User's Manual for the code in Matlab

1 Generating Random Variables from 8 UARS Distributions

In the simulation for a random 3×3 rotation matrix from a UARS distribution, we would use the misorientation angle $r(r \in (-\pi, \pi])$, the Euler angles α, β and $\gamma(\alpha \in [0, 2\pi], \beta \in [0, \pi], \gamma \in [0, 2\pi])$. A UARS distribution has two parameters: the location parameter $\boldsymbol{S}$ and the concentration parameter $\kappa(\kappa \in [0, \infty))$.

In the code, α, β and γ in the location parameter $\boldsymbol{S}$ are indicated by `a,b,g` respectively. $\boldsymbol{S}$ is indicated by `S`. The concentration parameter κ is indicated by `k`.

The ranges for α, β, γ and κ are as follows: $\alpha \in [0, 2\pi], \beta \in [0, \pi], \gamma \in [0, 2\pi], \kappa \in (0, \infty)$.

(1) Function used: `randraw.m` `vmUARS.m`
(`randraw.m` is downloaded online: https://www.mathworks.com/matlabcentral /fileexchange/7309-randraw/content/randraw.m by Alex Bar-Guy Copyright (c) 2005, Alex Bar-Guy All rights reserved.)
`[O,S]=vmUARS(k,a,b,g,n)` generates n random variables from Von Mises UARS distribution with location parameter `S (a, b, g)` and concentration parameter `k`. `S` is the calculated parameter from `a, b, g`. `O` are the generated `n` number of 3 by 3 matrix. The dimension of `O` is $3n$ by 3.

(2) Function used: `randraw.m` `MFUARS.m`
(`randraw.m` is downloaded online,see above)
`[O,S]=MFUARS(k,a,b,g,n)` generates `n` random variables from Matrix Fisher UARS distribution with location parameter `S (a, b, g)` and concentration parameter `k`. `S` is the calculated parameter from `a, b, g`. `O` are the generated `n` number of 3 by 3 matrix. The dimension of `O` is $3n$ by 3.

(3) Function used: `wnUARS.m`
`[O,S]=wnUARS(k,a,b,g,n)` generates `n` random variables from wrapped normal UARS distribution with location parameter `S (a, b, g)` and concentration parameter `k`. `S` is the calculated parameter from `a, b, g`. `O` are the generated `n` number of 3 by 3 matrix. The dimension of `O` is $3n$ by 3.

(4) Function used: `rwmb.m` `WTNUARS.m`

[O,S]=WTNUARS(k,a,b,g,n) generates n random variables from wrapped trivariate normal UARS distribution with location parameter S (a, b, g) and concentration parameter k. S is the calculated parameter from a, b, g. O are the generated n number of 3 by 3 matrix. The dimension of O is $3n$ by 3.

(5) Function used: densitywmb.m rwmb.m BungeUARS.m
[O,S]=BungeUARS(k,a,b,g,n) generates n random variables from Bunge UARS distribution with location parameter S (a, b, g) and concentration parameter k. S is the calculated parameter from a, b, g. O are the generated n number of 3 by 3 matrix. The dimension of O is $3n$ by 3.

(6) Function used: densitylorentz.m LorentzianUARS.m
[O,S]=LorentzianUARS(k,a,b,g,n) generates n random variables from Lorentzian UARS distribution with location parameter S (a, b, g) and concentration parameter k. S is the calculated parameter from a, b, g. O are the generated n number of 3 by 3 matrix. The dimension of O is $3n$ by 3.

(7) Function used: densitycayley.m densitywmb.m rwmb.m CayleyUARS.m
[O,S]=CayleyUARS(k,a,b,g,n) generates n random variables from Cayley UARS distribution with location parameter S (a, b, g) and concentration parameter k. S is the calculated parameter from a, b, g. O are the generated n number of 3 by 3 matrix. The dimension of O is $3n$ by 3.

(8) Function used: densityig.m densitywmb.m rwmb.m igUARS.m
[O,S]=igUARS(k,a,b,g,n) generates n random variables from Isotropic Gaussian UARS distribution with location parameter S (a, b, g) and concentration parameter k. S is the calculated parameter from a, b, g. O are the generated n number of 3 by 3 matrix. The dimension of O is $3n$ by 3.

2 Bayesian Inference for Parameters in Matrix Fisher UARS Distribution

(1) Bayesian estimate and credible set for the location parameter S and the concentration parameter k
Function used: SUMO.m posteriordensityMFUARS.m mcmcburnin.m
[Shat,S95,Khat,K025,K975]
=mcmcburnin(k,a,b,g,delta,sigma,n,OS,m,burnin) returns Bayesian estimate Shat, 95% credible set for S, Bayesian estimate of k, 95% credible set for k after one simulates m number of Ss and ks from the posterior distribution and discards the first burnin number of Ss and ks. In the function,

`k` is the starting value for κ. `a, b, g` can decide the starting value for $\boldsymbol{S}$. `delta` is the parameter for r in Metropolis-Hastings within Gibbs algorithm. `sigma` is the parameter for the proposal of κ. `OS` is the data set used for the Bayesian inference. `n` is the number of 3 by 3 matrices included in the data set `OS`. The dimension of `OS` is $3n$ by 3. The credible set for $\boldsymbol{S}$ is viewed in terms of the set of 3 cones of constant angle `S95` centered at `Shat`.

(2) Trace plots
Function used: `mcmc.m getmatrix.m plots.m`
`[mm,Khatm,Shatm1,Shatm2,Shatm3,Shatm4,Shatm5,`
`Shatm6,Shatm7,Shatm8,Shatm9]`
`=getmatrix(k,a,b,g,delta,sigma,n,OS,m0,h)` generates the results needed for the trace plots. The explanation for `k, a, b, g, delta, sigma, n, OS` is the same as that in (1). `m0` is the starting value for the iteration. `h` is the number of Bayesian estimates one can obtain.

For example, if the starting value `m0` is 300 and `h` is 3, then one can obtain Bayesian estimate for 300 posterior draws from the posterior distribution at the first time and then one can obtain the Bayesian estimate for 350 posterior draws from the posterior distribution at the second time. Totally, one can obtain 3 Bayesian estimates for each parameter respectively.
One can obtain 10 plots including one for `k`, and nine for the 9 elements of `S`.