MATLAB implementation of UWerrTexp

The program that implements the gamma method with the tail truncation bias correction is an extension of the code by U. Wolff publicly available[1] on the web. The function we implement is

```
function
  [value,dvalue,ddvalue,tauint,
   dtauint,qval,W, gammaout,drho]
  = UWerrTexp(Data,Parm,Nrep,Name,Quantity,varargin)
```

we have kept an interface that is fully compatible with the original code of U. Wolff. We describe here the meaning of the inputs and outputs, but practitioners with a working knowledge of `UWerr` will find all the extra information that is needed in the definition of the input argument `Parm`.

Input

Data it is an N x N_α matrix of measured (equilibrium!) data where N is the total number of measurements and N_α is the number of (primary) observables

Parm It is a vector of (up to 7) values:

1. Estimate of the ratio $S = \tau_*/\tau_{\rm int}$. If $S = 0$, absence of auto-correlations is *assumed*.
2. Value of τ_* used to add a tail and give an upper bound to the error. If $\tau_* = 0$ the code performs a "standard" `UWerr` analysis.
3. It is the N_σ parameter that defines the point $W_{\rm u}$ that satisfies $\overline{\rho}(W_{\rm u}) - N_\sigma \delta\overline{\rho}(W_{\rm u}) \leq 0$. If $\tau_* \neq 0$ the exponential tail is attached at $W_{\rm u}$.
4. A parameter $W_{\rm s}$ that defines a "small window". If $W_{\rm u} < W_{\rm s}$ a trial amplitude of the tail is taken to be either $\overline{\rho}(W_{\rm u}+1)$ or $2\delta\overline{\rho}(W_{\rm u}+1)$, whichever the largest. This new amplitude is accepted only if the resulting $\overline{\tau}^{\rm u}_{\rm int}$ is smaller than the previous one. This involved procedure prevents an excessive overestimate of $\tau^{\rm u}_{\rm int}$ in case when $\rho(\tau)$ decays very rapidly and the statistical errors are large. If $\overline{\rho}(W_{\rm u}) < 0$ this procedure is automatically applied.
5. This parameter is a Monte Carlo time conversion factor MCF. It is used in plots to rescale the time in user defined units.
6. This is a logical parameter, if set to 1 the output gives both the upper bound and the lower bound estimates for error, $\tau_{\rm int}$ and W.
7. This is a logical parameter, if set to 1 it allows to propagate the error of quantities for which only the central value, the statistical and eventually also the systematic error is known. The way to pass the extra quantities and their error to the function is described below.

[1]original `UWerr`: `http://www.physik.hu-berlin.de/com/ALPHAsoft/`

The default values for all these parameters are: [1.5 0 3 5 1 0 0]

Nrep It is a vector [N_1 N_2 $\ldots N_R$] specifying a breakup of the N rows of `Data` into replicas of length N_1, N_2, ... where $N = \sum N_r$. The replica distribution is plotted in a histogram and a Q-value (i.e. the probability to find this much or more scatter) is given when $R \geq 2$. Even though the code allows a splitting in realizations of different length, we recommend to use as often as possible replicas that have the exact same number of measurements. The default treats `Data` as a single chain of length N.

Name In case it is a string, it is the name of the observable in the titles of generated plots. Otherwise all plots are suppressed. The default is the string `''NoName''`.

Quantity It is a handle to a scalar function (@functionname) for the derived observable F. It has to operate on a row-vector of length N_α as first argument. Optional parameters P1, P2,... are passed on to this function as 2nd, 3rd, ... If `Quantity` is an integer between 1 and N_α the analysis is performed on the $\alpha_{\rm th}$ primary observable. The default value is 1.

If `Parm`(7) $\neq 0$ the function call changes to

```
function
  [value,dvalue,ddvalue,tauint,
   dtauint,qval,W, gammaout,drho]
  = UWerrTexp(Data,Parm,Nrep,Name,Quantity,UCData,varargin)
```

The extra parameter `UCData` is expected (i.e. if not set or set to `empty` it returns an error). All inputs are defined as before but the following

Quantity Scalar function handle (@functionname) for the derived observable F. It has to operate on a row-vector of length $N_\alpha +$ `NUCData` as first argument. Optional parameters P1, P2, ... are passed on to this function as 2nd, 3rd, ... argument.

UCData UnCorrelated Data. It is either an `NUCData x 2` or an `NUCData x 3` matrix. The first column contains the central value, the second contains the statistical error (that is summed in quadrature) and the third optional column is the systematic error (these contributions are summed linearly)

Output

value is the central estimate of `Quantity`.

dvalue is the statistical error (inclusive of auto-correlation effects). If `Parm`(6) = 1 it is a vector of 2 values, namely `Stat = [lowerbound upperbound]`. If

`Parm`(7) = 1 returns one extra value, namely `[lowerbound upperbound systematic]`.

ddvalue statistical error of the error (only for the lowerbound)

tauint integrated auto-correlation time. If `Parm`(6) = 1, it returns a vector of 2 values namely $[\tau_{\rm int}^{\rm l}\ \tau_{\rm int}^{\rm u}]$.

dtauint statistical error of tauint. If `Parm`(6) = 1, returns a vector of 2 values: $[\delta\tau_{\rm int}^{\rm l}\ \delta\tau_{\rm int}^{\rm u}]$. $\delta\tau_{\rm int}^{\rm u}$ is computed assuming no error on τ_*.

qval Q-value of the replica distribution if $R \geq 2$ (it is the goodness of fit to a constant)

W it is the numerical value of the summation window. If `Parm`(6) = 1, it returns a vector of 2 values: $[W_{\rm l}\ W_{\rm u}]$.

gammaFbb Auto-correlation function (only up to 2W)

drho Error on the normalized auto-correlation function.

By default the routine generates plots of $\overline{\rho}(\tau)$ and $\tau_{\rm int}^{\rm l}$ with error bars in the relevant range to inspect the required plateau behaviour. In case τ_* is an input the plot shows also $\tau_{\rm int}^{\rm u}$ and the exponential tail together with the value of $W_{\rm u}$. If there are two or more replicas their distribution is shown as a histogram with its Q-value in the title. In addition, in case that a primary observable is analyzed, a histogram of all estimates $a_\alpha^{i,r}$ is displayed.