StochMCMC.jl Documentation

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Contents

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Requires julia releases 0.4.1 or later

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Website https://github.com/alstat/StochMCMC.jl

A julia package for Stochastic Gradient Markov Chain Monte Carlo. The package is part of my master's thesis entitled **Bayesian Autoregressive Distributed Lag** *via* **Stochastic Gradient Hamiltonian Monte Carlo** or **BADL-SGHMC**, under the supervision of **Dr. Joselito C. Magadia** of School of Statistics, University of the Philippines Diliman. This work aims to accommodate other Stochastic Gradient MCMCs in the near future.

CHAPTER 1

Installation

To install the package, run the following

```
Pkg.clone("https://github.com/alstat/StochMCMC.jl")
```

And to load the package, run

```
using StochMCMC
```

Contents

Metropolis-Hasting

Implementation of the Metropolis-Hasting sampler for Bayesian inference.

MH(*logposterior::Function*, *proposal::Function*, *init_est::Array{Float64}*, *d::Int64*)
Construct a `Sampler` object for Metropolis-Hasting sampling.

Arguments

- `logposterior` : the logposterior of the parameter of interest.
- `proposal` : the proposal distribution for random steps of the MCMC.
- `init_est` : the initial/starting value for the markov chain.
- `d` : the dimension of the posterior distribution.

Value

Returns a `MH` type object.

Example

In order to illustrate the modeling, the data is simulated from a simple linear regression expectation function. That is the model is given by

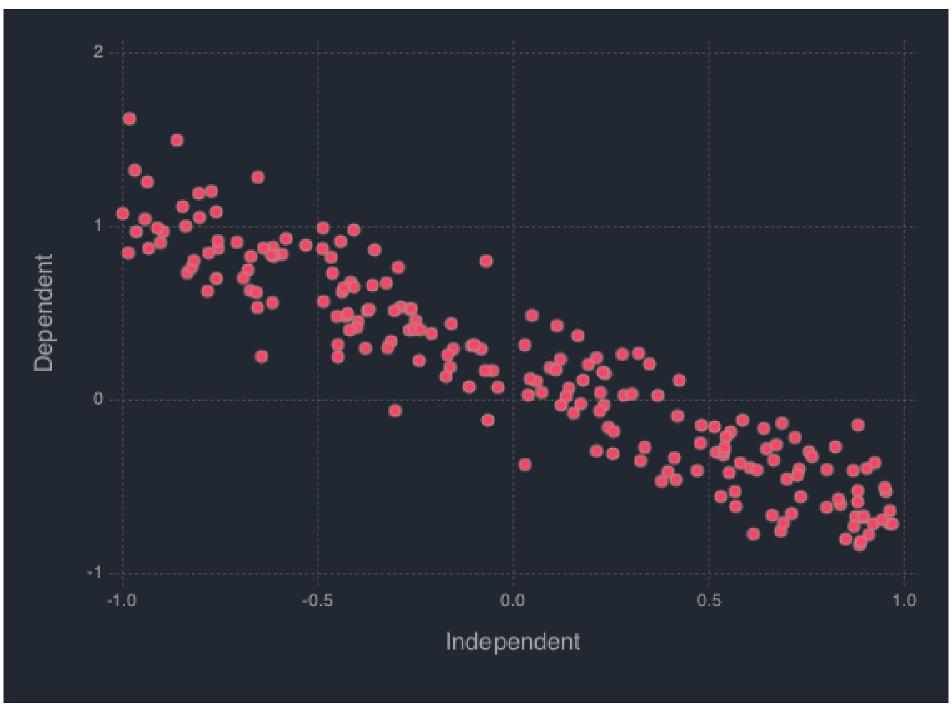
```
y_i = w_0 + w_1 x_i + e_i,    e_i ~ N(0, 1 / a)
```

To do so, let `B = [w_0, w_1]' = [.2, -.9]', a = 1 / 5`. Generate 200 hypothetical data:

```
using DataFrames
using Distributions
using Gadfly
using StochMCMC
Gadfly.push_theme(:dark)

srand(123);

# Define data parameters
w0 = -.3; w1 = -.5; stdev = 5.; a =  1 / stdev

# Generate Hypothetical Data
n = 200;
x = rand(Uniform(-1, 1), n);
A = [ones(length(x)) x];
B = [w0; w1];
f = A * B;
y = f + rand(Normal(0, a), n);

my_df = DataFrame(Independent = round(x, 4), Dependent = round(y, 4));
```

Next is to plot this data which can be done as follows:

```
plot(my_df, x = :Independent, y = :Dependent)
```



In order to proceed with the Bayesian inference, the parameters of the model is considered to be random modeled by a standard Gaussian distribution. That is, `B ~ N(0, I)`, where `0` is the zero vector. The likelihood of the data is given by,

```
L(w|[x, y], b) = _{i=1}^n N([x_i, y_i]|w, b)
```

Thus the posterior is given by,

```
P(w|[x, y])  P(w)L(w|[x, y], b)
```

To start programming, define the probabilities

```
"""
The log prior function is given by the following codes:
"""
function logprior(theta::Array{Float64}; mu::Array{Float64} = zero_vec,␣
↪s::Array{Float64} = eye_mat)
  w0_prior = log(pdf(Normal(mu[1, 1], s[1, 1]), theta[1]))
  w1_prior = log(pdf(Normal(mu[2, 1], s[2, 2]), theta[2]))
   w_prior = [w0_prior w1_prior]

  return w_prior |> sum
end

"""
The log likelihood function is given by the following codes:
"""
function loglike(theta::Array{Float64}; alpha::Float64 = a, x::Array{Float64}
↪ = x, y::Array{Float64} = y)
  yhat = theta[1] + theta[2] * x

  likhood = Float64[]
  for i in 1:length(yhat)
    push!(likhood, log(pdf(Normal(yhat[i], alpha), y[i])))
  end

  return likhood |> sum
end

"""
The log posterior function is given by the following codes:
"""
function logpost(theta::Array{Float64})
  loglike(theta, alpha = a, x = x, y = y) + logprior(theta, mu = zero_vec, s␣
↪= eye_mat)
end
```

To start the estimation, define the necessary parameters.

```
# Hyperparameters
zero_vec = zeros(2)
eye_mat = eye(2)
```

Run the MCMC:

```
srand(123);
mh_object = MH(logpost; init_est = zeros(2));
chain1 = mcmc(mh_object, r = 10000);
```

Extract the estimate

```
burn_in = 100;
thinning = 10;

# Expetation of the Posterior
est1 = mapslices(mean, chain1[(burn_in + 1):thinning:end, :], [1]);
est1
# 1×2 Array{Float64,2}:
#  -0.313208  -0.46376
```

Hamiltonian Monte Carlo

Implementation of the Hamiltonian Monte Carlo sampler for Bayesian inference.

HMC (*U::Function*, *K::Function*, *dU::Function*, *dK::Function*, *init_est::Array{Float64}*, *d::Int64*)

Construct a `Sampler` object for Hamiltonian Monte Carlo sampling.

Arguments

- `U` : the potential energy or the negative log posterior of the parameter of interest.
- `K` : the kinetic energy or the negative exponential term of the log auxiliary distribution.
- `dU` : the gradient or first derivative of the potential energy `U`.
- `dK` : the gradient or first derivative of the kinetic energy `K`.
- `init_est` : the initial/starting value for the markov chain.
- `d` : the dimension of the posterior distribution.

Value

Returns a `HMC` type object.

Example

In order to illustrate the modeling, the data is simulated from a simple linear regression expectation function. That is the model is given by

```
y_i = w_0 + w_1 x_i + e_i,   e_i ~ N(0, 1 / a)
```

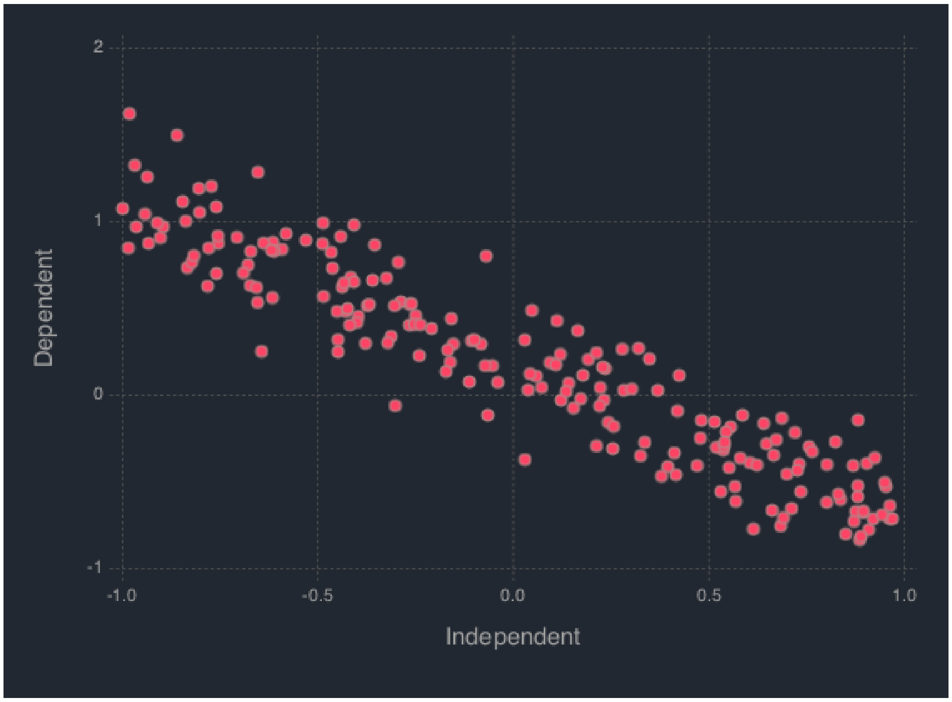
To do so, let `B = [w_0, w_1]' = [.2, -.9]', a = 1 / 5`. Generate 200 hypothetical data:

```
using DataFrames
using Distributions
using Gadfly
using StochMCMC
Gadfly.push_theme(:dark)

srand(123);

# Define data parameters
w0 = -.3; w1 = -.5; stdev = 5.; a =  1 / stdev

# Generate Hypothetical Data
n = 200;
x = rand(Uniform(-1, 1), n);
A = [ones(length(x)) x];
B = [w0; w1];
f = A * B;
```

```
y = f + rand(Normal(0, a), n);

my_df = DataFrame(Independent = round(x, 4), Dependent = round(y, 4));
```

Next is to plot this data which can be done as follows:

```
plot(my_df, x = :Independent, y = :Dependent)
```



In order to proceed with the Bayesian inference, the parameters of the model is considered to be random modeled by a standard Gaussian distribution. That is, `B ~ N(0, I)`, where `0` is the zero vector. The likelihood of the data is given by,

```
L(w|[x, y], b) = _{i=1}^n N([x_i, y_i]|w, b)
```

Thus the posterior is given by,

```
P(w|[x, y])  P(w)L(w|[x, y], b)
```

To start programming, define the probabilities

```
"""
The log prior function is given by the following codes:
"""
function logprior(theta::Array{Float64}; mu::Array{Float64} = zero_vec,
↪s::Array{Float64} = eye_mat)
  w0_prior = log(pdf(Normal(mu[1, 1], s[1, 1]), theta[1]))
  w1_prior = log(pdf(Normal(mu[2, 1], s[2, 2]), theta[2]))
   w_prior = [w0_prior w1_prior]

  return w_prior |> sum
end
```

```
"""
The log likelihood function is given by the following codes:
"""
function loglike(theta::Array{Float64}; alpha::Float64 = a, x::Array{Float64}
↪ = x, y::Array{Float64} = y)
  yhat = theta[1] + theta[2] * x

  likhood = Float64[]
  for i in 1:length(yhat)
    push!(likhood, log(pdf(Normal(yhat[i], alpha), y[i])))
  end

  return likhood |> sum
end

"""
The log posterior function is given by the following codes:
"""
function logpost(theta::Array{Float64})
  loglike(theta, alpha = a, x = x, y = y) + logprior(theta, mu = zero_vec, s␣
↪= eye_mat)
end
```

To start the estimation, define the necessary parameters

```
# Hyperparameters
zero_vec = zeros(2)
eye_mat = eye(2)
```

Setup the necessary paramters including the gradients. The potential energy is the negative logposterior given by `U`, the gradient is `dU`; the kinetic energy is the standard Gaussian function given by `K`, with gradient `dK`. Thus,

```
U(theta::Array{Float64}) = - logpost(theta);
K(p::Array{Float64}; Σ = eye(length(p))) = (p' * inv(Σ) * p) / 2;
function dU(theta::Array{Float64}; alpha::Float64 = a, b::Float64 = eye_
↪mat[1, 1])
  [-alpha * sum(y - (theta[1] + theta[2] * x));
   -alpha * sum((y - (theta[1] + theta[2] * x)) .* x)] + b * theta
end
dK(p::AbstractArray{Float64}; Σ::Array{Float64} = eye(length(p))) = inv(Σ) *␣
↪p;
```

Run the MCMC:

```
srand(123);
HMC_object = HMC(U, K, dU, dK, zeros(2), 2);
chain2 = mcmc(HMC_object, leapfrog_params = Dict([: => .09, :τ => 20]), r =␣
↪10000);
```

Extract the estimate

```
est2 = mapslices(mean, chain2[(burn_in + 1):thinning:end, :], [1]);
est2
# 1×2 Array{Float64,2}:
#  -0.307151  -0.458954
```

Stochastic Gradient Hamiltonian Monte Carlo

Implementation of the Hamiltonian Monte Carlo sampler for Bayesian inference.

SGHMC(*dU::Function, dK::Function, dKΣ::Array{Float64}, C::Array{Float64}, V::Array{Float64}, init_est::Array{Float64}, d::Int64*)

Construct a `Sampler` object for Hamiltonian Monte Carlo sampling.

Arguments

- `dU` : the gradient or first derivative of the potential energy `U`.
- `dK` : the gradient or first derivative of the kinetic energy `K`.
- `dKΣ` : the variance-covariance matrix in the gradient of the kinetic energy `dK`, this is set to identity matrix for the case of standard Gaussian distribution.
- `C` : the matrix factor in the frictional force term.
- `V` : the matrix factor in the random force term.
- `init_est` : the initial/starting value for the markov chain.
- `d` : the dimension of the posterior distribution.

Value

Returns a `SGHMC` type object.

Example

In order to illustrate the modeling, the data is simulated from a simple linear regression expectation function. That is the model is given by

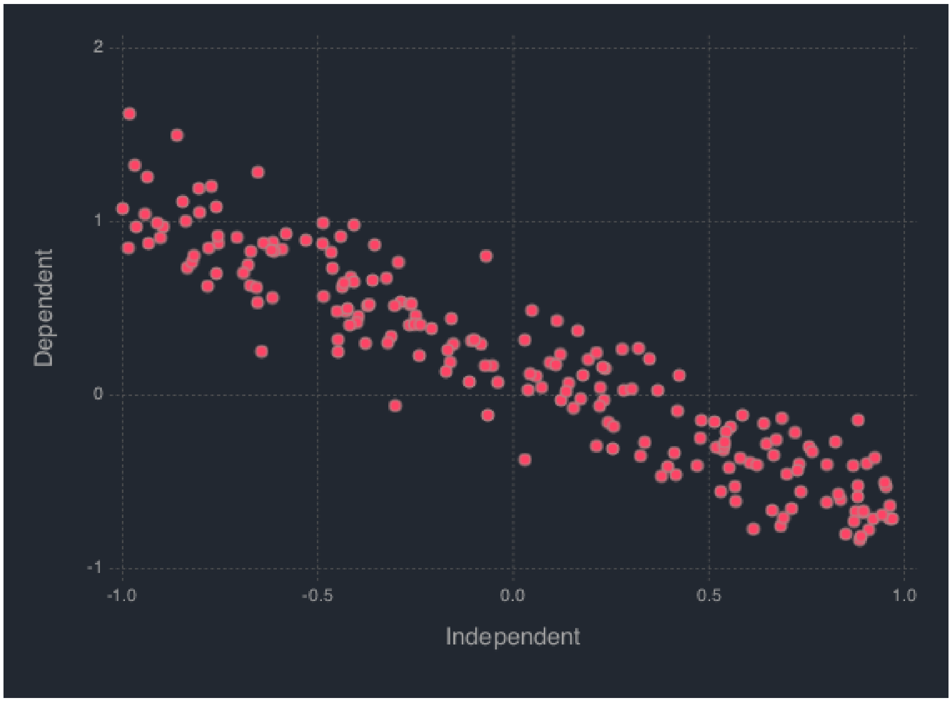
```
y_i = w_0 + w_1 x_i + e_i,    e_i ~ N(0, 1 / a)
```

To do so, let `B = [w_0, w_1]' = [.2, -.9]', a = 1 / 5`. Generate 200 hypothetical data:

```
using DataFrames
using Distributions
using Gadfly
using StochMCMC
Gadfly.push_theme(:dark)

srand(123);

# Define data parameters
w0 = -.3; w1 = -.5; stdev = 5.; a =  1 / stdev

# Generate Hypothetical Data
n = 200;
x = rand(Uniform(-1, 1), n);
A = [ones(length(x)) x];
B = [w0; w1];
f = A * B;
y = f + rand(Normal(0, a), n);

my_df = DataFrame(Independent = round(x, 4), Dependent = round(y, 4));
```

Next is to plot this data which can be done as follows:

```
plot(my_df, x = :Independent, y = :Dependent)
```



In order to proceed with the Bayesian inference, the parameters of the model is considered to be random modeled by a standard Gaussian distribution. That is, `B ~ N(0, I)`, where `0` is the zero vector. The likelihood of the data is given by,

```
L(w|[x, y], b) = _{i=1}^n N([x_i, y_i]|w, b)
```

Thus the posterior is given by,

```
P(w|[x, y])  P(w)L(w|[x, y], b)
```

To start programming, define the probabilities

```
"""
The log prior function is given by the following codes:
"""
function logprior(theta::Array{Float64}; mu::Array{Float64} = zero_vec,
↪s::Array{Float64} = eye_mat)
  w0_prior = log(pdf(Normal(mu[1, 1], s[1, 1]), theta[1]))
  w1_prior = log(pdf(Normal(mu[2, 1], s[2, 2]), theta[2]))
   w_prior = [w0_prior w1_prior]

  return w_prior |> sum
end

"""
The log likelihood function is given by the following codes:
"""
function loglike(theta::Array{Float64}; alpha::Float64 = a, x::Array{Float64}
↪ = x, y::Array{Float64} = y)
  yhat = theta[1] + theta[2] * x
```

```
  likhood = Float64[]
  for i in 1:length(yhat)
    push!(likhood, log(pdf(Normal(yhat[i], alpha), y[i])))
  end

  return likhood |> sum
end

"""
The log posterior function is given by the following codes:
"""
function logpost(theta::Array{Float64})
  loglike(theta, alpha = a, x = x, y = y) + logprior(theta, mu = zero_vec, s␣
↪= eye_mat)
end
```

To start the estimation, define the necessary parameters

```
# Hyperparameters
zero_vec = zeros(2)
eye_mat = eye(2)
```

Setup the necessary paramters including the gradients.

```
function dU(theta::Array{Float64}; alpha::Float64 = a, b::Float64 = eye_
↪mat[1, 1])
  [-alpha * sum(y - (theta[1] + theta[2] * x));
   -alpha * sum((y - (theta[1] + theta[2] * x)) .* x)] + b * theta
end
dK(p::AbstractArray{Float64}; Σ::Array{Float64} = eye(length(p))) = inv(Σ) *␣
↪p;
```

Define the gradient noise and other parameters of the SGHMC:

```
function dU_noise(theta::Array{Float64}; alpha::Float64 = a, b::Float64 =␣
↪eye_mat[1, 1])
  [-alpha * sum(y - (theta[1] + theta[2] * x));
   -alpha * sum((y - (theta[1] + theta[2] * x)) .* x)] + b * theta + randn(2,
↪1)
end
```

Run the MCMC:

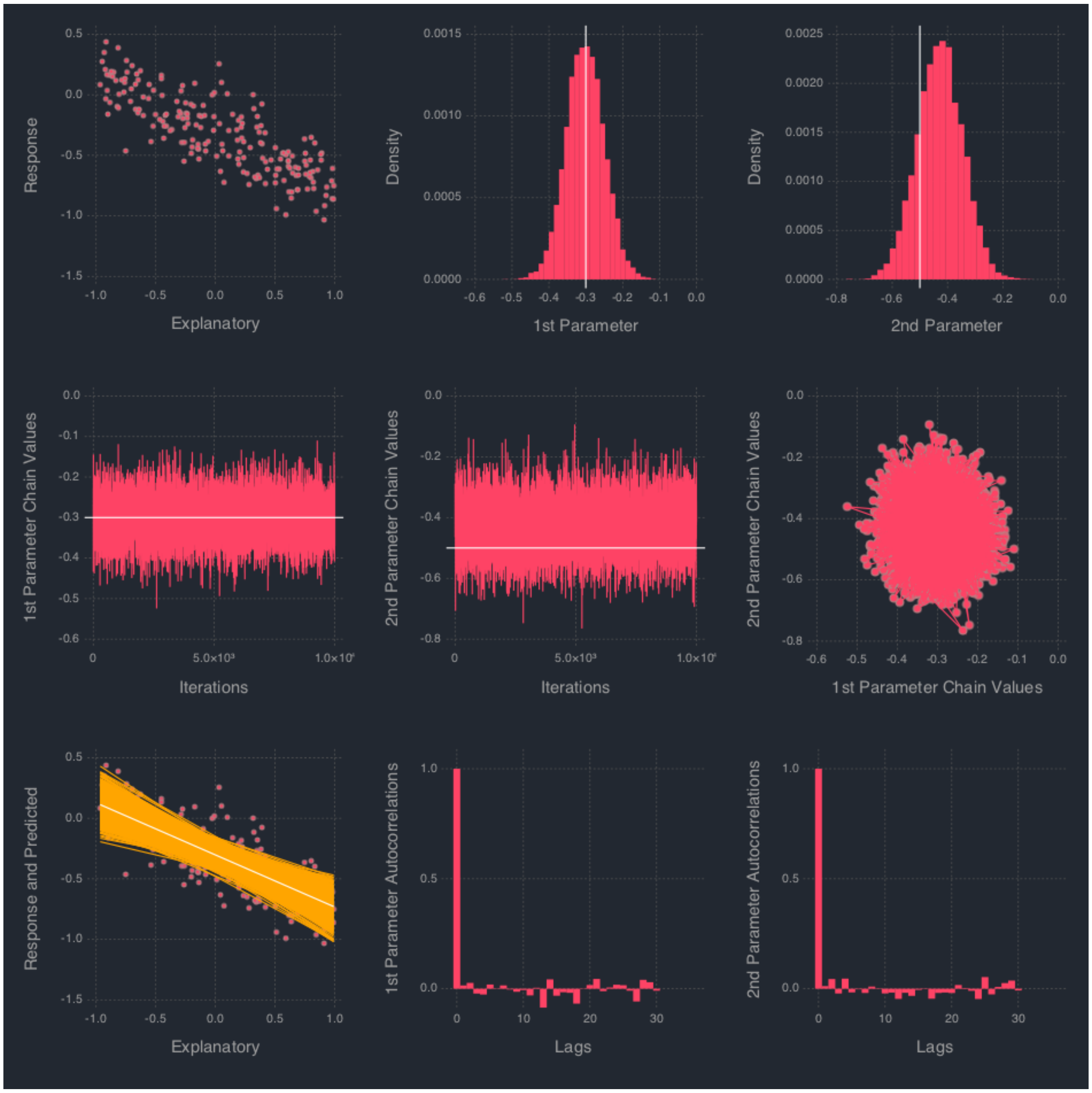
```
srand(123);
SGHMC_object = SGHMC(dU_noise, dK, eye(2), eye(2), eye(2), [0; 0], 2.);
chain3 = mcmc(SGHMC_object, leapfrog_params = Dict([: => .09, :τ => 20]), r␣
↪= 10000);
```

Extract the estimate:

```
est3 = mapslices(mean, chain3[(burn_in + 1):thinning:end, :], [1]);
est3
# 1×2 Array{Float64,2}:
#  -0.302745  -0.430272
```

Plot it

```
my_df_sghmc = my_df;
my_df_sghmc[:Yhat] = mapslices(mean, chain3[(burn_in + 1):thinning:end, :],␣
↪[1])[1] + mapslices(mean, chain3[(burn_in + 1):thinning:end, :], [1])[2] *␣
↪my_df[:Independent];

for i in (burn_in + 1):thinning:10000
    my_df_sghmc[Symbol("Yhat_Sample_" * string(i))] = chain3[i, 1] +␣
↪chain3[i, 2] * my_df_sghmc[:Independent]
end

my_stack_sghmc = DataFrame(X = repeat(Array(my_df_sghmc[:Independent]),␣
↪outer = length((burn_in + 1):thinning:10000)),
                           Y = repeat(Array(my_df_sghmc[:Dependent]), outer␣
↪= length((burn_in + 1):thinning:10000)),
                           Var = Array(stack(my_df_sghmc[:, 4:end])[1]),
                           Val = Array(stack(my_df_sghmc[:, 4:end])[2]));
ch1cor_df = DataFrame(x = collect(0:1:(length(autocor(chain3[(burn_in +␣
↪1):thinning:10000, 1])) - 1)),
                      y1 = autocor(chain3[(burn_in + 1):thinning:10000, 1]),
                      y2 = autocor(chain3[(burn_in + 1):thinning:10000, 2]));

p0 = plot(my_df, x = :Independent, y = :Dependent, Geom.point, style(default_
↪point_size = .05cm), Guide.xlabel("Explanatory"), Guide.ylabel("Response
↪"));
p1 = plot(DataFrame(chain3), x = :x1, xintercept = [-.3], Geom.vline(color =␣
↪colorant"white"), Geom.histogram(bincount = 30, density = true), Guide.
↪xlabel("1st Parameter"), Guide.ylabel("Density"));
p2 = plot(DataFrame(chain3), x = :x2, xintercept = [-.5], Geom.vline(color =␣
↪colorant"white"), Geom.histogram(bincount = 30, density = true), Guide.
↪xlabel("2nd Parameter"), Guide.ylabel("Density"));
p3 = plot(DataFrame(chain3), x = collect(1:nrow(DataFrame(chain3))), y = :x1,
↪ yintercept = [-.3], Geom.hline(color = colorant"white"), Geom.line, Guide.
↪xlabel("Iterations"), Guide.ylabel("1st Parameter Chain Values"));
p4 = plot(DataFrame(chain3), x = collect(1:nrow(DataFrame(chain1))), y = :x2,
↪ yintercept = [-.5], Geom.hline(color = colorant"white"), Geom.line, Guide.
↪xlabel("Iterations"), Guide.ylabel("2nd Parameter Chain Values"));
p5 = plot(DataFrame(chain3), x = :x1, y = :x2, Geom.path, Geom.point, Guide.
↪xlabel("1st Parameter Chain Values"), Guide.ylabel("2nd Parameter Chain␣
↪Values"));
p6 = plot(layer(my_df_sghmc, x = :Independent, y = :Yhat, Geom.line,␣
↪style(default_color = colorant"white")),
          layer(my_stack_sghmc, x = :X, y = :Val, group = :Var, Geom.line,␣
↪style(default_color = colorant"orange")),
          layer(my_df_sghmc, x = :Independent, y = :Dependent, Geom.point,␣
↪style(default_point_size = .05cm)),
          Guide.xlabel("Explanatory"), Guide.ylabel("Response and Predicted
↪"));
p7 = plot(ch1cor_df, x = :x, y = :y1, Geom.bar, Guide.xlabel("Lags"), Guide.
↪ylabel("1st Parameter Autocorrelations"), Coord.cartesian(xmin = -1, xmax␣
↪= 36, ymin = -.05, ymax = 1.05));
p8 = plot(ch1cor_df, x = :x, y = :y2, Geom.bar,  Guide.xlabel("Lags"), Guide.
↪ylabel("2nd Parameter Autocorrelations"), Coord.cartesian(xmin = -1, xmax␣
↪= 36, ymin = -.05, ymax = 1.05));

vstack(hstack(p0, p1, p2), hstack(p3, p4, p5), hstack(p6, p7, p8))
```



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