## **Chapter 9. Markov Chain Monte Carlo.**

#### 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 × 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.ed
u.cn/julia
JULIA_REVISE_WORKER_ONLY = 1
```

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

1 using Pkg, DrWatson, PlutoUI

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```
begin
plutoUI.TableOfContents()
and
```

```
1 begin
      using Random
      using StatsBase
3
      using Distributions
      using StatsPlots
      using StatsFuns
6
      using Logging
8
9
      using CSV
      using DataFrames
11
      using Optim
12
      using MCMCChains
13
       using Optim
15
       using Turing
       using StatisticalRethinking
16
17 end
```

Error requiring 'Turing' from 'StatisticalRethinking'

```
LoadError: UndefVarError: `ModeResult` not defined

in expression starting at /y/home/huangyu/.julia/packages/Statistical Rethinking/RYYWV/src/require/turing/turing_optim_sample.jl:5

in expression starting at /y/home/huangyu/.julia/packages/Statistical Rethinking/RYYWV/src/require/turing/turing.jl:7
```

### **Stack trace**

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

```
begin

Plots.default(labels=false)

# Comment out the following (Do not disable
Logging.Warn) and restart the Pluto notebook. So that

console/terminal output can appear.

#Logging.disable_logging(Logging.Warn);
end
```

name	size	summary
BuiltinsNotebook	1.381 MiB	Module
Button	140 bytes	DataType
CheckBox	140 bytes	DataType
Clock	188 bytes	DataType
ClockNotebook	1.305 MiB	Module
ColorPicker	40 bytes	UnionAll
ColorStringPicker	140 bytes	DataType
ConfirmNotebook	1.303 MiB	Module
CounterButton	140 bytes	DataType
DateField	156 bytes	DataType
DatePicker	156 bytes	DataType
DetailsNotebook	16.806 KiB	Module
DownloadButton	148 bytes	DataType
Dump	148 bytes	DataType
FilePicker	140 bytes	DataType
LabelButton	140 bytes	DataType
LocalResource	0 bytes	LocalResource (generic function with 1 method)
MultiCheckBox	80 bytes	UnionAll
MultiCheckBoxNotebook	1.307 MiB	Module
MultiSelect	80 bytes	UnionAll
NumberField	188 bytes	DataType
PasswordField	140 bytes	DataType
PlutoUI	1.686 MiB	Module
Print	0 bytes	Print (generic function with 1 method)
Radio	164 bytes	DataType
RangeSlider	236 bytes	DataType
RangeSliderNotebook	1.305 MiB	Module
RemoteResource	252 bytes	DataType
Resource	252 bytes	DataType
Scrubbable	244 bytes	DataType
ScrubbableNotebook	1.306 MiB	Module
Select	148 bytes	DataType
Show	80 bytes	UnionAll
Slider	40 bytes	UnionAll

```
172
TableOfContents
                                    DataType
                            bytes
                            1.325
TableOfContentsNotebook
                                    Module
                              MiB
                            1.317
TerminalNotebook
                                    Module
                              MiB
                               204
TextField
                                    DataType
                            bytes
                              156
TimeField
                                    DataType
                            bytes
                                    TimePicker (generic
TimePicker
                          0 bytes
                                    function with 2 methods)
                              196
WebcamInput
                                    DataType
                            bytes
                            1.322
WebcamInputNotebook
                                    Module
                              MiB
                               40
WithIOContext
                                    UnionAll
                            bytes
                                    #4 (generic function with
as_html
                          0 bytes
                                    1 method)
                                    as_mime (generic function
as_mime
                          0 bytes
                                    with 2 methods)
                                    #4 (generic function with
                          0 bytes
as_png
                                    1 method)
                                    #4 (generic function with
as_svg
                          0 bytes
                                    1 method)
                                    #4 (generic function with
                          0 bytes
as_text
                                    1 method)
                               20
                                    HTML{String}
                            bytes
                                    confirm (generic function
confirm
                          0 bytes
                                    with 1 method)
                                    details (generic function
                          0 bytes
details
                                    with 2 methods)
                                    with_terminal (generic
function with 1 method)
with_terminal
                          0 bytes
1 begin
      PlutoUI.with_terminal() do
3
           println("Hola")
4
       end
```

```
varinfo(PlutoUI)
5
6 end
```

#### 0.000000 seconds

```
1 with_terminal(show_value=false) do
      @time x=sum(1:100000)
3 end
```

#### 5000050000

1 Qtime sum(1:100000)

? 0.000001 seconds

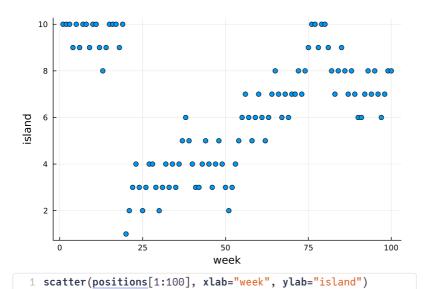
### 9.1 Good King Markov and his island kingdom.

#### Code 9.1

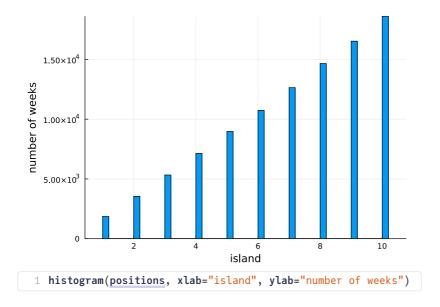
```
1 begin
2   Random.seed!(1)
3   num_weeks = 10^5
4   positions = []
5   current = 10
6 end;
```

```
1 for i ∈ 1:num_weeks
2  # record current position
3  push!(positions, current)
4  # flip coin to generate proposal
5  proposal = current + sample([-1, 1])
6  # handle loops around
7  proposal < 1 && (proposal = 10)
8  proposal > 10 && (proposal = 1)
9  # move?
10  prob_move = proposal / current
11  rand() < prob_move && (current = proposal)
12 end</pre>
```

#### Code 9.2 Island vs Week



### Code 9.3 The number of weeks spent at each island

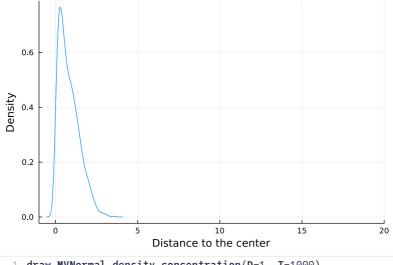


### 9.2 Metropolis algorithms

### Code 9.4 Curse of dimensionality in MVNormal

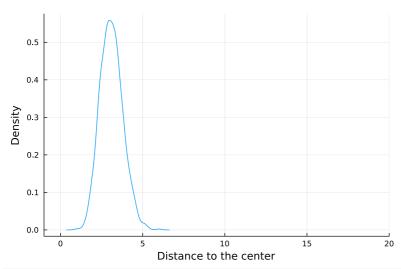
```
draw_MVNormal_density_concentration (generic function with 1 meth

1 function draw_MVNormal_density_concentration(; D=10, T=1000)
2  # D is #dimensions.
3  # T is #samples.
4  #for D in [1,10,100,1000]
5  # Normal mean at 0, stddev=1.
6  @time Y = rand(MvNormal(zeros(D), ones(D)), T)
7  @time Rd = sqrt.(sum.(eachcol(Y.^2)))
8  plot(density(Rd), xlim = (-1, 20))
9  xlabel!("Distance to the center")
10  ylabel!("Density")
11 end
```



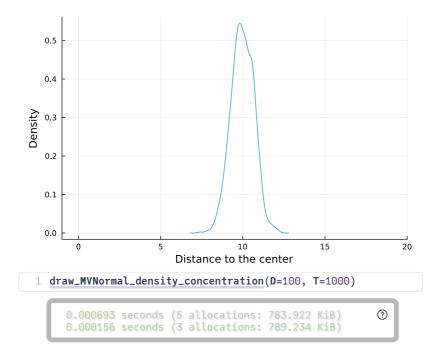
 ${\scriptsize 1\ \underline{draw\_MVNormal\_density\_concentration}(D=1,\ T=1000)}$ 

0.003463 seconds (400 allocations: 36.398 KiB, 9 ② 9.00% compilation time) 0.000010 seconds (2 allocations: 15.875 KiB)



1 draw\_MVNormal\_density\_concentration(D=10, T=1000)

0.000098 seconds (5 allocations: 78.594 KiB) 0.000030 seconds (3 allocations: 86.109 KiB)



#### 9.3 Hamiltonian Monte Carlo

#### Code 9.5 Simulate some data

```
begin
Random.seed!(7)

x = rand(Normal(), 50)
y = rand(Normal(), 50)
x = standardize(ZScoreTransform, x)
y = standardize(ZScoreTransform, y);
end;
```

```
U (generic function with 1 method)

1 function U(q::Vector{Float64}; a=0, b=1, k=0, d=1)::Float64

2 μy, μx = q

3 U = sum(normlogpdf.(μy, 1, y)) + sum(normlogpdf.(μx, 1, 4 x))

5 U += normlogpdf(a, b, μy) + normlogpdf(k, d, μx)

6 -U
end
```

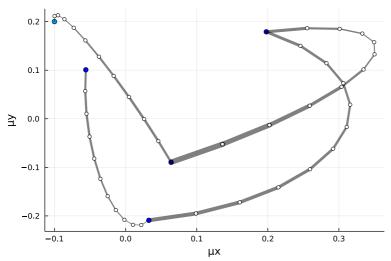
#### **Code 9.6 Gradient ∇U**

```
∇U (generic function with 1 method)
```

### Codes 9.8 - 9.10 (HMC2 function)

HMC2 (generic function with 1 method) 1 function HMC2(U, ∇U, €::Float64, L::Int, 2 current\_q::Vector{Float64}) q = current\_q p = rand(Normal(), length(q)) # random flick - p is 5 momentum current\_p = p 7 # make a half step for momentum at the beginning 8 p -= ε .\* ∇U(q) ./ 2 9 # initialize bookkeeping - saves trajectory 11 12 qtraj = [q]13 ptraj = [p] 14 # Alternate full steps for position and momentum 15 16 for  $i \in 1:L$ 17  $q += 0. \in * p$  # full step for the position # make a full step for the momentum except at the 18 19 end of trajectory 20 if i != L 21 p -= ε \* ∇U(q) 22 push!(ptraj, p) 23 end 24 push!(qtraj, q) 25 end 26 27 # Make a half step for momentum at the end  $p -= \varepsilon * \nabla U(q) / 2$ 28 29 push!(ptraj, p) 30 # negate momentum at the end of trajectory to make the 32 proposal symmetric 33 p = -p34 35 # evaluate potential and kinetic energies at the start 36 and the end of trajectory 37 current\_U = U(current\_q) 38 current\_K = sum(current\_p.^2)/2 39  $proposed_U = U(q)$ 40  $proposed_K = sum(p.^2)/2$ 41 42 # accept or reject the state at the end of trajectory, 43 returning either # the position at the end of the trajectory or the 44 45 initial position accept = (rand() < exp(current\_U - proposed\_U +</pre> current\_K - proposed\_K)) if accept  $current_q = q$ (q=current\_q, traj=qtraj, ptraj=ptraj, accept=accept)

#### Code 9.7 Plot the trace of HMC2



```
1 begin
       Random.seed!(1)
 3
       Q = (q=[-0.1, 0.2],)
       pr = 0.3
       step1 = 0.03
 5
       L = 11
       n_samples = 4
       p = scatter([Q.q[1]], [Q.q[2]], xlab="\mu x", ylab="\mu y")
 9
10
       for i \in 1:n\_samples
11
            Q = HMC2(U, \nabla U, step1, L, Q.q)
12
13
            if n_samples < 10</pre>
14
                cx, cy = [], []
                for j \in 1:L
15
                    K0 = sum(Q.ptraj[j].^2)/2
16
17
                    plot!(
18
                         [Q.traj[j][1], Q.traj[j+1][1]],
                         [Q.traj[j][2], Q.traj[j+1][2]],
20
                         lw=1+2*K0,
                         c=:black,
22
                         alpha=0.5
23
                    )
24
                    push!(cx, Q.traj[j+1][1])
25
                    push!(cy, Q.traj[j+1][2])
26
27
                scatter!(cx, cy, c=:white, ms=3)
28
29
            scatter!([Q.q[1]], [Q.q[2]], shape=(Q.accept ?
        :circle : :rect), c=:blue)
31
32
   end
```

### 9.4 Easy HMC: ulam. A package that calls Stan.

### Code 9.11 Load terrain ruggedness dataset

```
begin

d = CSV.read(sr_datadir("rugged.csv"), DataFrame)

dd = d[completecases(d, :rgdppc_2000),:]

dd[:,:log_gdp] = log.(dd.rgdppc_2000);

dd[:,:log_gdp_std] = dd.log_gdp / mean(dd.log_gdp)

dd[:,:rugged_std] = dd.rugged / maximum(dd.rugged)

dd[:,:cid] = @. ifelse(dd.cont_africa == 1, 1, 2);

end;
```

### Code 9.12 MAP() estimates of m8\_3

```
model_m8_3 (generic function with 2 methods)
 1 @model function model_m8_3(rugged_std, cid, log_gdp_std,
 2 rugged_mean)
       σ ~ Exponential()
       a ~ MvNormal([1, 1], 0.1)
       b ~ MvNormal([0, 0], 0.3)
       μ = @. a[cid] + b[cid] * (rugged_std - rugged_mean)
       log_gdp_std \sim MvNormal(\mu, \sigma)
   end
@time m8_3_MAP =
ModeResult with maximized lp of 137.00
[0.10948706712790776, 0.8865582229554612, 1.0505754634252704, 0.1
 1 @time m8_3_MAP = optimize(model_m8_3(dd.rugged_std, dd.cid,
    dd.\log_gdp_std, \bar{r}), MAP())
     14.415919 seconds (18.43 M allocations: 1.159 GiB,
    5.90% gc time, 99.93% compilation time)
 NamedArrays.NamedVector{Float64, Vector{Float64}, Tuple{Ordered
 1 coef(m8_3_MAP)
 (:values, :optim_result, :lp, :f)
 1 propertynames(m8_3_MAP)
 (:values, :optim_result, :lp, :f)
 1 fieldnames(typeof(m8_3_MAP))
 NamedArrays.NamedVector{Float64, Vector{Float64}, Tuple{Ordered
 1 m8_3_MAP.values
```

### 9.12.2 HMC/NUTS() estimates of model m8\_3

```
variable
                                 min
                                           median
                     mean
                                                        max
1 Symbol("a[1]") 0.886093
                              0.831898
                                          0.886028
                                                     0.937784
2 Symbol("a[2]") 1.05025
                              1.01955
                                          1.05013
                                                     1.08829
3 Symbol("b[1]") 0.131964
                              -0.0798954 0.132143
                                                     0.367039
4 Symbol("b[2]") -0.140506
                              -0.326315
                                          -0.142743 0.0488674
                   0.111486
                              0.0946746
                                          0.111045
                                                     0.137369
5 : \sigma
```

 NUTS with or without initial parameter estimates makes little difference.

```
variable
                                         median
                    mean
                                min
                                                     max
1 Symbol("a[1]") 0.886086
                             0.832369
                                        0.885509
                                                  0.940338
2 Symbol("a[2]") 1.05042
                             1.01933
                                        1.0506
                                                  1.08246
3 Symbol("b[1]") 0.132552
                                                  0.378509
                             -0.1447
                                        0.134152
4 Symbol("b[2]") -0.143058
                                                  0.0142253
                             -0.356798 -0.142808
5 : o
                  0.111456
                             0.0934895
                                        0.111501
                                                  0.130875
```

```
1 begin
2 @time m8_3_NUTSO_df =
DataFrame(sample(model_m8_3(dd.rugged_std, dd.cid,
dd.log_gdp_std, ₸), NUTS(), 1_000))
describe(m8_3_NUTSO_df)
end

100%

Found initial step size
€: 0.2

3.182691 seconds (2.37 M allocations: 496.417 Mi ②
B, 3.46% gc time, 57.56% compilation time)
```

### Code 9.13 Slim down datasets (remove unused columns from the data frame

#### For Turing this is not needed

	variable	mean	min	median	max	nmis
1	:log_gdp_std	1.0	0.721556	1.00718	1.28736	0
2	:rugged_std	0.21496	0.000483715	0.157933	1.0	0
3	:cid	1.71176	1	2.0	2	0
1	hegin					•

```
1 begin
2   dat_slim = dd[!,[:log_gdp_std, :rugged_std, :cid]]
3   describe(dat_slim)
4 end
```

# Code 9.14 m9\_1, was supposedly to call Stan to optimize. But it is the same as NUTS version of m8\_3, as both uses Turing.jl in Julia

• The following  $m9\_1$  result is almost identical to  $m8\_3\_NUTS0\_df$ 

#### One chain will be produced by default

```
1 @time m9_1 = sample(model_m8_3(dd.rugged_std, dd.cid, dd.log_gdp_std, r), NUTS(), 1000);

100%

Found initial step size

e: 0.2

0.941466 seconds (1.49 M allocations: 413.139 Mi   )

B, 7.85% gc time)
```

### Code 9.15 m9\_1 estimates

	variable	mean	min	median	max	
1	Symbol("a[1]")	0.887002	0.842436	0.887238	0.936285	
2	Symbol("a[2]")	1.05064	1.012	1.05053	1.08042	
3	Symbol("b[1]")	0.136678	-0.0797008	0.135572	0.370708	
4	Symbol("b[2]")	-0.143541	-0.34901	-0.14319	0.0339764	
5	<b>:</b> σ	0.111769	0.0959122	0.111605	0.132429	
					•	
1 describe(DataFrame(m9_1))						

### Code 9.16 Sample 4 chains simultaneously

For this to use multiple cores, julia has to be started with --threads 4 parameter, otherwise chains will be sampled sequentially

```
1 @time m9_1_4 = sample(model_m8_3(dd.rugged_std, dd.cid, dd.log_gdp_std, r̄), NUTS(), MCMCThreads(), 500, 4);

100%

Found initial step size
€: 0.2

Found initial step size
€: 0.025

Found initial step size
€: 0.2

Found initial step size
€: 0.05

3.882802 seconds (5.93 M allocations: 1.162 GiB, ②
4.84% gc time, 235.09% compilation time)
```

### Code 9.17 Combined chain results

# This shows combined chains statistics. To get information about individual chains, use $m9_1_4[:,:,1]$

	iteration	chain	σ	a[1]	a[2]	b[1]		
1	251	1	0.115365	0.862147	1.05205	0.00825668		
2	252	1	0.108155	0.916316	1.05186	0.172376		
3	253	1	0.115473	0.878241	1.05082	-0.00200212		
4	254	1	0.111862	0.912823	1.05784	0.255254		
5	255	1	0.113163	0.882214	1.03235	0.111389		
6	256	1	0.116453	0.873397	1.03836	0.106406		
7	257	1	0.108644	0.886925	1.03033	0.00341997		
8	258	1	0.115241	0.869615	1.0702	0.335698		
9	259	1	0.10633	0.906558	1.03387	0.0697053		
10	260	1	0.126833	0.865614	1.05916	0.125642		
	more							
4								
1	m9_1_4							
(5	00, 17, 4)							
1	1 size( <u>m9_1_4</u> )							

						_
	variable	mean	min	median	max	
1	Symbol("a[1]")	0.886732	0.832128	0.886847	0.942331	_
2	Symbol("a[2]")	1.05055	1.01846	1.05074	1.08512	1
3	Symbol("b[1]")	0.133572	-0.137065	0.133999	0.392913	1
4	Symbol("b[2]")	-0.143107	-0.315074	-0.142219	0.13312	1
5	<b>:</b> σ	0.111772	0.092706	0.111459	0.134023	1

1 describe(DataFrame(m9\_1\_4))

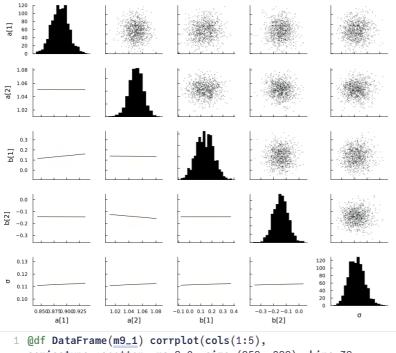
#### Code 9.18 Estimates of the 1st chain

	variable	mean	min	median	max	
1	Symbol("a[1]")	0.88628	0.843781	0.885974	0.930676	_
2	Symbol("a[2]")	1.05028	1.01846	1.05067	1.08177	
3	Symbol("b[1]")	0.134518	-0.117074	0.136525	0.345704	
4	Symbol("b[2]")	-0.142815	-0.303729	-0.143753	0.13312	
5	<b>:</b> σ	0.11199	0.0961834	0.111582	0.134023	

1 describe(DataFrame(m9\_1\_4[:,:,1]))

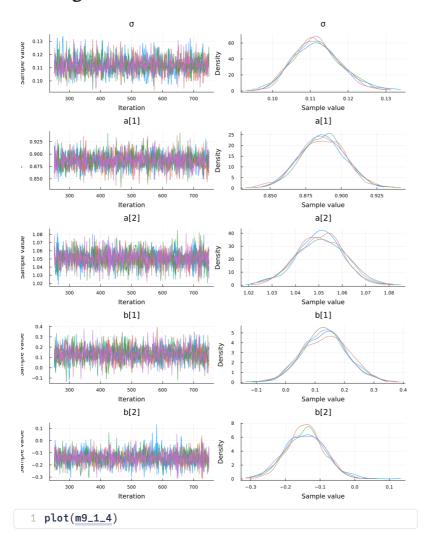
### Code 9.19 Correlation/histogram plots of all estimated parameters

- Little correlation among pairs.
- Multivariat normal is OK.

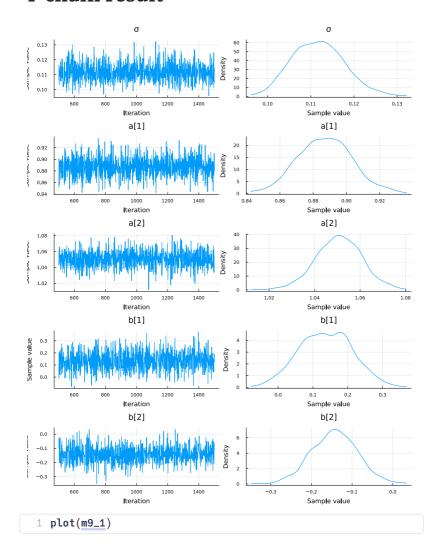


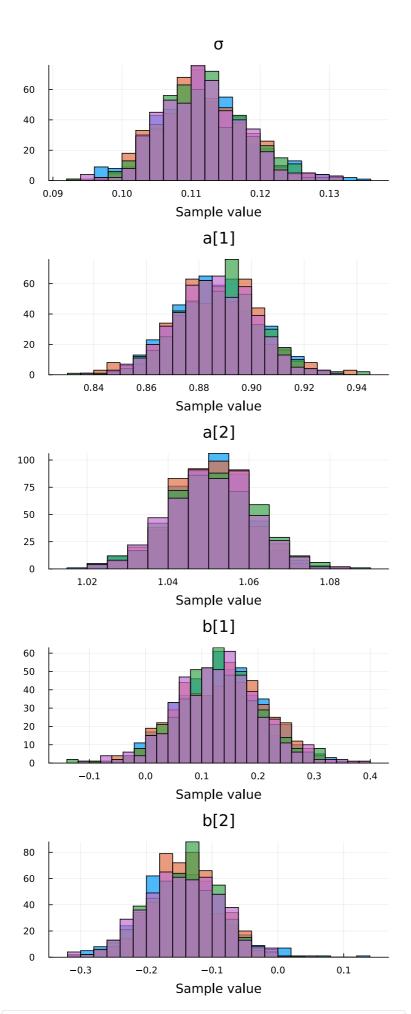
@df DataFrame(m9\_1) corrplot(cols(1:5),
seriestype=:scatter, ms=0.2, size=(950, 800), bins=30,
grid=false)

### Code 9.20 Check 4 chains: traceplot, histogram



### Code 9.21 Traceplot and histogram of 1-chain result





### 9.5 Care and feeding of your Markov chain.

# Codes 9.22 - 9.23 A poor MCMC chain with very flat prior and two data points.

• To make it diverging with Turing, we need to increase exp() argument (from 0.0001 to 1/0.0001).

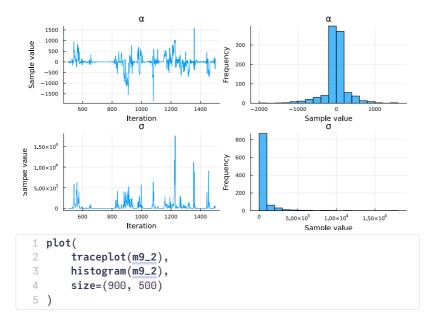
	variable	mean	min	median	max	nmissing
1	:α	-7.00748	-1837.35	-0.189339	1582.93	0
2	:σ	526.252	8.59881	76.6043	17567.1	0

```
1 let
      # To make it diverting with Turing, it was needed to
       increase exp() argument.
       Random.seed!(1)
      y = [-1., 1.]
 6
      @model function model_m9_2(y)
       \alpha \sim Normal(0, 1000)
9
           \sigma \sim Exponential(1/0.0001)
          y \sim Normal(\alpha, \sigma)
11
12
      global m9_2 = sample(model_m9_2(y), NUTS(), 1000)
       m9_2_df = DataFrame(m9_2)
       describe(m9_2_df)
   end
```

Found initial step size

 $\in$ : 0.00625

### Code 9.23 Check the estimates, traceplot, histogram



### Code 9.24 Narrow the prior

```
TaskLocalRNG()

1 Random.seed!(2)

model_m9_3 (generic function with 2 methods)

1 @model function model_m9_3(y)

2 α ~ Normal(1, 10)

3 σ ~ Exponential(1)

4 y ~ Normal(α, σ)

5 end
```

```
variable
                                       median
               mean
                             min
                                                    max
                                                            nm
            -0.00149585
                         -0.480793
                                     -0.00523852
                                                  0.403978
                                                            0
1 :α
             1.01593
                          0.754992
                                     1.00712
                                                  1.51101
2
   :σ
```

```
1 begin
2    m9_3 = sample(model_m9_3(y), NUTS(), 1000)
3    m9_3_df = DataFrame(m9_3)
4    describe(m9_3_df)
5 end
```

Found initial step size  $\epsilon$ : 0.2

100%

	parameters	ess	rhat	ess_per_sec
1	:α	1004.88	0.999312	530.842
2	<b>:</b> σ	983.644	1.00215	519.622

```
1 ess_rhat(m9_3)
```

### Code 9.25 - 9.26 Non-identifiable parameters and Flat priors

1 md"### Code 9.25 - 9.26 Non-identifiable parameters and Flat priors"

	variable	mean	min	median	max	nmissing	•
1	:a1	76.0651	-527.086	-17.116	1280.98	0	Fl
2	:a2	-76.1075	-1280.85	17.0966	526.908	0	Fl
3	<b>:</b> σ	1.02494	0.833166	1.01593	1.3076	0	Fl

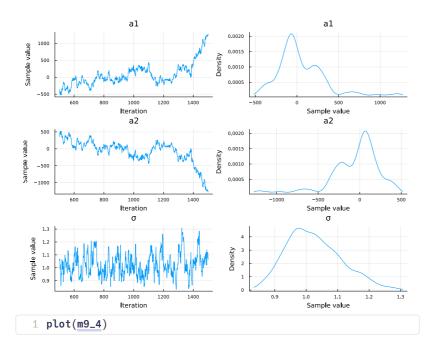
```
1 let
       Random.seed!(41)
       y = rand(Normal(), 100)
       Random.seed!(384)
 5
 6
 7
      @model function model_m9_4(y)
         a1 ~ Normal(0, 1000)
9
           a2 ~ Normal(0, 1000)
          \sigma \sim Exponential(1)
10
11
           \mu = a1 + a2
           y \sim Normal(\mu, \sigma)
12
13
      end
14
      global m9_4 = sample(model_m9_4(y), NUTS(), 1000)
15
       m9_4_df = DataFrame(m9_4)
16
17
       describe(m9_4_df)
18
19 end
```

100%

Found initial step size ∈: 0.000390625

	parameters	ess	rhat	ess_per_sec
1	:a1	3.65021	1.39632	0.201469
2	:a2	3.65033	1.39627	0.201475
3	<b>:</b> σ	62.8801	1.00418	3.47059

```
1 ess_rhat(m9_4)
```



### Code 9.27 Narrow the prior.

 HMC converges but the model is probably wrong due to large stddevs of estimates

```
TaskLocalRNG()

1 Random.seed!(384)

model_m9_5 (generic function with 2 methods)

1 @model function model_m9_5(y)
2    a1 ~ Normal(0, 10)
3    a2 ~ Normal(0, 10)
4    σ ~ Exponential(1)
5    μ = a1 + a2
6    y ~ Normal(μ, σ)
7 end
```

```
variable
               mean
                           min
                                    median
                                                 max
                                                         nmissing
             -0.453194
                         -21.3018
                                   -0.309591
                                               18.5956
             0.451404
                         -18.7207
                                   0.355443
                                               21.3758
                                                         0
   :a2
             1.00409
                         0.748858
                                   0.99868
                                               1.46932
                                                         0
3
   :0
```

Found initial step size ∈: 0.0125

100%

	parameters	ess	rhat	ess_per_sec
1	:a1	206.309	1.01768	52.4426
2	:a2	205.848	1.01787	52.3254
3	<b>:</b> σ	456.427	0.99935	116.021



