Computational modeling in RStan --basics and practices

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Self introduction

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 University
- Education: BSc of Human Resource Management in SWUFE; Exchange student in UCR
- Research Interests: Interested in decision making, learning (reinforcement learning, social learning and group learning) via computational neuroscience approach.



This tutorial is not to:

- Introduce how to create a good model;
- Introduce a specific family of models;

But we expect to:

- Develop an interest in combining computational models in your own research
- Know a basic routine to conduct computational model work
- Use MCMC and Rstan to fit your own models

Content

Basics about computational modeling

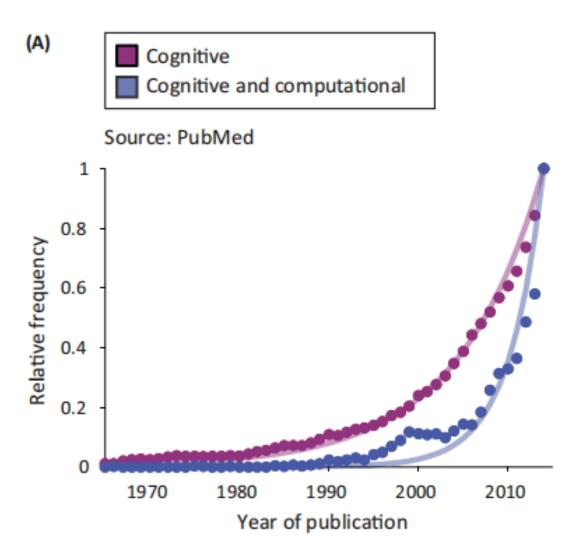
Standard approaches of modeling

MCMC and Rstan

Practices: implementing a reinforcement learning model in Rstan

Basics about computational modeling

- What is computational modeling?
 - computational modeling is a technique that applies mathematical models and computer science in complex systems (e.g., ecological environment, biology, physics and etc.,) to better understand the underlying mechanisms.
- What can computational modeling relate to psychology and neuroscience?
 - better understand behavioral mechanisms (choice behavior, RT, eye movement and etc.)
 - better understand neural mechanisms (DCM, neuronal spikes and etc.)
- Why is it special?
 - high precision on predicting data
 - inference on laten variables (states)
 - capability of coping large-scale, high-dimensional data
 - **—** ...

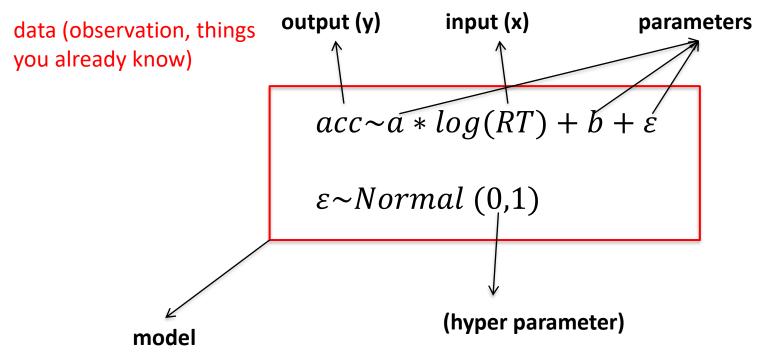


Computational cognitive research is growing rapidly, due to the development of machine learning techniques and AI.

New interdisciplinary fields emerged:

- neuroeconomics
- computational neuroscience
- computational psychiatry
- ...

- Basic concepts of a computational model:
 - suppose you have a set of data concerning RT and choice accuracy....



goal (things you wish to know...)

relationship (hypotheis, things you think you know)

Model fitting:

- get to the goal
- optimize the parameters that best suit to your data, given your model
- how to optimize: minimize the errors between data and model predictions, by adjusting the parameters.

Cost functions (measurement of 'errors'):

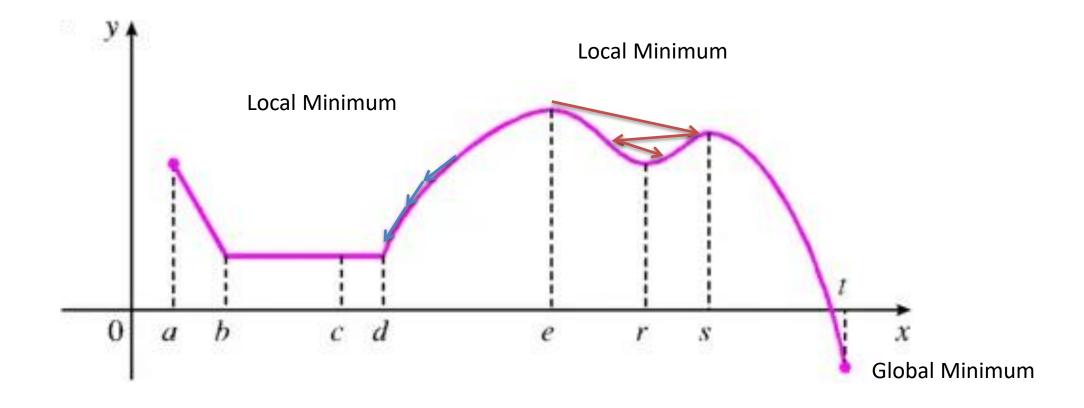
- mean squared error (MSE)
- log-likelihood
- TD error (in deep reinforcement learning)
- dis-similarities

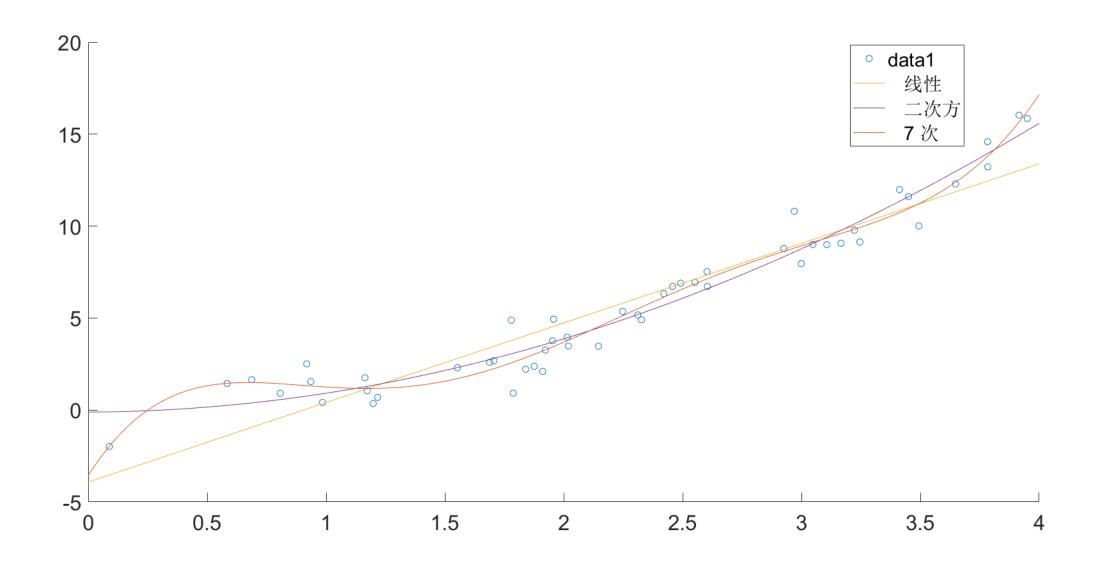
— ...

Two general approaches of estimating the parameters:

- iterative approaches
 - » Gradient descent (MLE), Variational Bayesian Analysis, (mean-field, newton, ...)
 - » Quick computing, but may reach a local minimum

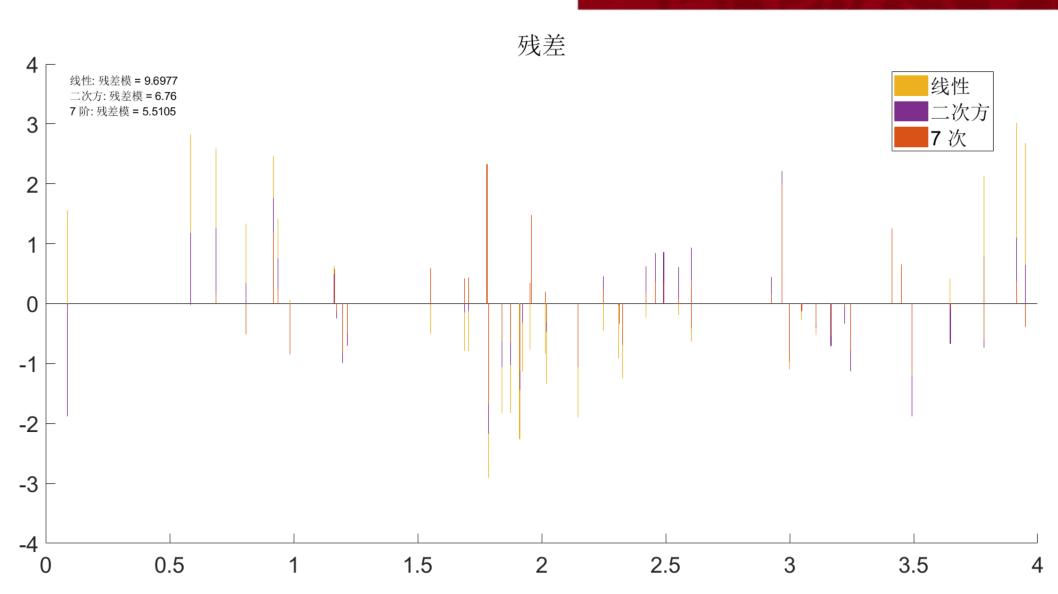
- sampling approaches
 - » MCMC, Gibson sampling, Grid search...
 - » Computationally expensive, hard to sample for extreme complex models





北京大学心理与认知科学学院

School of Psychological and Cognitive Sciences, Peking University



First order polynomial (Linear regression)

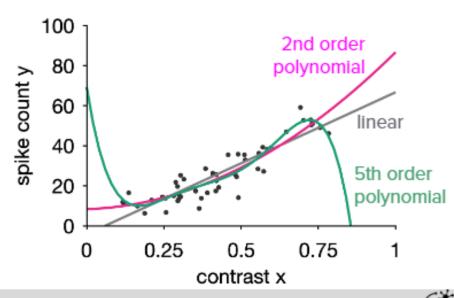
 $y = \theta_1 x + \theta_0$

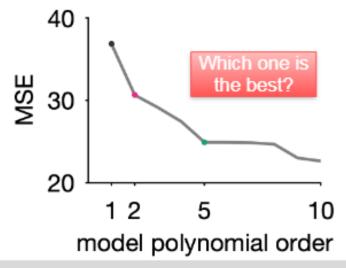
Second order polynomial

$$y = \theta_2 x^2 + \theta_1 x + \theta_0$$

Higher order polynomial

$$y = \sum_{p=0}^{5} \theta_p x^p$$





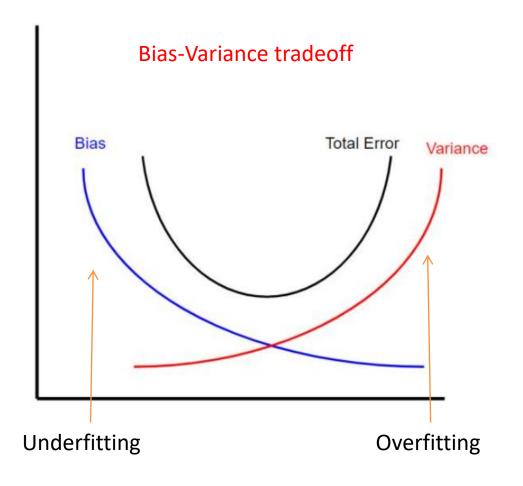
Angi Wu • Model Fitting

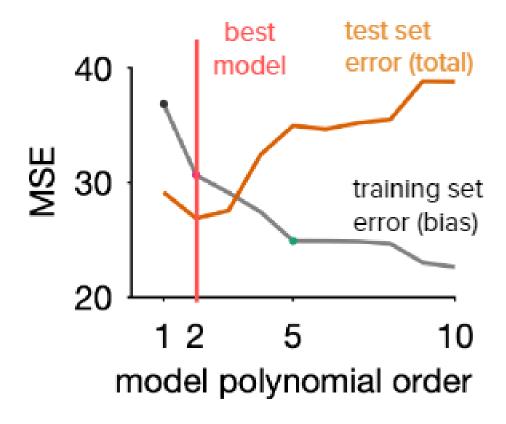
Week 1 • Day 3 • Tutorial 5

45

Neuromatch Academy Computational Neuroscience Summer school

Overfitting!





• How to avoid overfitting?

- Train with more data!
- Machine learning:
 - Regularization
 - Cross-validation
 - Dropout
 - •
- Psychology:
 - Model comparison (a simpler model)
 - Information criteria (AIC, BIC, DIC, LOOIC...)

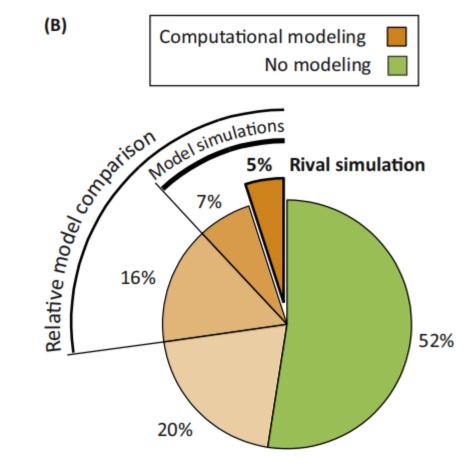
Summary

- What is computational modeling? Why do we need computational modeling?
- Basic concepts of a model
- What is model fitting? Two general approaches for fitting.
- What is overfitting? Why do we need to avoid overfitting?

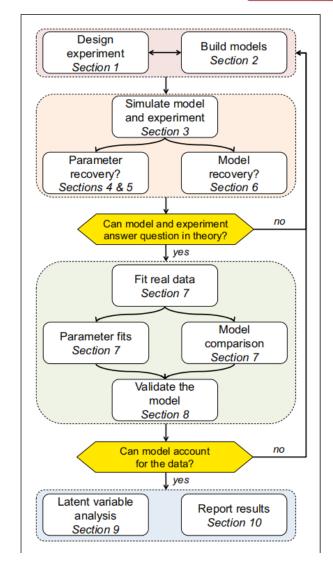
Standard approaches of modeling

Modeling requires standards

 Like all other tools, computational modeling requires golden standards to be used.

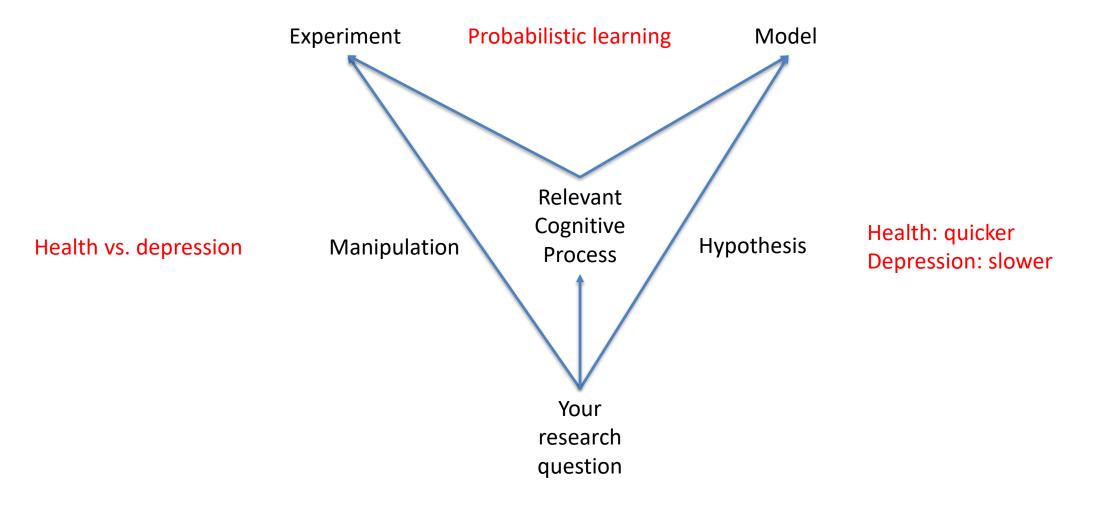


Ten Simple Rules



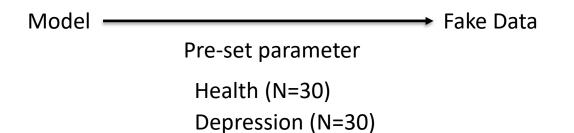
Wilson, Colins, 2019

Step 1: experiment vs. model



e.g. What is difference between healthy people and those with depression in probabilistic learning?

Step2: Simulation



Model: Reinforcement learning model

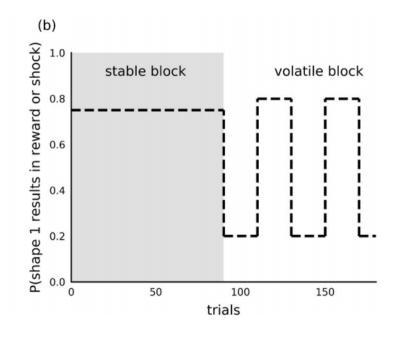
$$PE = R - v_{i,t}$$
 Prediction Error

$$v_{i,t+1} = v_{i,t} + \alpha * PE$$
 α :learning rate

$$P(i, t + 1) = \frac{e^{v_{i,t+1}}}{\sum e^{v_{i,t+1}}}$$

Rescorla, R. A., & Wagner, A. R. (1972)

Environment(Task): Probability reversal learning task



Step-by-Step Simulation

1.Define the environment

```
#adopt WSLS strategy
p_reward1=c(0.8,0.2)
p_reward2=c(0.2,0.8)
```

2. Define (an) agent(s)

- Action(choice)
- Reward(feedback)
- Policy (strategy)
- Hidden States...

```
if (t==1){
  choice[t]=sample(c(1:2), size = 1, replace = T, prob = p_choose)
```

3. Define the environment response

tmp_reward=sample(c(1,-1), size = 1, replace = T, prob = p_reward[choice[t],])
accumulated_reward2[t]=accumulated_reward2[t-1]+tmp_reward

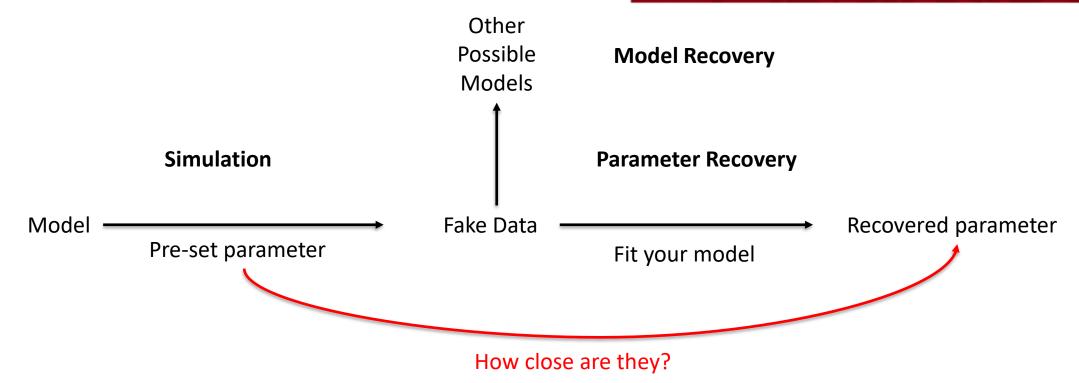
4.Set and run the simulation process!

for-loop: trials and agents

5. Analyze and visualize your simulated data!

v[choice[t]]=v[choice[t]]+lr*(tmp_reward-v[choice[t]])

Model Validation



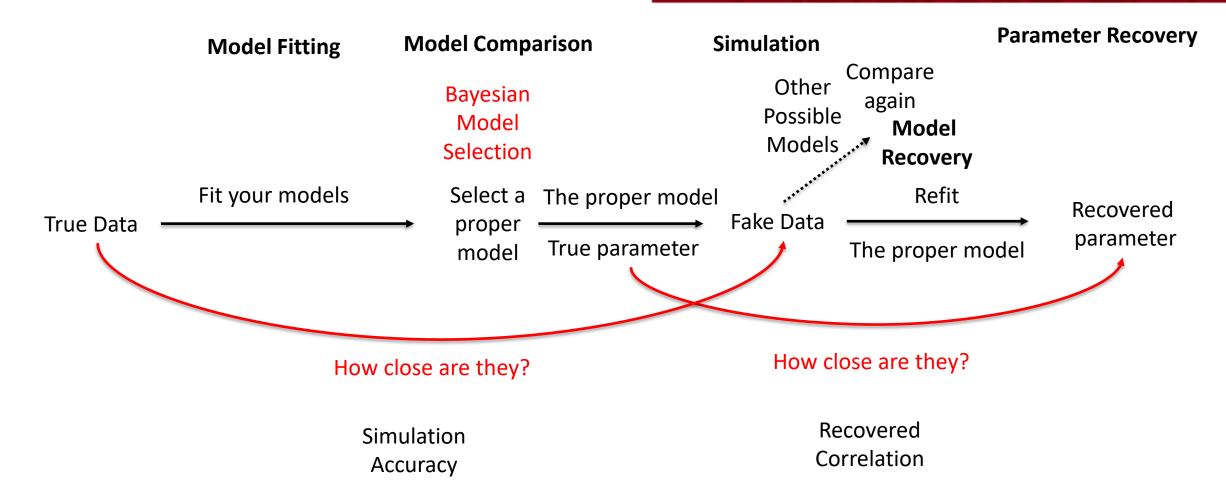
Collect your own data

If your model is fine with your experiment...

Run the experiment!

Why not run your model while collecting your data?

After you collect your data



Analyze results from your model

Your parameters:

- Compare different parameters across your conditions;
- Correlate your parameters with something you measure;
- Even more flexible analysis approach (depends on your questions)

Your latent variables:

- Value
- Prediction error/ TD error
- Compare, correlate, cluster.....
- Also more flexible analysis approach

Report your model result

- What your model (usually winning model) reflects about the cognitive, psychological or neuronal process?
- What your parameters mean? How are they bounded?
- Your fitting methods (specific details)
- Your parameter results (usually winning model); frequentist vs. Bayesian.
- Model Comparison (the criterion you choose, BMS result)
- How well is your model fitted, simulated(predicted) and recovered?
- How's your model relevant analysis conducted?
- How are the results above able to help answer your questions?

Model Philosophy

Three levels of description (David Marr, 1982)

Computational

Why do things work the way they do? What is the goal of the computation? What are the unifying principles?

Algorthmic

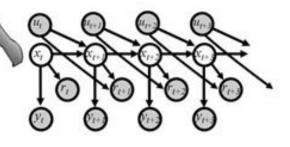
What representations can implement such computations?
How does the choice of representations determine the algorithm?

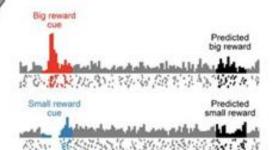
Implementational

How can such a system be built in hardware?
How can neurons carry out the computations?

maximize:

$$R_t = r_{t+1} + r_{t+2} + \dots + r_T$$

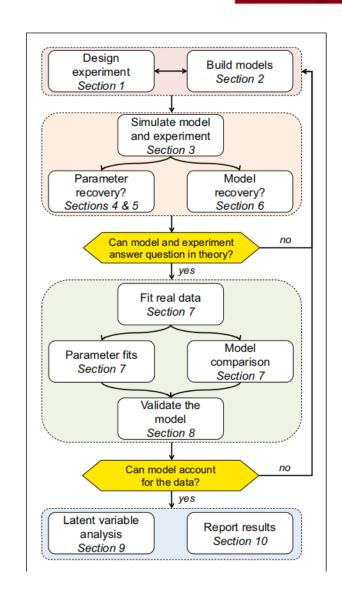




All models are wrong, **but** some are useful......
---- George E. P. Box

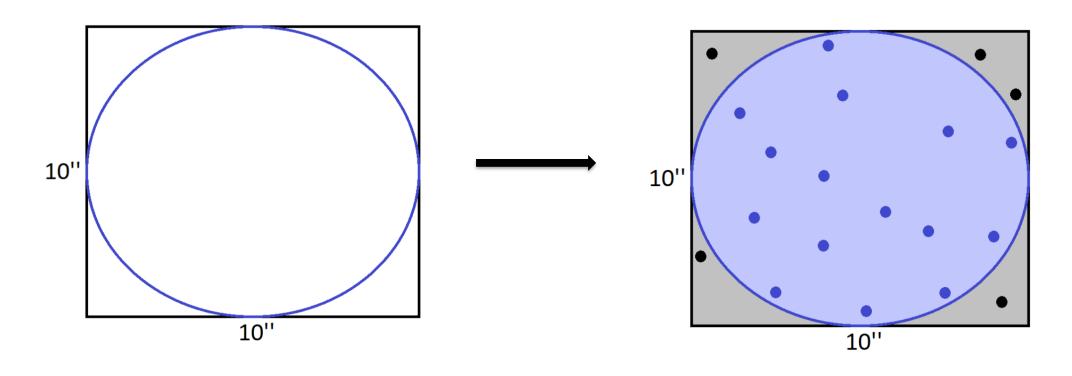
All models are imperfect, **but** some are useful.....

Summary



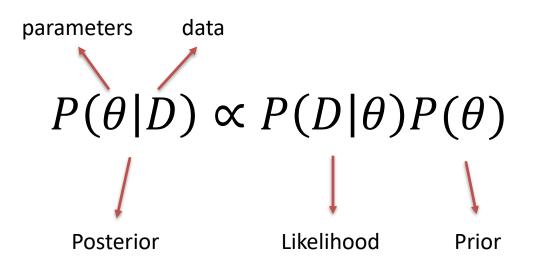
MCMC and Stan

Monte Carlo Sampling

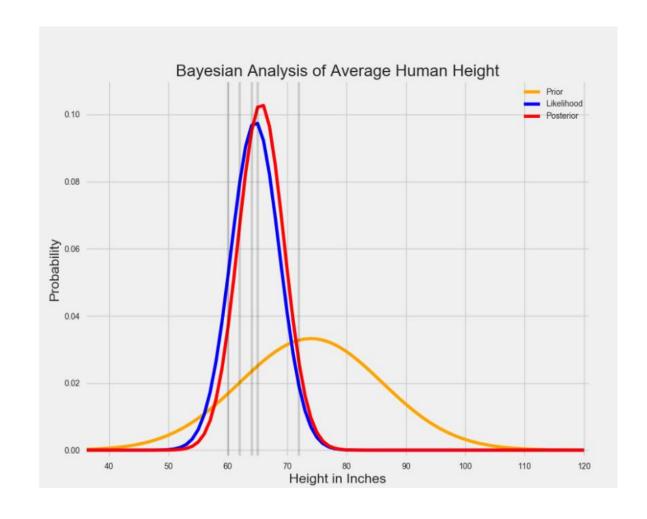


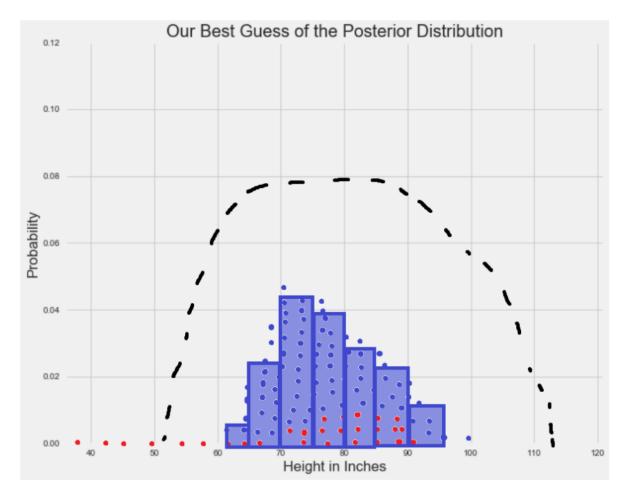
A Zero-Math Introduction to Markov Chain Monte Carlo Methods

Bayes Theorem



MC and Bayesian Theorem





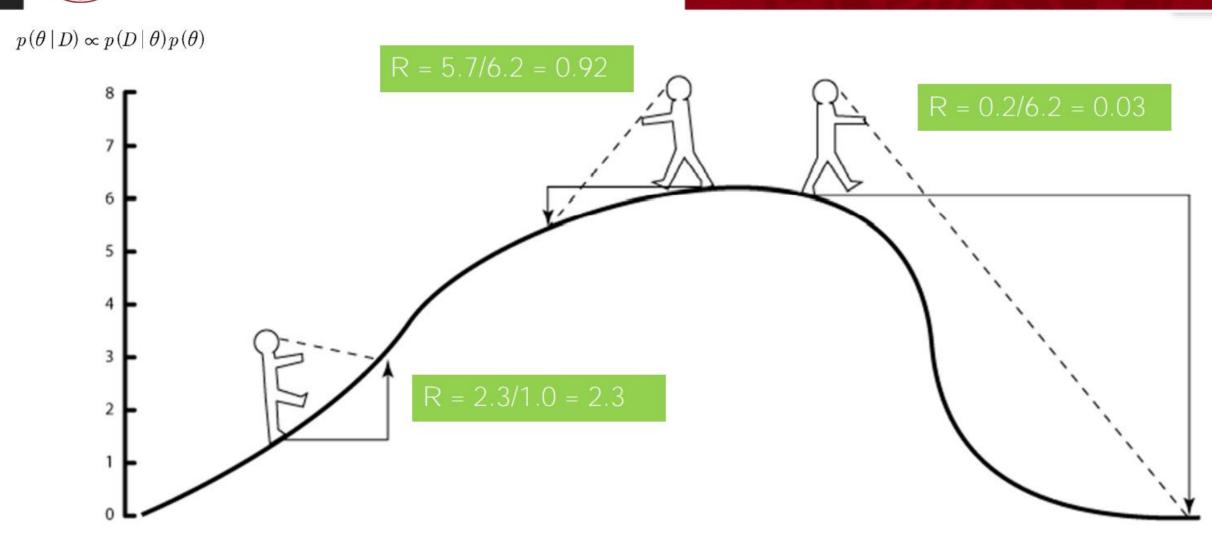
If Only Monte Carlo

What is different from grid search?

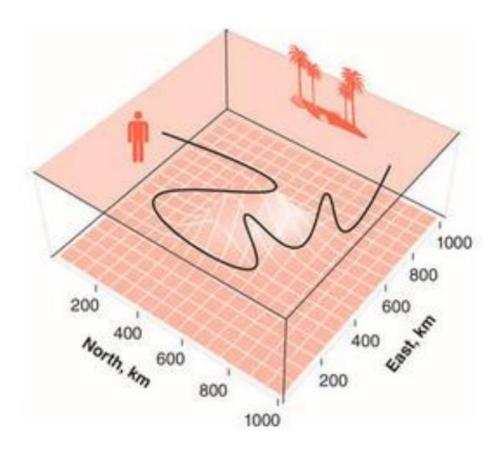
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School of Psychological and Cognitive Sciences, Peking University

Markov Chain



An MCMC Robert in 3D



Lambert (2018)

Algorithms

- Rejection Sampling
- Importance Sampling
- Metropolis Sampling
- Gibbs Sampling
- Hamilton MC (Stan)

- 1. an independent programming language based on C++
- 2. Can be interacted with different platforms (e.g., R, Matlab and Python)

Steps to use Stan

- 1. Prepare your data
- 2. Write your model in Stan
- 3. Check with stan codes
- 4. Set up Stan options
- 5. Run/Call Stan files
- 6. Post-analysis

Stan file

```
transformed data {
parameters {
transformed parameters {
model {
generated quantities {
```



Stan Syntax Cheatsheet.pdf

A minimal Stan program implementing a binomial model.

```
data {
  int n;
  int x;
parameters {
  real<lower=0, upper=1> p;
model {
 p ~ uniform(0, 1);
  x ~ binomial(n, p);
```

Call Stan file

Running a Stan program is usually done from another language such as Python or R.

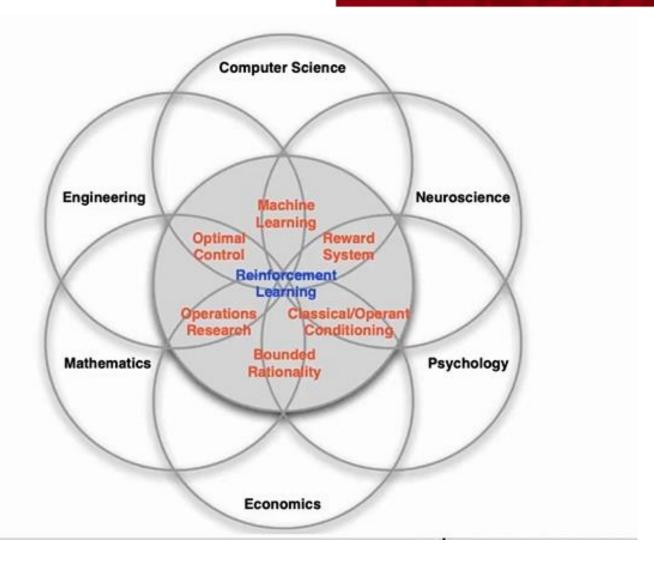
(Here assuming model_string contains the model from the last slide.)

Summary

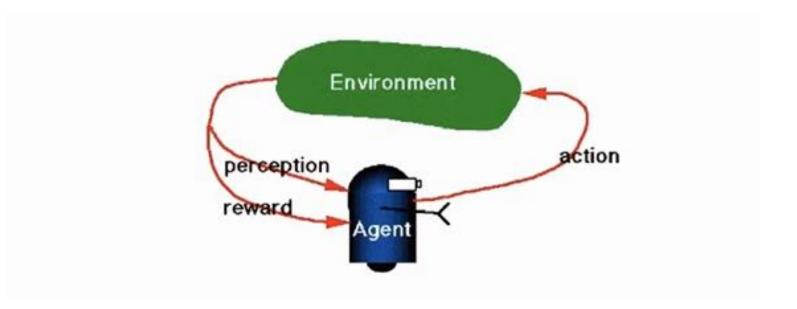
- 1. What is MCMC?
- 2. What is Stan?
- 3. How to use Stan?

Practices: implementing a reinforcement learning model in Rstan

Brief introduction about RL



Brief introduction about RL



- Agent perceives the environment state s
- Agent takes action a
- Agent receive reward r
- And agent adjust his action a'

RL tutorial

Rescorla-Wagner Model

$$PE = R - v_{i,t}$$

Prediction Error

$$v_{i,t+1} = v_{i,t} + \alpha * PE$$

 α :learning rate

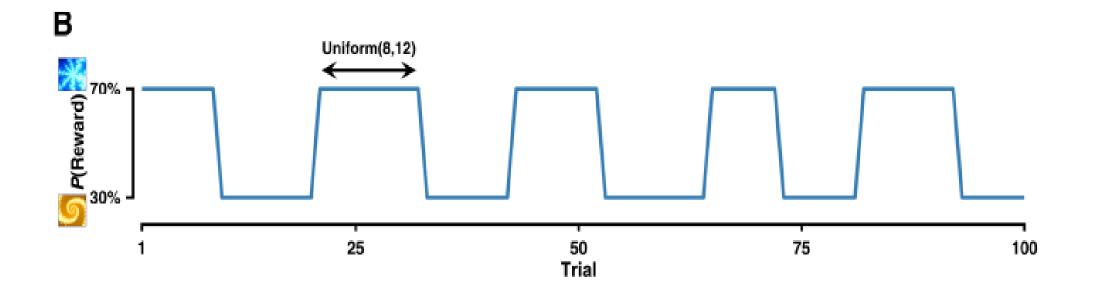
$$P(i, t + 1) = \frac{e^{v_{i,t+1}*\beta}}{\sum e^{v_{i,t+1}*\beta}}$$

Softmax function

$$\beta = 3^{\tau} - 1$$

Rescorla, R. A., & Wagner, A. R. (1972)

Probability Reversal Learning



(Zhang, Glascher, 2020)

Run the simulation

Task setting

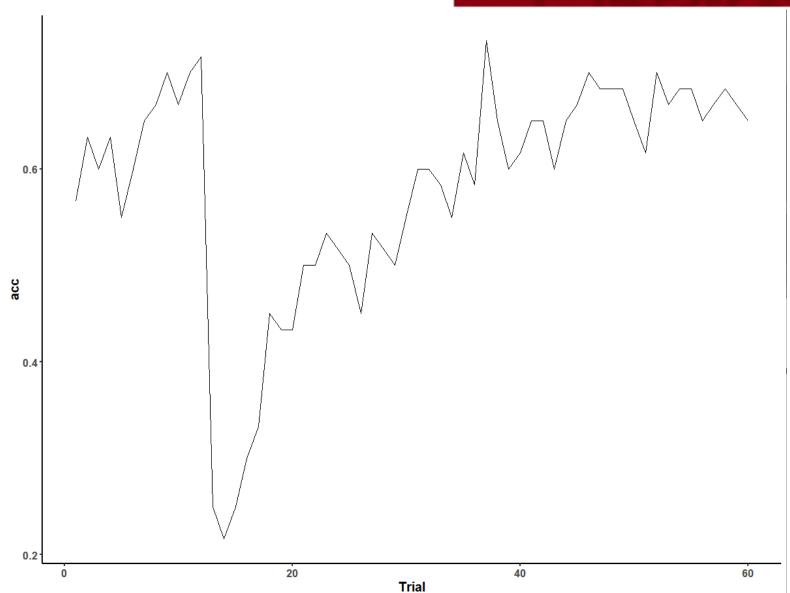
```
##task setting (probability reversal learing task)
set.seed(2021)
reverse_trials=sample(c(8,9,10,11,12,13), replace = F)
ntrials=60
reward_prob=matrix(c(0,7,0.3,0.3,0.7),ncol=2,nrow=2)
```

Agent setting

```
##agent setting
nsubjects=60
lr=rnorm(n=nsubjects,mean=0.4,sd=0.2)
tau=rnorm(n=nsubjects,mean=3,sd=1)
```

```
#run the simulation
agent_data=list()
for (i in 1:nsubjects){
 tmp_lr=lr[i]
 tmp_tau=tau[i]
  v=matrix(rep(0,2*ntrials),nrow=2,ncol=ntrials)
  p=c(0,0)
  consistency=3**tmp_tau-1
  choice=rep(0,ntrials)
 reward=rep(0,ntrials)
 correct=rep(0,ntrials)
  n_reverse=1
  count trial=0
  for (t in 1:ntrials){
   if(t>1){
     v[choice[t-1],t] < -v[choice[t-1],t-1] + tmp_lr*(reward[t-1]-v[choice[t-1],t-1])
   p<-softmax(v[,t]*consistency)</pre>
   choice[t]=sample(c(1,2),prob = p,replace=T)
   reward[t]=sample(c(1.0).prob = reward_prob[choice[t].].replace=T)
    count_trial=count_trial+1
   if(count_trial==reverse_trials[n_reverse]){
     reward_prob=1-reward_prob
      count_trials=0
      n_reverse=n_reverse+1
    if (reward_prob[choice[t],1]==0.7){
     correct[t]=1
   }else{
     correct[t]=0
 agent_data[[i]]=list(c(1:ntrials),choice,reward,correct,v,tmp_lr,tmp_tau)
```

Visualization



R and RStan



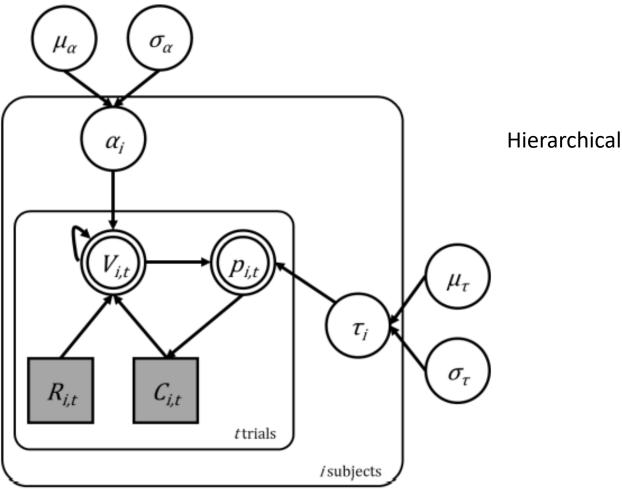
Stan model

Define your data

```
data {
  int<lower=1> nSubjects;
  int<lower=1> nTrials;
  int<lower=1, upper=2> choice[nSubjects, nTrials];
  real<lower=0, upper=1> reward[nSubjects, nTrials];
}
```

```
transformed data {
  vector[2] initv; // initial values for v
  initv = rep_vector(0.0, 2);
}
```

Stan model



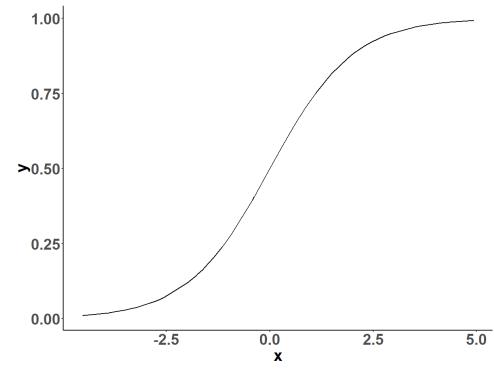
Hierarchical Bayesian Model

Stan model

```
parameters {
 // group-level parameters
 real lr_mu_raw;
 real tau_mu_raw;
 real<lower=0> lr_sd_raw;
 real<lower=0> tau_sd_raw;
 // subject-level raw parameters
 vector[nSubjects] lr_raw;
 vector[nSubjects] tau_raw;
transformed parameters {
 vector<lower=0,upper=1>[nSubjects] lr;
 vector<lower=0,upper=5>[nSubjects] tau;
 for (s in 1:nSubjects) {
   lr[s] = Phi_approx( lr_mu_raw + lr_sd_raw * lr_raw[s] );
   tau[s] = Phi_approx( tau_mu_raw + tau_sd_raw * tau_raw[s] ) * 5;
```

Phi approx: sigmoid

$$y = \frac{1}{1 + e^{-x}} \qquad y \in (0,1)$$

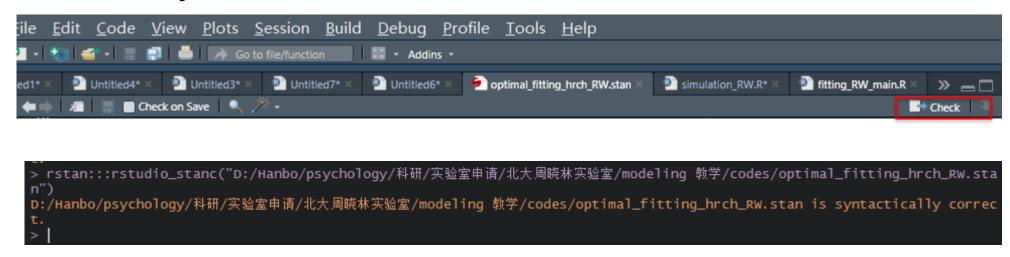


```
model {
  lr_{mu}_{raw} \sim normal(0,1);
  tau_mu_raw \sim normal(0,1);
  lr_sd_raw \sim cauchy(0,3);
  tau_sd_raw \sim cauchy(0,3);
  lr_raw \sim normal(0,1);
  tau_raw \sim normal(0,1);
  for (s in 1:nSubjects) {
    vector[2] v;
    real pe;
    V = initV;
    for (t in 1:nTrials) {
      choice[s,t] \sim categorical_logit((pow(3,tau[s])-1)* v );
      pe = reward[s,t] - v[choice[s,t]];
      v[choice[s,t]] = v[choice[s,t]] + lr[s] * pe;
```

```
generated quantities {
 real<lower=0,upper=1> lr_mu;
 real<lower=0,upper=3> tau_mu;
 real log_lik[nSubjects];
 int y_pred[nSubjects, nTrials];
 lr_mu = Phi_approx(lr_mu_raw);
 tau_mu = Phi_approx(tau_mu_raw) * 5;
 y_pred = rep_array(-999,nSubjects ,nTrials);
  { // local block
   for (s in 1:nSubjects) {
       vector[2] v;
       real pe;
        log_lik[s] = 0;
       v = initV;
       for (t in 1:nTrials) {
          log_lik[s] = log_lik[s] + categorical_logit_lpmf(choice[s,t] | ((pow(3,tau[s])-1) * v));
         y_pred[s,t] = categorical_logit_rng( (pow(3,tau[s])-1) * v );
          pe = reward[s,t] - v[choice[s,t]];
          v[choice[s,t]] = v[choice[s,t]] + lr[s] * pe;
```

Stan file

Check your codes



Bugs?

The Stan Forums (mc-stan.org)

- Prepare data
- Specify stan file
- Set options for fitting
- Run the fitting process

```
#suppose we have completed simulation process and get the agent_data
nSubjects <- length(agent_data)
nTrials <- length(agent_data[[1]][[1]])
##reshape the data from a list to an array to be fitted
data_array<-array(rep(0,nSubjects*nTrials*2),dim=c(nSubjects, nTrials, 2))</pre>
for (i in 1:nSubjects){
    for(t in 1:nTrials){
        data_array[i,t,1]=agent_data[[i]][[2]][t]
        data_array[i,t,2]=agent_data[[i]][[3]][t]
dataList <- list(nSubjects=nSubjects,</pre>
                 nTrials=nTrials,
                 choice=data_array[,,1],
                 reward=data_array[,,2])
```

```
Your
own
path
```

```
rstan_options(auto_write = TRUE)
options(mc.cores = 4)
➡modelFile <- 'D:\\Hanbo\\psychology\\科研\\实验室申请\\北大周晓林实验室\\modeling 教学\\codes\\optimal_fitt
          <- 16000
nIter
nChains
          <- floor(nIter/2)
nWarmup
nThin
cat("Estimating", modelFile, "model... \n")
startTime = Sys.time(); print(startTime)
cat("Calling", nChains, "simulations in Stan... \n")
fit_rl <- stan(modelFile,
                       = dataList,
               data
               chains = nChains,
               iter
                       = nIter.
               warmup = nWarmup,
               thin = nThin,
               init
                       = "random",
               control = list(adapt_delta=0.999, max_treedepth=100),
               seed
                       = 2021
cat("Finishing", modelFile, "model simulation ... \n")
endTime = Sys.time(); print(endTime)
cat("It took", as.character.Date(endTime - startTime), "\n")
```

R file

Run the whole function to define the function

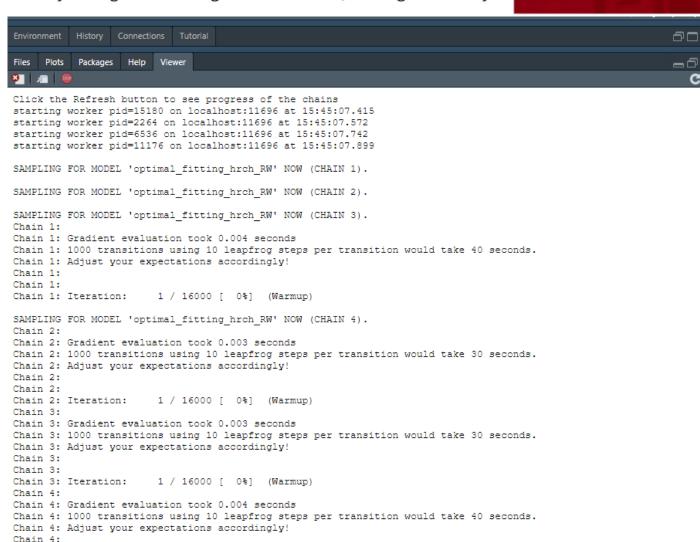
```
> fit_rl<-run_RW_fitting()
```

Call the function through command

Chain 4:

Chain 4: Iteration:

1 / 16000 [0%] (Warmup)



Result Diagnose

```
print(fit_r1)
Inference for Stan model: optimal_fitting_hrch_RW.
 chains, each with iter=16000; warmup=8000; thin=1;
post-warmup draws per chain=8000, total post-warmup draws=32000.
                                                                       97.5% n_eff Rhat
                                sd
                                       2.5%
                                                25%
                                                         50%
                                                                 75%
                 mean se_mean
                                              -0.62
                -0.50
                         0.00 0.18
                                      -0.87
                                                       -0.49
                                                               -0.38
                                                                       -0.16 2701
lr_mu_raw
tau_mu_raw
                 1.83
                         0.00 0.42
                                       1.12
                                               1.53
                                                       1.79
                                                                2.08
                                                                        2.77 11334
lr_sd_raw
                 1.06
                         0.00 0.16
                                       0.78
                                               0.94
                                                       1.05
                                                                1.16
                                                                        1.42 3042
tau_sd_raw
                                               1.58
                                                                2.34
                                                                        3.41 4095
                 2.00
                         0.01 0.61
                                       1.03
                                                       1.93
                                      -2.78
                                              -1.82
                                                       -1.08
                                                               -0.07
                                                                        1.55
                                                                              9682
lr_raw[1]
                -0.91
                         0.01 1.18
lr_raw[2]
                 0.69
                         0.00 0.36
                                       0.05
                                               0.44
                                                       0.67
                                                                0.92
                                                                        1.46 14462
lr_raw[3]
                -0.22
                         0.00 0.46
                                      -1.15
                                              -0.54
                                                       -0.21
                                                                0.10
                                                                        0.65 17157
                 0.49
                                      -0.13
                                               0.26
                                                       0.47
                                                                0.71
                                                                        1.24 13418
lr_raw[4]
                         0.00 0.35
                                                                        2.78 13315
lr_raw[5]
                 1.84
                         0.00 0.49
                                       0.85
                                               1.52
                                                       1.85
                                                                2.16
1r_raw[6]
                -0.27
                         0.00 0.50
                                      -1.28
                                              -0.60
                                                       -0.25
                                                                0.09
                                                                        0.64 19402
lr_raw[7]
                 0.49
                         0.00 0.34
                                      -0.10
                                               0.26
                                                       0.46
                                                                0.70
                                                                        1.25 12884
lr_raw[8]
                -0.70
                         0.00 0.28
                                      -1.25
                                              -0.88
                                                      -0.69
                                                               -0.51
                                                                       -0.15 3689
lr_raw[9]
                 0.63
                         0.00 0.45
                                      -0.42
                                               0.39
                                                       0.69
                                                                0.93
                                                                        1.39 12864
lr_raw[10]
                 1.57
                         0.01 0.68
                                       0.24
                                               1.08
                                                       1.63
                                                                2.06
                                                                        2.81 12984
                -1.31
                                                       -1.31
                                                                       -0.61 3577
lr_raw[11]
                         0.01 0.37
                                      -2.05
                                              -1.56
                                                               -1.07
                                                                        2.35 7887
lr_raw[12]
                 0.77
                         0.01 0.75
                                      -0.43
                                               0.23
                                                       0.63
                                                                1.29
lr_raw[13]
                 0.61
                         0.00 0.43
                                      -0.13
                                               0.31
                                                       0.57
                                                                0.86
                                                                        1.57 15384
                                              -0.10
                                                       0.48
                                                                0.87
lr_raw[14]
                 0.36
                         0.01 0.70
                                      -1.16
                                                                        1.46 18117
                         0.000.28
                                      0.01
                                               0.33
```

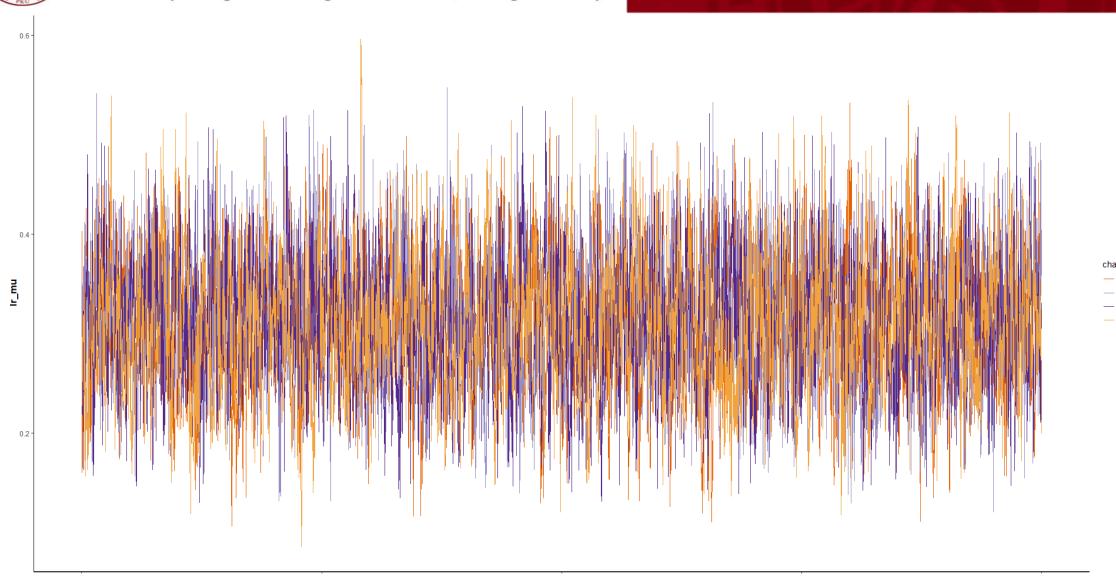
Rhat should generally be smaller than 1.01

<u>'shinystan'</u>

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A good example



Result Diagnose

Stan Sampling Parameters

cognitive model statistics

computing

| parameter | description | constraint | default |
|-------------------------|------------------------------------|-------------------------|---------|
| iterations | number of MCMC samples (per chain) | int, > 0 | 2000 |
| delta: δ | target Metropolis acceptance rate | $\delta \in [0,1]$ | 0.80 |
| stepsize: ε | initial HMC step size | real, $\varepsilon > 0$ | 2.0 |
| $\max_$ treedepth: L | maximum HMC steps per iteration | int, $L > 0$ | 10 |

Typical adjustments

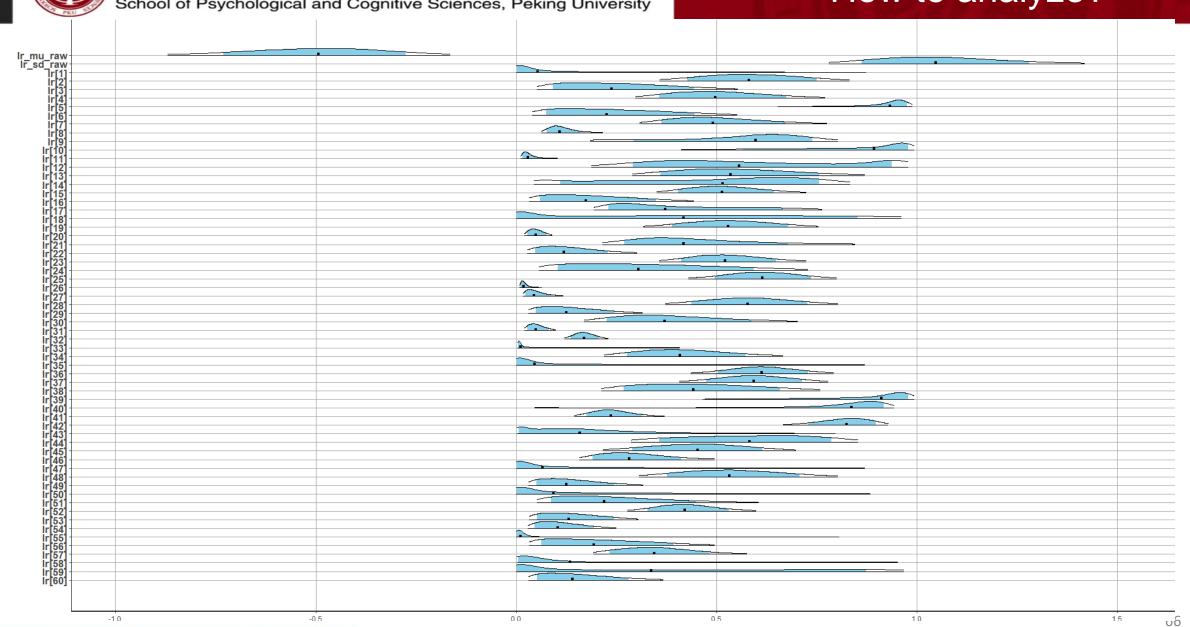
- Increase iterations
- Increase delta
- Decrease stepsize
- Might have to increase max_treedepth



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How to analyze?



- Mean
- HDI=highest density interval (credential interval)

```
Compute Highest-Density Interval
  @description
  Computes the highest density interval from a sample of representative values, estimated as shortest credible into
  Downloaded from John Kruschke's website \url{http://www.indiana.edu/~kruschke/DoingBayesianDataAnalysis/}
  @param sampleVec A vector of representative values from a probability distribution (e.g., MCMC samples).
  @param credMass A scalar between 0 and 1, indicating the mass within the credible interval that is to be estimate
  @return A vector containing the limits of the HDI
  @export
HDIofMCMC = function(samplevec,
                    credMass = 0.95) {
   if ( class(samplevec) == "mcmc.list" ) {
       samplevec = as.matrix(samplevec)
   sortedPts = sort( samplevec )
   ciIdxInc = floor( credMass * length( sortedPts ) )
   nCIs = length( sortedPts ) - ciIdxInc
   ciWidth = rep( 0 , nCIs )
   for ( i in 1:nCIs ) {
       ciWidth[ i ] = sortedPts[ i + ciIdxInc ] - sortedPts[ i ]
   HDImin = sortedPts[ which.min( ciWidth ) ]
   HDImax = sortedPts[ which.min( ciWidth ) + ciIdxInc ]
   HDIlim = c( HDImin , HDImax )
   return( HDIlim )
```

How to analyze?

Statistical Rethinking

A Bayesian Course with Examples in R and Stan

Richard McElreath

Model Comparison

Generally, you can compare your models by using various indicators:

- > Log-likelihood
- ➤ Alike Information Criterion (AIC)
- Bayesian Information Criterion (BIC)
- **➤** Leave-one-out Information Criterion (LOOIC)

```
##model comparison
library(loo)
loo(fit_rl)
```

```
Computed from 32000 by 60 log-likelihood matrix

Estimate SE
elpd_loo -879.4 104.2
p_loo 62.8 4.2
looic 1758.8 208.5
-----
Monte Carlo SE of elpd_loo is NA.
```

Summary

- 1. How to write a stan code?
- 2. How to write an R code?
- 3. How to diagnose the fitting result?
- 4. How to analyze the result?

- We introduce concepts of computational modeling and why we need to learn about it in psychology and cognitive sciences.
- We introduce standard approaches (ten simple rules) on conducting a computational modeling research.
- We briefly go through how Stan works with MCMC.
- We dived into the codes to realize from the very beginning of simulation to analyze model fitting results.

- How to create/think up a good model?
 - Sorry, I don't know either…

- How to learn about computational modeling?
 - Knowledge perspective:
 - Math (linear algebra, theory of probability, Calculus)
 - Programming languages (R, Matlab, Python, Julia, C++, Java.....)
 - Algorithms (basics about machine learning)
 - Practice perspective:
 - Learn by demanding, doing and achieving!

Recommended resources

Summer schools:

- Neuromatch Academy Summer School (Annually)
- Computational Psychiatry Course @ Zürich, CH (annual)
- London Computational Psychiatry Course @ London, UK (annual)
- Brains, Minds & Machines Summer Course @ MIT, US (annual)
- And so on (keep searching!)

Recommended resources

Online courses:

- Machine learning (@Coursera- Andrew Ng)
- Bayesian Modeling (@Bilibili- Lei Zhang)
- Reinforcement learning model basics (myself)
- Reinforcement learning (@coursera)

Recommended resources

• Books:

- R语言实战
- Statistical Rethinking
- 认知和行为的计算建模

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