

# Gaussian Mixture

```
1 # margin-left: 1%;
2 # margin-right: 5%;
3 html"""<style>
4 main {
5     margin: 0 auto;
6     max-width: 90%;
7     padding-left: max(50px, 1%);
8     padding-right: max(253px, 10%);
9     # 253px to accomodate TableOfContents(aside=true)
10 }
11 """
```

```
1 using Pkg, DrWatson, PlutoUI
```

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```
1 begin
2     PlutoUI.TableOfContents()
3 end
```

```
1 versioninfo()
```

```
Julia Version 1.10.2
Commit bd47eca2c8a (2024-03-01 10:14 UTC)
Build Info:
  Official https://julialang.org/ release
Platform Info:
  OS: Linux (x86_64-linux-gnu)
  CPU: 32 x Intel(R) Xeon(R) CPU E5-2630 v3 @ 2.40GHz
  WORD_SIZE: 64
  LIBM: libopenlibm
  LLVM: libLLVM-15.0.7 (ORCJIT, haswell)
Threads: 16 default, 0 interactive, 8 GC (on 32 virtual cores)
Environment:
  JULIA_PKG_SERVER = https://mirrors.tuna.tsinghua.edu.cn/julia
  JULIA_REVERSE_WORKER_ONLY = 1
```

# 1.0 Import all packages

```
TaskLocalRNG()

1 begin
2   using Distributions
3   using FillArrays
4   using StatsPlots
5
6   using LinearAlgebra
7   using Random
8   using Turing
9
10  # Set a random seed.
11  Random.seed!(3)
12 end
```

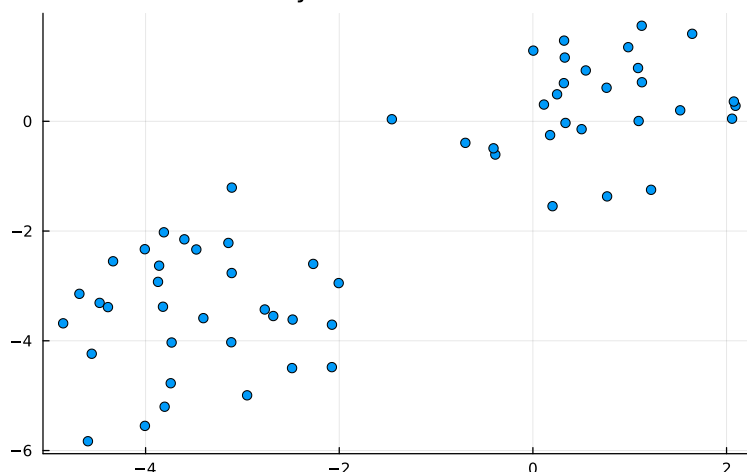
## 1.1 Simulate some data

```
2×60 Matrix{Float64}:
-3.80334 -3.87173 2.09236 1.64516 ... -4.68366 0.24971 -3
-5.20162 -2.9261 0.282404 1.59448 ... -3.14423 0.491857 -4
```

```
1 begin
2   # Define Gaussian mixture model.
3   w = [0.5, 0.5]
4   μ = [-3.5, 0.5]
5   mixturemodel = MixtureModel([MvNormal(Fill(μk, 2),
6     Distributions.I) for μk in μ], w)
7
8   # We draw the data points.
9   N = 60
10  @time x = rand(mixturemodel, N)
end
```

```
0.573396 seconds (491.87 k allocations: 33.482 MiB, 99.98% compilation time)
```

Synthetic Dataset



```
1 scatter(x[1, :], x[2, :]; legend=false, title="Synthetic Dataset")
```

## 1.2 Establish Turing model

=====

```
gaussian_mixture_model (generic function with 2 methods)

1 @model function gaussian_mixture_model(x)
2   # Draw the parameters for each of the K=2 clusters from
   a standard normal distribution.
3   K = 2
4    $\mu \sim \text{MvNormal}(\text{Zeros}(K), I)$ 
5
6   # Draw the weights for the K clusters from a Dirichlet
   distribution with parameters  $\alpha_k = 1$ .
7    $w \sim \text{Dirichlet}(K, 1.0)$ 
8   # Alternatively, one could use a fixed set of weights.
9   #  $w = \text{fill}(1/K, K)$ 
10
11   # Construct categorical distribution of assignments.
12   distribution_assignments = Categorical(w)
13
14   # Construct multivariate normal distributions of each
15 cluster.
16   D, N = size(x)
17   distribution_clusters = [MvNormal(Fill( $\mu_k$ , D), I) for
18  $\mu_k$  in  $\mu$ ]
19
20   # Draw assignments for each datum and generate it from
21 the multivariate normal distribution.
22   k = Vector{Int}(undef, N)
23   for i in 1:N
24     k[i] ~ distribution_assignments
25     x[:, i] ~ distribution_clusters[k[i]]
26   end
27
28   return k
29 end
```

## 1.3 Sampling by PG+HMC

=====

- PG for the discrete K. HMC for continuous  $\mu$  and  $w$ .

	iteration	chain	$\mu[1]$	$\mu[2]$	w[1]	w[2]	
1	1	1	-3.17473	-0.338518	0.493137	0.506863	:
2	2	1	-2.95212	0.358465	0.648418	0.351582	:
3	3	1	-3.85494	0.536792	0.422491	0.577509	:
4	4	1	-2.98575	0.291792	0.545014	0.454986	:
5	5	1	-3.71472	0.548404	0.744618	0.255382	:
6	6	1	-3.34117	0.374166	0.558974	0.441026	:
7	7	1	-3.34117	0.374166	0.558974	0.441026	:
8	8	1	-3.47253	0.562244	0.55249	0.44751	:
9	9	1	-3.37564	0.294521	0.537982	0.462018	:
10	10	1	-3.50283	0.48389	0.436915	0.563085	:
more							

```

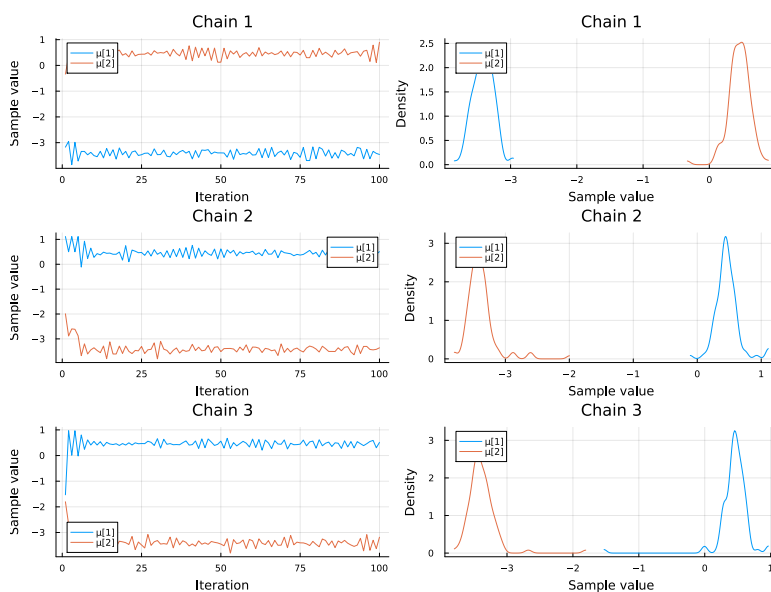
1 begin
2   model = gaussian_mixture_model(x);
3   # k,  $\mu$ , w are all mapped into the sampler?
4   sampler = Gibbs(PG(100, :k), HMC(0.05, 10, : $\mu$ , :w))
5   nsamples = 100
6   nchains = 3
7   @time chains = sample(model, sampler, MCMCThreads(),
8   nsamples, nchains);
end

```

100%

246.782446 seconds (1.30 G allocations: 108.373 GiB, 9.86% gc time, 29.66% compilation time) ?

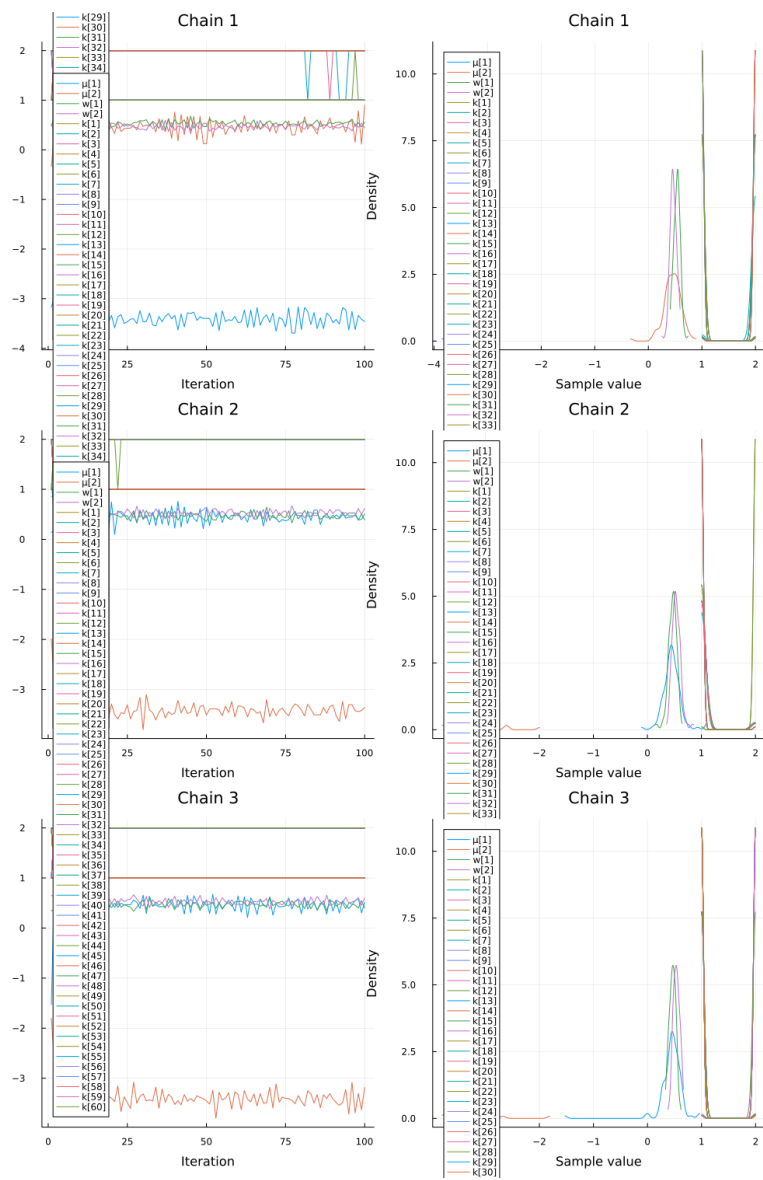
1 chains



```

1 plot(chains[[" $\mu[1]$ ", " $\mu[2]$ "]]; colordim=:parameter,
   legend=true)

```



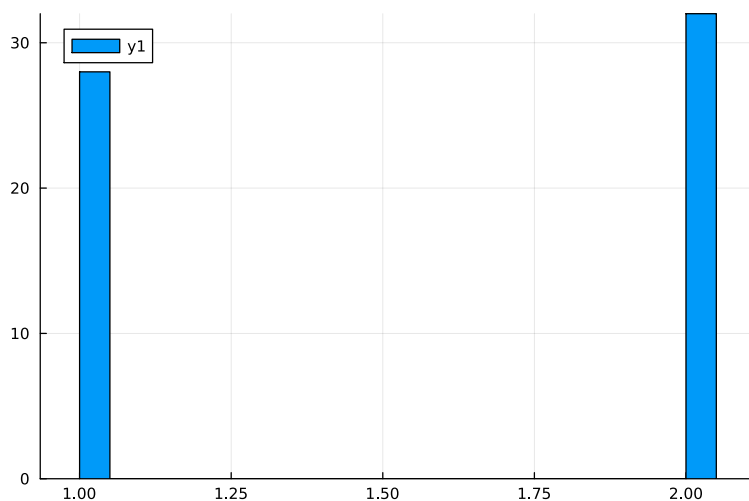
```
1 plot(chains; colordim=:parameter, legend=true, size=(1000,1500))
```

```

3-dimensional AxisArray{Float64,3,...} with axes:
  :iter, 1:1:100
  :var, [Symbol("μ[1]"), Symbol("μ[2]"), Symbol("w[1]"), Symbol("w[2]"), Symbol("w[3]")]
  :chain, 1:3
And data, a 100×65×3 Array{Float64, 3}:
[:, :, 1] =
-3.17473 -0.338518 0.493137 0.506863 ... 2.0 2.0 1.0 1.0
-2.95212 0.358465 0.648418 0.351582 ... 1.0 1.0 1.0 2.0
-3.85494 0.536792 0.422491 0.577509 ... 1.0 1.0 1.0 2.0
-2.98575 0.291792 0.545014 0.454986 ... 1.0 1.0 1.0 2.0
-3.71472 0.548404 0.744618 0.255382 ... 1.0 1.0 1.0 2.0
-3.34117 0.374166 0.558974 0.441026 ... 1.0 1.0 1.0 2.0
-3.34117 0.374166 0.558974 0.441026 ... 1.0 1.0 1.0 2.0
⋮
-3.629 0.550979 0.561428 0.438572 ... 1.0 1.0 1.0 2.0
-3.25971 0.589129 0.620074 0.379926 ... 1.0 1.0 1.0 2.0
-3.62434 0.153246 0.475385 0.524615 ... 1.0 1.0 1.0 2.0
-3.33782 0.788136 0.54756 0.45244 ... 1.0 1.0 1.0 2.0
-3.41603 0.113558 0.463805 0.536195 ... 1.0 1.0 1.0 2.0
-3.45961 0.897516 0.555307 0.444693 ... 1.0 1.0 1.0 2.0
⋮
[:, :, 2] =
1.11545 -1.99098 0.138071 0.861929 ... 2.0 2.0 2.0 2.0
0.501362 -2.88465 0.183156 0.816844 ... 2.0 2.0 2.0 1.0
1.11487 -2.5986 0.289975 0.710025 ... 2.0 2.0 2.0 1.0
0.500535 -2.61454 0.349798 0.650202 ... 2.0 2.0 2.0 1.0
1.11584 -2.87466 0.285701 0.714299 ... 2.0 2.0 2.0 1.0
-0.112998 -3.67492 0.574123 0.425877 ... 2.0 2.0 2.0 1.0
0.928263 -3.1998 0.497663 0.502337 ... 2.0 2.0 2.0 1.0
⋮
0.443253 -3.30328 0.52756 0.47244 ... 2.0 2.0 2.0 1.0
0.443253 -3.30328 0.52756 0.47244 ... 2.0 2.0 2.0 1.0
⋮

```

```
1 chains.value
```



```

1 #last iteration of the 3rd chain of 60 k values (cluster
2 assignments)
histogram(chains.value[iter=100][5:64,3], bins=20)

```

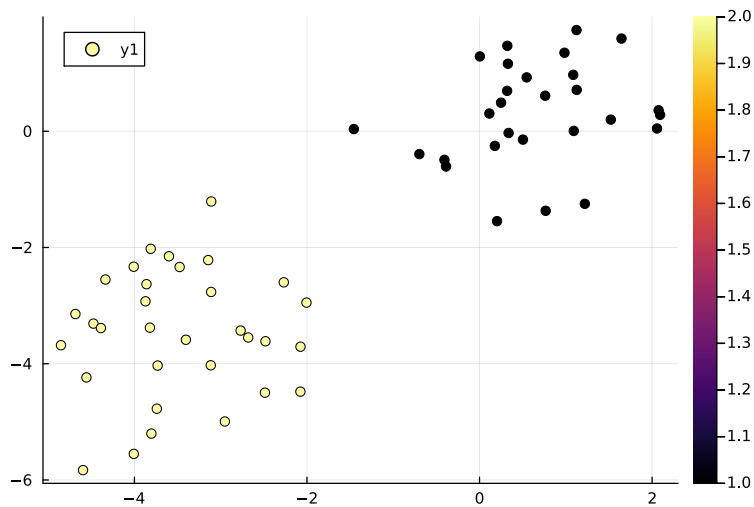
```
(varname_to_symbol = OrderedDict(μ[1] ⇒ Symbol("μ[1]"), μ[2] ⇒
```

```
1 chains.info
```

```
[0.460472, 0.531358, 0.533908]
```

```
1 begin
2   @show median.(eachcol(chains[:"μ[1]"']))
3   @show median.(eachcol(chains[:"μ[2]"']))
4   @show median.(eachcol(chains[:"w[1]"']))
5   @show median.(eachcol(chains[:"w[2]"']))
6 end
```

```
median.(eachcol(chains[:(QuoteNode("μ[1]"))])) = [- ②
3.405617489183758, 0.44674296000216607, 0.46345993339,
3022]
median.(eachcol(chains[:(QuoteNode("μ[2]"))])) = [0.45
82280003677017, -3.420573823097018, -3.406275476316240
6]
median.(eachcol(chains[:(QuoteNode("w[1]"))])) = [0.53
95282753183839, 0.4686417827884136, 0.466092321742558
7]
median.(eachcol(chains[:(QuoteNode("w[2]"))])) = [0.46
047172468161607, 0.5313582172115864, 0.533907678257441
2]
```



```
1 begin
2   cmap = Dict{1 => :red, 2 => :blue}
3   # Color function based on color map
4   color_func(value) = cmap[get(cmap, value, :gray)] #
5   Default to gray if not in map
6   color_vec = chains.value[iter=100][5:64,3]
7   scatter(x[1, :], x[2, :]; marker_z=color_vec) #
8   markerfacecolor=map(color_func, color_vec),
9   title="Synthetic Dataset")
10 end
```

	iteration	chain	$\mu[1]$	$\mu[2]$	w[1]	w[2]	
1	1	1	-0.917817	0.514631	0.88358	0.11642	:
2	2	1	-2.23336	1.17691	0.638822	0.361178	:
3	3	1	-2.73592	0.438788	0.752347	0.247653	:
4	4	1	-3.77493	0.554984	0.441144	0.558856	:
5	5	1	-3.0009	0.43676	0.721961	0.278039	:
6	6	1	-3.61718	0.811352	0.476689	0.523311	:
7	7	1	-3.4402	0.278046	0.527244	0.472756	:
8	8	1	-3.43152	0.478669	0.385599	0.614401	:
9	9	1	-3.45661	0.411029	0.638697	0.361303	:
10	10	1	-3.27962	0.564529	0.441955	0.558045	:
	more						

```

1 begin
2 @time sample(model, sampler, MCMCThreads(), nsamples,
3 nchains)
end

```

100%

226.930748 seconds (1.27 G allocations: 106.401 GiB, 10.05% gc time) ?

## 1.4 Sampling by NUTS(). Failed due to ForwardDiff error.

- $k$  is discrete, so NUTS/HMC sampler will fail (no gradient).



```
ArgumentError: invalid index:  
Dual{ForwardDiff.Tag{DynamicPPL.DynamicPPLTag,  
Float64}}  
(2.0,0.0,0.0,0.0,1.0,0.0,0.0,0.0,0.0,0.0,0.0) of  
type  
ForwardDiff.Dual{ForwardDiff.Tag{DynamicPPL.DynamicPPLT  
ag, Float64}, Float64, 11}
```

## Stack trace

Here is what happened, the most recent locations are first:

1. `to_index(i::ForwardDiff.Dual{ForwardDiff.Tag{DynamicPPL.DynamicPPLTag, Float64}, Float64, 11})`  
@ `(indices.jl:300)`
2. `to_index(A::Vector{Distributions.MvNormal{ForwardDiff.Dual{ForwardDiff.Tag{DynamicPPL.DynamicPPLTag, Float64}, Float64, 11}, PDMats.ScalMat{ForwardDiff.Dual{ForwardDiff.Tag{DynamicPPL.DynamicPPLTag, Float64}, Float64, 11}}, FillArrays.Fill{ForwardDiff.Dual{ForwardDiff.Tag{DynamicPPL.DynamicPPLTag, Float64}, Float64, 11}, 1, Tuple{Base.OneTo{Int64}}}}, i::ForwardDiff.Dual{ForwardDiff.Tag{DynamicPPL.DynamicPPLTag, Float64}, Float64, 11})` @ `(indices.jl:277)`
3. `_to_indices1(A::Vector{Distributions.MvNormal{ForwardDiff.Dual{ForwardDiff.Tag{DynamicPPL.DynamicPPLTag, Float64}, Float64, 11}, PDMats.ScalMat{ForwardDiff.Dual{ForwardDiff.Tag{DynamicPPL.DynamicPPLTag, Float64}, Float64, 11}}, FillArrays.Fill{ForwardDiff.Dual{ForwardDiff.Tag{DynamicPPL.DynamicPPLTag, Float64}, Float64, 11}, 1, Tuple{Base.OneTo{Int64}}}}, inds::Tuple{Base.OneTo{Int64}}, I1::ForwardDiff.Dual{ForwardDiff.Tag{DynamicPPL.DynamicPPLTag, Float64}, Float64, 11})` @ `(indices.jl:359)`
4. `to_indices` @ `indices.jl:354`
5. `to_indices` @ `indices.jl:345`
6. `getindex` @ `abstractarray.jl:1291`
7. `gaussian_mixture_model(__model__::DynamicPPL.Model{typeof(Main.var"workspace#4".gaussian_mixture_model), (:x,), (), (), Tuple{Matrix{Float64}}, Tuple{(), DynamicPPL.DefaultContext}, __varinfo__::DynamicPPL.ThreadSafeVarInfo{DynamicPPL.TypedVarInfo{@NamedTuple{μ::DynamicPPL.Metadata{Dict{AbstractPPL.VarName{μ}, Setfield.IdentityLens}, Int64}, Vector{Distributions.ZeroMeanIsoNormal{Tuple{Base.OneTo{Int64}}}}, Vector{AbstractPPL.VarName{μ}, Setfield.IdentityLens}}, Vector{ForwardDiff.Dual{ForwardDiff.Tag{DynamicPPL.DynamicPPLTag, Float64}, Float64, 11}}, Vector{Set{DynamicPPL.Selector}}}, w::DynamicPPL.Metadata{Dict{AbstractPPL.VarName{w}, Setfield.IdentityLens}, Int64}, Vector{Distributions.Dirichlet{Float64}, FillArrays.Fill{Float64, 1, Tuple{Base.OneTo{Int64}}}}, Float64}}, Vector{AbstractPPL.VarName{w},`

```

Setfield.IdentityLens}},
Vector{ForwardDiff.Dual{ForwardDiff.Tag{DynamicPPL.DynamicPPLTag, Float64}, Float64, 11}},
Vector{Set{DynamicPPL.Selector}}},
k::DynamicPPL.Metadata{Dict{AbstractPPL.VarName{:k,
Setfield.IndexLens{Tuple{Int64}}}}, Int64},
Vector{Distributions.Categorical{Float64,
Vector{Float64}}}, Vector{AbstractPPL.VarName{:k,
Setfield.IndexLens{Tuple{Int64}}}},
Vector{ForwardDiff.Dual{ForwardDiff.Tag{DynamicPPL.DynamicPPLTag, Float64}, Float64, 11}},
Vector{Set{DynamicPPL.Selector}}}},
ForwardDiff.Dual{ForwardDiff.Tag{DynamicPPL.DynamicPPLTag, Float64}, Float64, 11}},
Vector{Base.RefValue{ForwardDiff.Dual{ForwardDiff.Tag{DynamicPPL.DynamicPPLTag, Float64}, Float64, 11}}}},
__context__::DynamicPPL.SamplingContext{DynamicPPL.Sampler{Turing.Inference.NUTS{ADTypes.AutoForwardDiff{0,
Nothing}, (), AdvancedHMC.DiagEuclideanMetric}},
DynamicPPL.DefaultContext, Random.TaskLocalRNG},
x::Matrix{Float64}) @ (Other cell: line 22

```

```

20     for i in 1:N
21         k[i] ~ distribution_assignments
22         x[:, i] ~ distribution_clusters[k[i]]
23     end
24
cell preview

```

8. [Show more...](#)

```
1 @time chains_NUTS = sample(model, NUTS(), 1000)
```

100%

Another cell defining `chains_NUTS` contains errors.

```
1 plot(chains_NUTS; colordim=:parameter, legend=true)
```

# 1.5 Sampling via PG+NUTS.

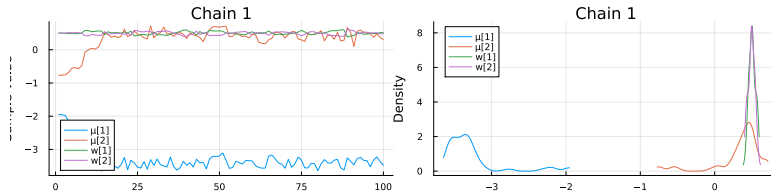
@time chains\_PG\_NUTS =

	iteration	chain	$\mu[1]$	$\mu[2]$	w[1]	w[2]
1	1	1	-1.94838	-0.773854	0.506241	0.493759
2	2	1	-1.96032	-0.760893	0.502367	0.497633
3	3	1	-1.97654	-0.753359	0.499932	0.500068
4	4	1	-2.14837	-0.676939	0.481817	0.518183
5	5	1	-2.17949	-0.554959	0.49149	0.50851
6	6	1	-2.21794	-0.53658	0.48612	0.51388
7	7	1	-2.26144	-0.570986	0.483773	0.516227
8	8	1	-2.3283	-0.478795	0.50734	0.49266
9	9	1	-2.73912	-0.0723776	0.581018	0.418982
10	10	1	-2.79475	-0.00475192	0.57743	0.42257
more						

```
1 @time chains_PG_NUTS = sample(model, Gibbs(PG(100, :k),
2   NUTS(200, 0.65, init_ε=0.003, :μ, :w)), 100)
```

100%

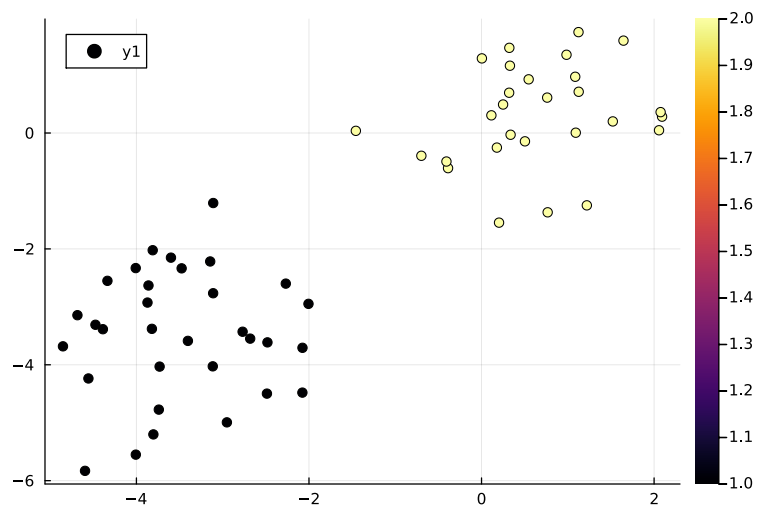
194.602903 seconds (426.31 M allocations; 35.779 Gi B, 4.84% gc time, 2.60% compilation time)



```
1 plot(chains_PG_NUTS[["μ[1]", "μ[2]", "w[1]", "w[2]"]];
   colordim=:parameter, legend=true)
```

3-dimensional AxisArray{Float64,3,...} with axes:  
 :iter, 1:1:100  
 :var, [Symbol("μ[1]"), Symbol("μ[2]"), Symbol("w[1]"), Symbol("w[2]")]  
 :chain, 1:1  
 And data, a 100×65×1 Array{Float64, 3}:  
 [:, :, 1] =  
 -1.94838 -0.773854 0.506241 0.493759 ... 1.0 1.0 1.0 2.0  
 -1.96032 -0.760893 0.502367 0.497633 ... 1.0 1.0 1.0 2.0  
 -1.97654 -0.753359 0.499932 0.500068 ... 1.0 1.0 1.0 2.0  
 -2.14837 -0.676939 0.481817 0.518183 ... 1.0 1.0 1.0 2.0  
 -2.17949 -0.554959 0.49149 0.50851 ... 1.0 1.0 1.0 2.0  
 -2.21794 -0.53658 0.48612 0.51388 ... 1.0 1.0 1.0 2.0  
 -2.26144 -0.570986 0.483773 0.516227 ... 1.0 1.0 1.0 2.0  
 ⋮ ⋮ ⋮ ⋮ ⋮ ⋮ ⋮ ⋮  
 -3.33896 0.495269 0.471419 0.528581 ... 1.0 1.0 1.0 2.0  
 -3.5244 0.474689 0.495744 0.504256 ... 1.0 1.0 1.0 2.0  
 -3.32019 0.373059 0.488997 0.511003 ... 1.0 1.0 1.0 2.0  
 -3.22497 0.483376 0.489564 0.510436 ... 1.0 1.0 1.0 2.0  
 -3.3667 0.36694 0.517047 0.482953 ... 1.0 1.0 1.0 2.0  
 -3.47571 0.304172 0.515882 0.484118 ... 1.0 1.0 1.0 2.0

```
1 chains_PG_NUTS.value
```



```
1 begin
2   scatter(x[1, :], x[2, :];
3   marker_z=chains_PG_NUTS.value[iter=100][5:64,1])
4   # markerfacecolor=map(color_func, color_vec),
   title="Synthetic Dataset")
end
```