RRA Optimization GUI User's Manual

This user's manual will provide instructions on how to use the optimization graphical user interface (GUI) for use in the Residual Reduction Algorithm in the OpenSim software. This GUI will require the use of both OpenSim and MATLAB.

The users of this GUI are asked to kindly cite the manuscripts listed below in publications that use this open-source tool.

1. Samaan, M.A., *et al*. 2016 "Determining Residual Reduction Algorithm Kinematic Tracking Weights for a Sidestep Cut via Numerical Optimization." Computer Methods in Biomechanics and Biomedical Engineering, 19(16): 1721-1729.
2. Weinhandl, J.T., *et al.* 2013 "Anticipatory Effects on Anterior Cruciate Ligament Loading During Sidestep Cutting." Clinical Biomechanics, 28(6): 655-663.

The objective function (generic form) used in this GUI was adapted from Weinhandl *et al*. (2013) is:

$$\min_{w_{\dot{q}}} \left[\sum_{i=i}^{nq} \left(\frac{rms(q_i^{err})}{wq_i} \right)^{pq_i} + \sum_{j=i}^{nR} \left(\frac{rms(R_j)}{wR_j} \right)^{pR_j} \right]$$

w_q = OpenSim task weights found in *RRA_Tasks.xml

nq = number of degrees-of-freedom

$rms(q^{err})$ = root mean square error between the experimentally measured kinematics and the model estimated kinematics.

wq = OPTRRA kinematic weights (i.e., maximal allowable $rms(q^{err})$)

pq = OPTRRA kinematic powers (larger pq increases the penalty for exceeding wq)

nR = number of residual forces and torques (generally 6)

$rms(R)$ = root mean square magnitude of the residual

wR = OPTRRA residual weights (i.e., maximal allowable $rms(R)$)

pR = OPTRRA kinematic powers (larger pR increases the penalty for exceeding wR)

Please note that the objective function (equation 3) listed in the Samaan et al, 2016 has a typo in which the exponent of 3 should be listed on the outside of the larger parentheses.

GUI Instructions

Download the folder called "RRA_OPT_GUI " and make sure that the entire contents of this folder are added to the current path in MATLAB.

Right click on “RRA_OPT_GUI.m” and select “Run” in order to start the GUI. A GUI (Figure 1) should appear on your screen. **If the GUI docks to the MATLAB command window, close the GUI figure window and then right click “RRA_OPT_GUI.m” and select “Run” again to display the undocked GUI.**

The GUI consists of 3 steps, where each step is contained within its own panel in the GUI.

Step 1: Allows the user to select the version of OpenSim being used, the choice to use either the particle swarm optimization (PSO) or simplex simulated annealing (SIMPSA) algorithms.

Step 2: Allows the user to select the OpenSim motion file, RRA setup and RRA tasks files that are to be used in the GUI.

Step 3: Allows the user to adjust various optimizer parameters, objective function constraints, initial guess for the RRA tracking weights, etc.

Step 1: Select Parameters

1) Select the version of OpenSim that will be used by the GUI by using the pulldown menu. If the user does not make a selection, the GUI will use OpenSim 3.0 as the default. This first step will add the desired OpenSim path to MATLAB.
2) Select the either the PSO or SIMPSA optimization routine for optimization of tracking weights. The GUI will use the PSO algorithm by default.
3) If the PSO algorithm is selected, the user can edit the swarm size for the PSO algorithm. A default value of 25 will be used by the GUI, if no selection is made. A swarm size of 25 was selected as the default as a swarm size of 20 – 30 was stated to be a reasonable compromise between cost and reliability [1].

Step 2: Select RRA Files

1) Click the “Select Motion File” button and navigate to the directory where the motion (.mot or .sto) file of the trial that will be optimized is located. Select the motion file and click “Open”.

2) Click the “Select RRA Setup File” button and navigate to the directory where the RRA setup (.xml) file of the trial that will be optimized is located. Select the RRA setup file and click “Open”.

    a) A new RRA Setup File with the extension “_GUI” will be created. This new RRA Setup File will create a folder called “RRA_Results” within the same directory as the RRA Setup File, in order to simplify the specification of the directory of the RRA Results folder.

3) Click the “Select RRA Tasks File” button and navigate to the directory where the RRA tasks (.xml) file of the trial that will be optimized is located. Select the RRA tasks file and click “Open”.

a) This step will take a few moments to complete as MATLAB reads in the OpenSim model degrees of freedom. A wait bar will appear after the RRA tasks file is selected and will disappear after the process is completed.

b) The total number of model degrees of freedom (DOFs) will be displayed underneath the name of the RRA tasks file in the step 2 panel.

Step 3: Select Optimizer Parameters

1) The user can modify the run time (minutes), tolerance level of the objective function, kinematic and residual powers as well as the root mean square (RMS) Force/Moment Allowance.

   a) **Run time** – the user can modify the length of time for which the RRA optimization is allowed to run. The default value is set to 2,880 minutes (48 hours).

   b) **Tolerance Level** – the user can modify the objective function tolerance level, which will be used in determining the set of optimal task tracking weights, by assessing the difference between the global worst and best solutions of the objective function. If the difference in costs between the global worst and best solutions to the objective function exceed the prescribed function tolerance, the optimizer will stop as the optimal solution has been determined. The default value is set to 0.001

   c) **Kinematic Power** – the power to which the kinematic RMS errors are raised to in the objective function. A default value of 3 will be used if the user does not modify this value.

   d) **Residual Power** – the power to which the residual force and moment RMS errors are raised to in the objective function. A default value of 3 will be used if the user does not modify this value.

   e) **RMS Force/Moment Allowance** – the largest RMS error of the residual forces and moments that the optimizer will try to obtain with the optimal set of task tracking weights. A default value of 10N and 10Nm will be used if the user does not modify this value.

2) The user has the option of adjusting the intial guess (i.e. initial task tracking weights), max RMS kinematic errors that will try to be obtained as well as the lower and upper bounds of the task tracking weights that will be used by the optimizer.

   a) Click the "Adjust RRA Tasks Parameters?" button, which will open up an Excel file called "trial_name_RRA_Tasks_Parameters.xlsx" (Figure 2) where "trial_name" is the name of the motion file selected in step 2. This file is located in the same directory as the RRA setup file. The initial task weights are read from the RRA tasks.xml file that the user selected in Step 2.3

   b) The first row in the "trial_name_RRA_Tasks_Parameters.xlsx" file are the model DOFs.

   c) The initial task tracking weights are located in the second row of the "trial_name_RRA_Tasks_Parameters.xlsx" file and are selected from the task tracking

weights from the RRA tasks file selected in step 2. The user can modify these values as desired.

d) The max RMS errors for each model DOF is listed in the third row of the "trial_name_RRA_Tasks_Parameters.xlsx" file and can be modified by the user.

e) The lower and upper bounds of the task tracking weights are located in the fourth and fifth rows, respectively, of the "trial_name_RRA_Tasks_Parameters.xlsx" file and can be modified by the user. The lower and upper bounds are set by the optimizer to be 0.01 and 10 times the initial task tracking weights by default.

f) Once all changes are made, save the file and close the "trial_name_RRA_Tasks_Parameters.xlsx" file. **Do not change the name or directory of this file!**

g) If modifications are made to the initial guess values for the RRA task weights, these modified task weights will be written to the original RRA Tasks (.xml) file.

h) If modifications are made to the max RMS errors or task weight bounds for any model DOF, these modifications will be automatically recognized by the GUI and used during the optimization routines.

3) Click the "START OPTIMIZATION!" button to start the optimization routine. A new figure window will appear and will display the RMS kinematic and residual forces/moments data as well as plot the cost of the current iteration of the objective function. It should be noted that the SIMPSA algorithm may not immediately produce actual plots due to the algorithm properties but will display these plots after the algorithm achieves a certain solution state.

4) A display of the objective function cost, along with other information will be displayed in the MATLAB command window.

5) Two files labeled "trial_name_RRA_Tasks_rms_errors.out" and "trial_name_RRA_Tasks_task_weights.out" will be created and located in the same directory as the RRA setup file. These two files will contain the RMS errors and task weights for each iteration of the optimization routine.

6) Once the optimizer has determined the optimal solution or exceeds the prescribed time limit, two Excel files will be created which contain the RMS errors of the model DOFs and the residual forces/moments and the optimal task tracking weights. These files will be located in the same directory as the RRA setup file.

a) "trial_name_RMS_Errors_OptType.xlsx" file is the file containing the RMS errors. The term "OptType" refers to SIMPSA or PSO, depending on the optimization algorithm used.

b) "trial_name_Opt_Task_Weights_OptType.xlsx" file is the file containing the optimal task tracking weights for the trial.

7) A figure containing a plot of the cost and associated RMS errors using the optimal task weights determined by the optimizer will be created and saved to the directory where the RRA setup file is located.

8) All of the workspace variables created will be saved to a file called "trial_name_OptType_Results.mat", which is located in the directory where the RRA setup file is located.

9) Upon completion of the optimization routine, either when the Run Time is exceeded or the Tolerance level is met, the GUI will display the Cost Function Value and Total Run Time in the Step 3 Panel.

10) The optimal task tracking weights of a previously optimized trial (from the same subject and same set of tasks) can be used for another trial of the same task and subject without running through the entire optimization routine.

    a) Re-run Step 2: Select Motion, RRA Setup and RRA Tasks Files for the trial that the user would like to "optimize". Make sure that the trial is from the same set of tasks and from the same subject.

    b) Click the "Process Next File!" button and select the "trial_name_RRA_Tasks_task_weights.out" file from a particular subject that was successfully run through the optimizer. **After selecting the appropriate task weights file, please wait (displayed in MATLAB command window) until the GUI performs the necessary calculations for the chosen trial.**

    c) The task weights from this optimized trial will be written to the new RRA tasks file selected and RRA will be run with these optimal task weights. The cost of the objective function for this selected trial will be displayed in the Step 3 panel.

    d) The RMS and optimal task tracking weights files as well as the results figure, similar to those in Step 3.7 above will be written to the same directory as the recently selected RRA setup file in Step 3.10a.

    e) Also a file called "trial_name_Results.mat" with all of the workspace variables will be saved to the same directory as the recently selected RRA setup file selected in Step 3.10a.

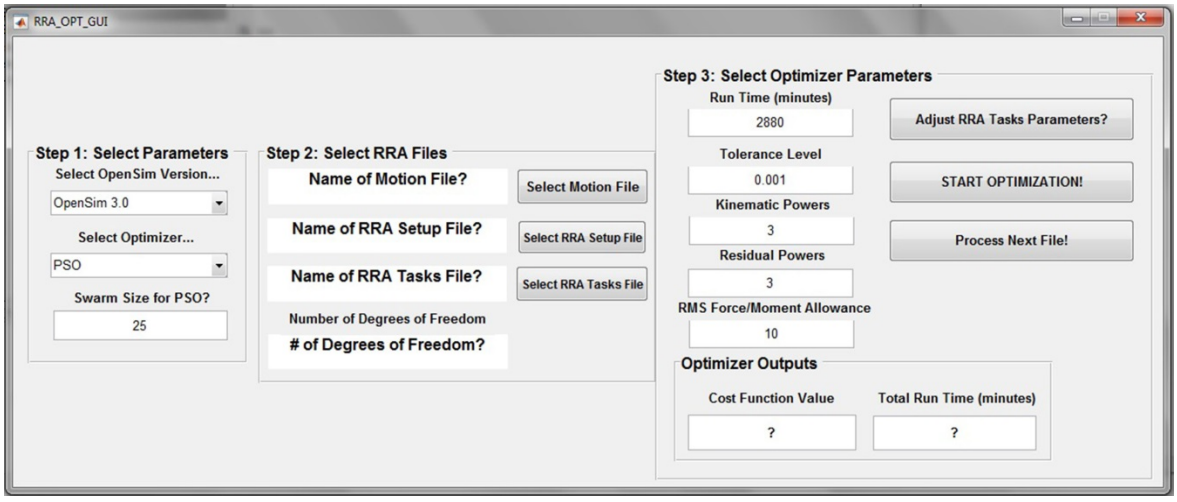

Figure 1: The graphical user interface (GUI) that will be used in MATLAB to select the various optimizer, optimizer parameters, RRA files for OpenSim and run the numerical optimization routine.

	pelvis_tx	pelvis_ty	pelvis_tz	pelvis_tilt	pelvis_list	pelvis_rot	hip_flexic	hip_addu	hip_rotati	knee_flex
Initial Guess (xo)	1499.885	1003.503	746.9851	56.4435	236.5301	22.8205	29.4389	143.2943	132.8264	85.8572
Max RMS Errors	1	1	1	2	2	2	2	2	2	2
Lower Bound (LB)	14.99885	10.03503	7.469851	0.564435	2.365301	0.228205	0.294389	1.432943	1.328264	0.858572
Upper Bound (UB)	14998.85	10035.03	7469.851	564.435	2365.301	228.205	294.389	1432.943	1328.264	858.572

Figure 2: An example of the RRA Tasks Parameter file created by the GUI. The model degrees of freedom (DOFs) are listed on the first row, the initial task tracking weights (row 2), the max RMS error for each DOF (row 3: centimeters for translations and degrees for rotations), the lower (row 4) and upper (row 5) bounds of the task tracking weights. The values in rows 2 – 5 can be modified by the user.

References

1. Schutte, J.F. and A.A. Groenwold, *A Study of Global Optimization Using Particle Swarms.* J Global Optim, 2005. **31**: 93-108.

2. Weinhandl, J.T., Earl-Boehm, J.E., Ebersole, K.T., Huddleston, W.E., Armstrong, B.S.R., O'Connor, K.M., *Anticipatory Effects on Anterior Cruciate Ligament Loading during Sidestep Cutting.* Clin. Biomech., 2013. **28**(6): 655-663.

3. Samaan, M.A., Weinhandl, J.T., Bawab, S.Y., Ringleb, S.I., *Determing Residual Reduction Algorithm Kinematic Tracking Weights for a Sidestep Cut via Numerical Optimization*. Comp. Meth. Biomech. Biomed. Eng., 2016. 19(16): 1721-1729.