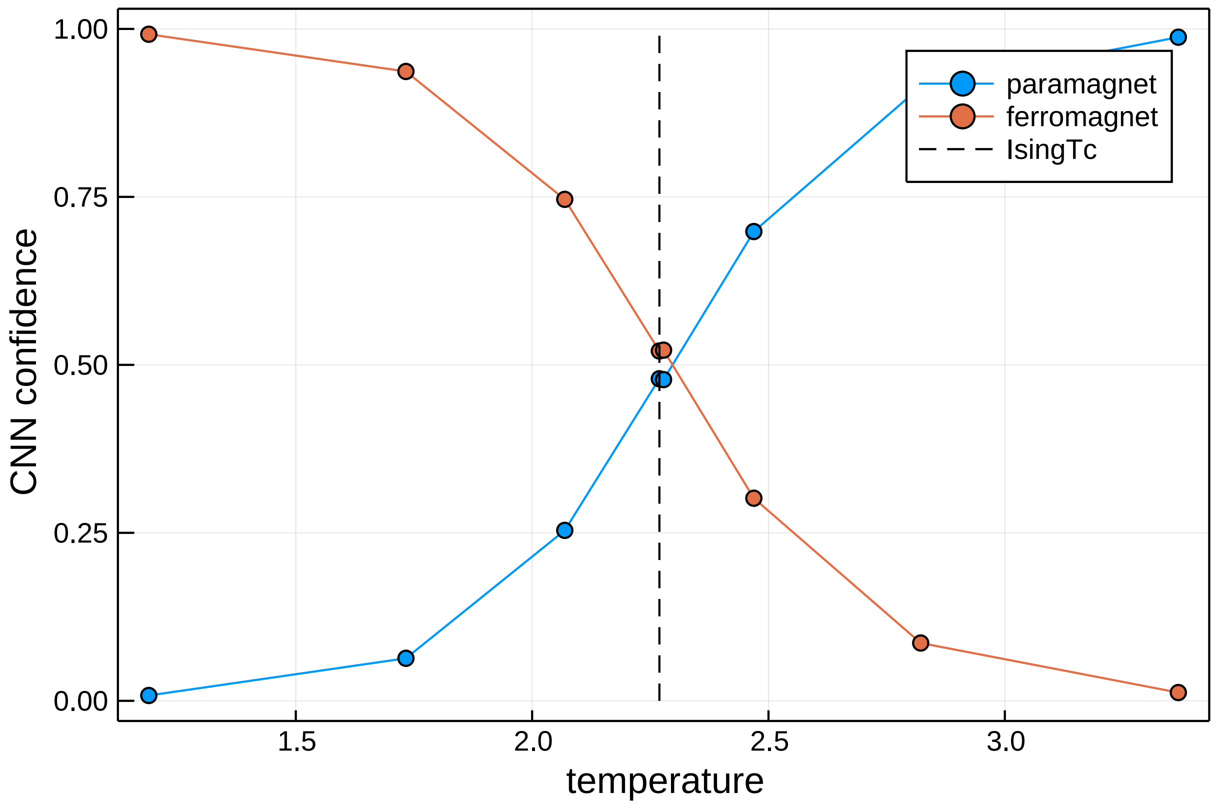
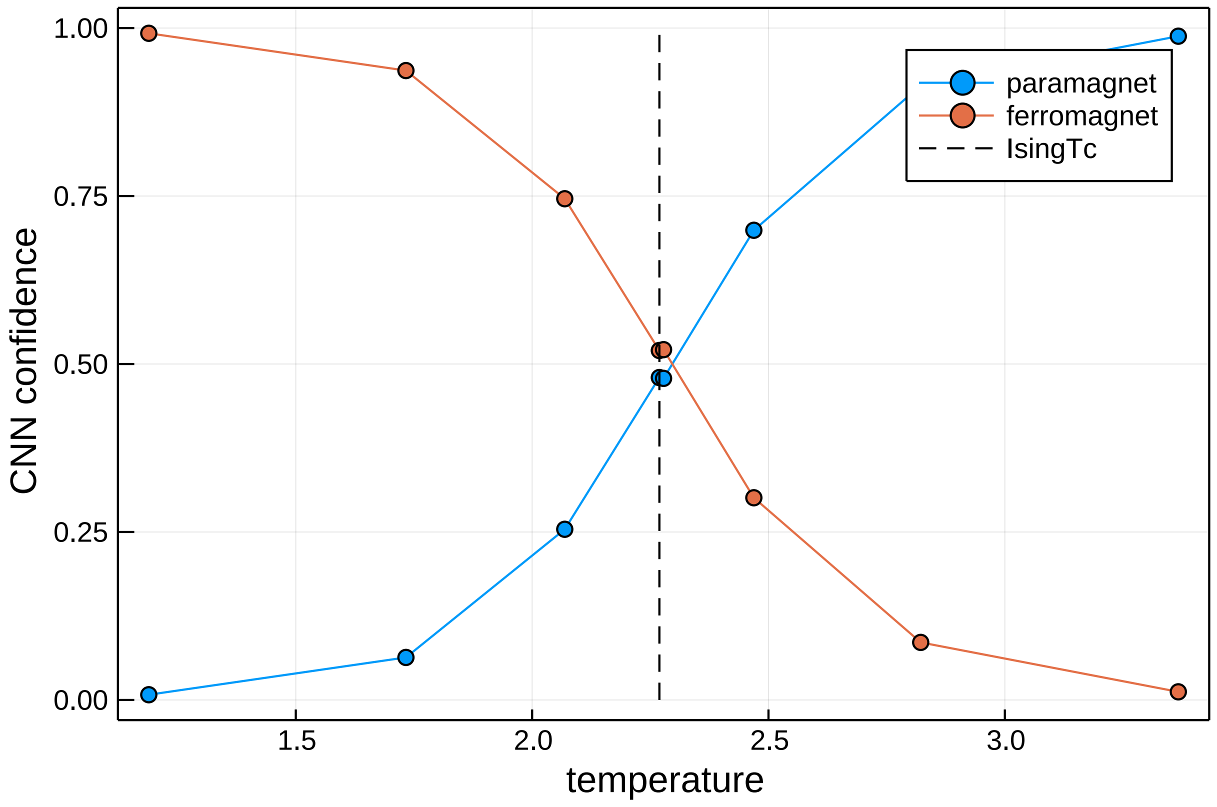
IsingTc





2.1 Appendix

This tutorial is part of the PhysicsTutorials.jl repository.