General Gauss-Markov noise tests; comparison of est_noise, hector, and cats

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This report compares the results from simulations of noisy time series from three programs that quantify the amount of generalized Gauss-Markov noise (GGM). There are two motivations. The first motivation comes from analysis of decades long creepmeter data that measure aseismic slip on the San Andreas fault; these data suggest that the background, natural variations in creep are consistent with a GGM process with a very steep power-law component. Secondly is the observation that, in many cases, the standard deviation of rates calculated by one program, est_noise, can exceed its calculated rate uncertainty by a factor of three. In principle, these two values should be nearly equivalent. On the other hand, for the same set of simulations, the program hector (estimatetrend) yields nearly equivalent values of the standard deviation in rate with its calculated rate uncertainty, as expected. However, results from the program cats are similar to those from from est_noise.

A summary of this comparison is shown in Figure 1 for a variety of different sets of simulations. Specifically, these simulations were carried out as follows; Specify the level of power law noise and its index, the amount of white noise, the characteristic frequency of GGM noise, f_o, and the length of the time series. To obtain the results shown in Figure 1, the power-law amplitude is specified to be 2.7 with an index of 2.5, no white noise, and 10 year long time series with daily sampling and no gaps. The specified GM frequency was varied between 0.01 and 15 cycles/year. A represented power spectra is shown in Figure 2. For each set of simulations, 42 different time series were generated. Each time series was analyzed by each of the three programs and the calculated rates and their uncertainties were tabulated. For est_noise, the program was instructed to calculate the rate and uncertainty using the specified parameters of the simulated time-series. For hector, its parameter, ϕ, was held fixed, and the program optimized the values of power law amplitude and its index. ($\phi = 1 - 2\pi f_o/t_s$, where $t_s = 365.25$) For cats, the power law index and the GM frequency were held fixed while the power-law amplitude optimized. In addition, from the est_noise program, a second rate was also saved as that rate assumed that the time series had no temporal correlations (ie, a diagonal covariance matrix); that is identified as the white-noise solution.

In addition to Figure 1, scatter plots from all of the simulations were made and representative samples are shown in Figures 3 through 5. Each scatter plot shows the results of estimating rate and its uncertainty from each of the 42 simulations. The scatter plots show comparisons of rates calculated by hector and est_noise, hector and the white noise assumption of noise, hector and cats, and est_noise and cats. Ideally, for all four sequences of plots, the rates show fall on a linear, 1 to 1 line, which is provided for convenience. In general, the one-to-one adherence to this trend is found with hector and white noise, and est_noise and cats.

Figure 3 exemplifies the divergence between est_noise/cats and hector where the GM frequency, $f_o = 1.4$. There are two scatter plots where the rates calculated from hector are compared with those calculated by est_noise (upper left) and cats (lower left). Both show a lack of correlation between these sets with hector being in common. On the other hand, the rates calculated by both est_noise and cats show a very strong correlation (lower right) or equivalence. And, the the rates calculated by hector are nearly equivalent to the white-noise model (upper right). These relationships are also illustrated in Figure 1 when $f_o = 1.4$.

Two "end-member" cases are illustrated in Figures 4 and 5. In Figure 4, the GM frequency is specified to be low, $f_o = 0.03$ or equivalent to 33 years, or a factor of 3 longer than the 10 year long time-series. This represents the case where the underlying noise model is close to that of a power law. In that case, the scatter plots in all four cases show a high correlation or that all of the programs provide essentially equivalent values of rates. As expected, the comparison of rates using the white-noise model, show more scatter than those from the other three comparisons as the white noise assumption is clearly violated in the presence of strong temporal correlations.

The results in the other "end-member, Figure 5, show the comparison when the GM frequency is specified to be high, $f_o = 15$ or equivalent to about a month correlation time. In all cases, scatter plots show a strong correlation between the results of the programs and with the white noise model.

The divergence between est_noise/cats and hector for their rate estimates is shown in Figure 1 when $0.2 < f_o < 6$ cycles/yr illustrated by the solid lines. In addition, for a larger range in GM frequencies, $0.02 < f_o < 6$ cycles/yr, the rate uncertainties calculated by est_noise/cats are underestimated by as much as a factor of 4 ($f_o = 1.4$) when compared the standard deviation in rates. Unlike hector where the standard deviation of rates are nearly equivalent to the calculated rate uncertainty (ie, the solid blue line is nearly equivalent to the dashed blue line), the rate uncertainties calculated by both est_noise and cats lie below both their standard deviations in rate and also below the rate uncertainties computed by hector.

Table 1: Comparison of values of estimated power-law amplitude, index, and GM frequency when all are optimized

program	power-law index	power-law amplitude	GM frequency	std. dev rate	rate uncertainty
input noise	2.50	2.70	1.41		
hector	2.52 ± 0.13	2.71 ± 0.19	1.52 ± 0.29	0.0419	0.0376
est_noise	2.50 ± 0.15	2.69 ± 0.14	1.28 ± 0.30	0.1063	0.0263
cats	2.47 ± 0.03	2.64 ± 0.13	1.24 ± 0.29	0.1063	0.0268

error-bars are standard deviation about mean value of noise estimates

A similar relationship between hector and est_noise/cats that is shown in Figure 1 for a power law index of 2.5 also is shown in Figure 6 when the power-law index is 1.5.

I've also verified that all three programs can recover accurately the parameters of the underlying noise model. Again, this was done with 42 simulations of the same set of time series discussed above, but each program was allowed to optimize the parameters that describe the GGM noise. The results are summarized in Table 1. All three programs provide internally consistant values of the noise parameters that are close to the values of the simulations. As discussed above, however, the standard deviation of rates and uncertainties from hector differ from those from est_noise and cats.

I've also compared the log-likelihood metric for the simulations from Table 1. The average difference between est_noise and hector is -1.5 with a standard deviation of those difference is 3.5. Similarly, the difference in log-likelihood between cats and hector is -1.7 with a standard deviation of 3.6. Likewise, there is strong agreement between cats and est_noise with an average difference of -0,2 with a standard deviation of 0.6

So, it is a mystery to me about why the rates (and their uncertainties) differ between hector and the other two programs. One possibility for the differences is the construction of the data covariance matrix. est_noise constructs the covariance matrix from impulse response for GGM. Bos et al. (2014) provides a formula for the covariance matrix for GGM as:

$$Cov(i, i+k) \sim \frac{\Gamma(d+k)\phi^k}{\Gamma(d)\Gamma(1+k)} {}_2F_1(d+k; d; 1+k; \phi^2) \tag{1}$$

where Γ is the gamma function and ${}_2F_1$ is the hypergeometric function. I've coded that equation using the hypergeometric function from Numerical Recipes (it has some limitations). In Figure 7, I show a few comparisons of the first row (or column) of the covariance matrix computed for est_noise and the above covariance function. (Note that for the above equation that, although the lefthand indexes on both i *and* k, the i index is dropped for the righthand portion of the equation, so it doesn't appear complete.) Examining the covariances for two of the three cases, the functional relations between the two programs differ. For the case of first order Gauss-Markov noise (FOGM), where the power index is 2, both hector and est_noise have the same covariance function. However, comparisons that I made above for indices of 2.5 and 1.5 (Figures 1 and 6), FOGM have the same discrepancies. So, it would appear that possible differences in the make-up of the covariance matrices between the two programs is not an explanation.

With est_noise, I've noted previously the divergence between the standard deviations in rates from simulations and their calculated uncertainties. Consequently, I have thought that the calculated uncertainties were too small since the maximum likelihood procedure splits the optimization in two, one for the deterministic function and the other part for the noise model, but didn't consider any possible covariance between the two sets of parameters. For GGM noise, I have thought that there would be a strong linkage between the rate uncertainty and the GM frequency. However, the results from hector doesn't support that idea.

My conclusion, so far, is that both cats and est_noise provide the same results, so I don't think the difference between hector and est_noise/cats is a coding problem, and the problem lies elsewhere. In addition, hector seems to provide rate uncertainties consistent with the actual standard deviation of rates that one gets from simulations. In addition, with GGM as the underlying noise process, I would expect that the estimated rate would be close to that from a white noise model, which is provided by hector but not est_noise or cats.

So, I'm asking for ideas to resolve the differences; although all three programs provide good measures of the amount of GGM noise in time-series data, my results indicate that hector provides the most accurate estimate of rate and its uncertainty.

UPDATE: Work-around for cats and est_noise

After consulting with Machiel Bos and Simon Williams, I realized, at least for GGM noise, that the data covariance matrix needs to account for the time preceding the time series of interest; Machiel calls this "spin-up" time, but I'll call that interval "ghost data". Both est_noise and cats can be fooled to include ghost data by inserting single, phony observation that precedes the real data, then requesting that both programs estimate one additional parameter, that being an offset inserted between the phony observation and the real data. In addition, the input to est_noise needs to be modified such that it will include the phony observation. As a rule of thumb, the phony observation needs to precede the real data by at least 3 times the time constant of the GGM process; for example, if $f_{ggm} = 0.1$ c/yr, then the time constant is $1/(0.1 \times 2\pi)$ or 1.6 years. For est_noise, the work-around caused it to use Cholesky decomposition of the data covariance matrix rather than the *fast*, deconvolution algorithm, which could impact the computation time.

I re-ran the examples discussed above, and Figures 8 and 9 demonstrate the effectiveness of this work-around. For est_noise, as before, I prescribed the known noise parameters so that the program need not search for the optimal solution. Note that Figure 8 should be compared with Figure 1, and Figure 9 should be compared with Figure 3. For the summary plots, Figure 1 and 8, the bulged noted for Figure 1 has disappeared when the work-around was applied to est_noise and cats, Figure 8. Likewise, the scatter plots that compare the rates estimated for all three programs fall almost exactly on the one-to-one line shown in Figure 9.

A few other observations:

- From table above, the use of ghost data is not required to estimate the parameters that characterize GGM noise. But, it is required to estimate the rate and its uncertainty.
- The requirement of ghost data to precede the time series is not needed in the case of power-law noise; with a GGM, the impulse response has a "hump" within the time-constant of its initiation. Insertion of ghost data accounts for that hump. On the other hand, the impulse response for PL noise monotonically decreases (or increases) dependent upon the index consequently, ghost data are not required.

est_noise should be relatively easy to modify to better accommodate GGM noise-model, by slightly rewriting the final computation of the deterministic model (ie, rate and other parameters) by forcing est_noise to use Cholesky decomposition, inserting ghost data, but accounting for them as missing data. This modification should minimally impact the computation speed since, for estimating the noise parameters, the original "fast" (or deconvolution) algorithm is employed, but slower, Cholesky decomposition is employed only at the last step where the rate and its uncertainty is estimated.

UPDATE: Implementing the "fix" for est_noise.

As described above, I made some modifications to est_noise such that manually inserting "ghost" data and an offset is not required. The results are shown in Figures 10 and 11, which are analogues to Figures 8 and 9. Note that I have not used the "work-around" for cats in this example. Essentially, the fixed version of est_noise provides the same results using the "work-around" version described above.

For both hector and est_noise, at least for f_o between 0.03 and 0.1, the standard deviation of rate appears to be less than the rate uncertainties by about 10%. Although I haven't check the calculation, the standard deviation in rate is computed about the mean value of rate. In principle, that standard deviation should be computed about a rate of zero, which would increase the size of the standard deviation.

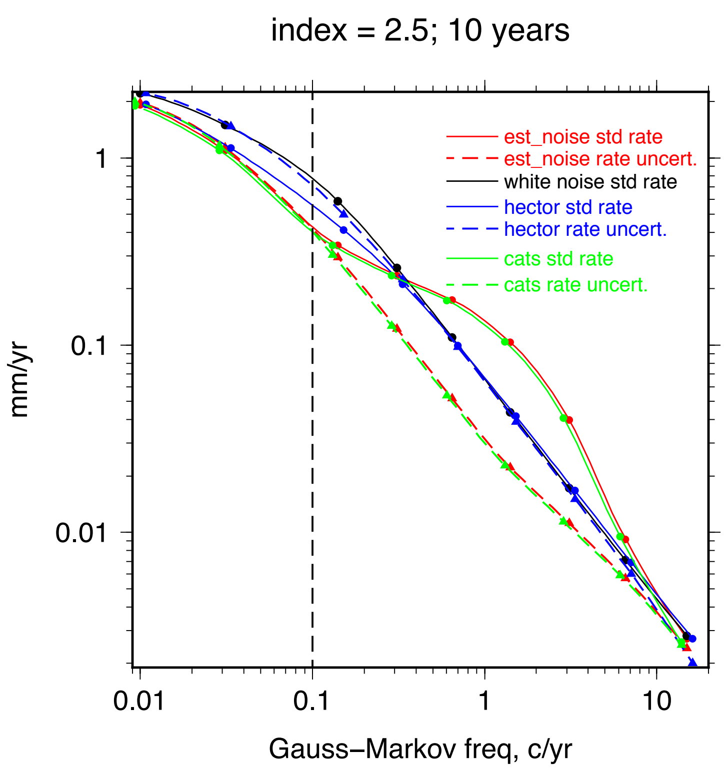

Figure 1: Comparison of standard deviation in rates and rate uncertainties from est_noise, hector, and cats from simulations of generalized, Gauss-Markov noise for a variety of cut-off frequencies, f_o, for power-law index of 2.5 and 10 year long time-series.

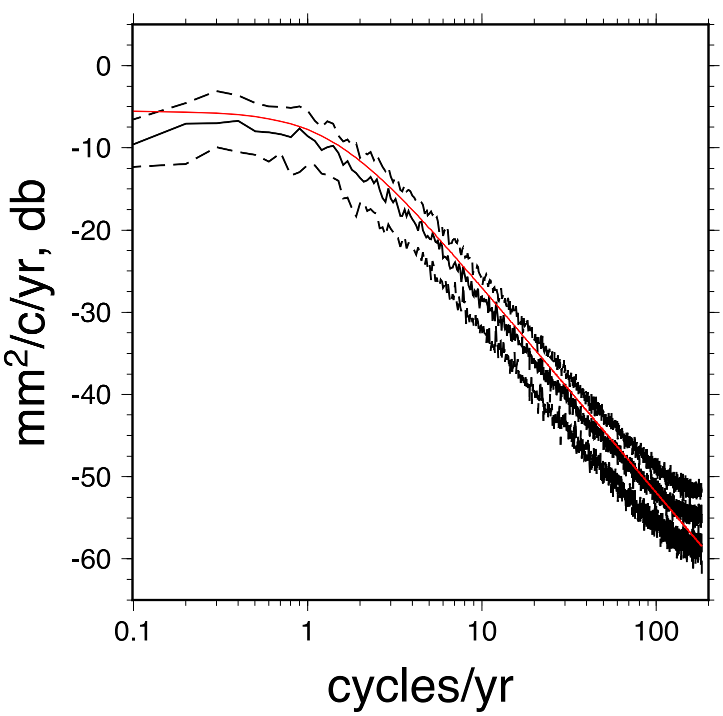

Figure 2: Power spectra for one of the sets of simulations of time series of GGM noise where the power law amplitude and index is 2.7 and 2.5 respectively. The GM frequency is specified to be 1.4 cycle/year. The red trace is the theoretical power spectra while the three black traces are the median and interquartile spectra based upon 100 simulations

GGM04_results_10_1_GGM_1.41_PL2.5.dat

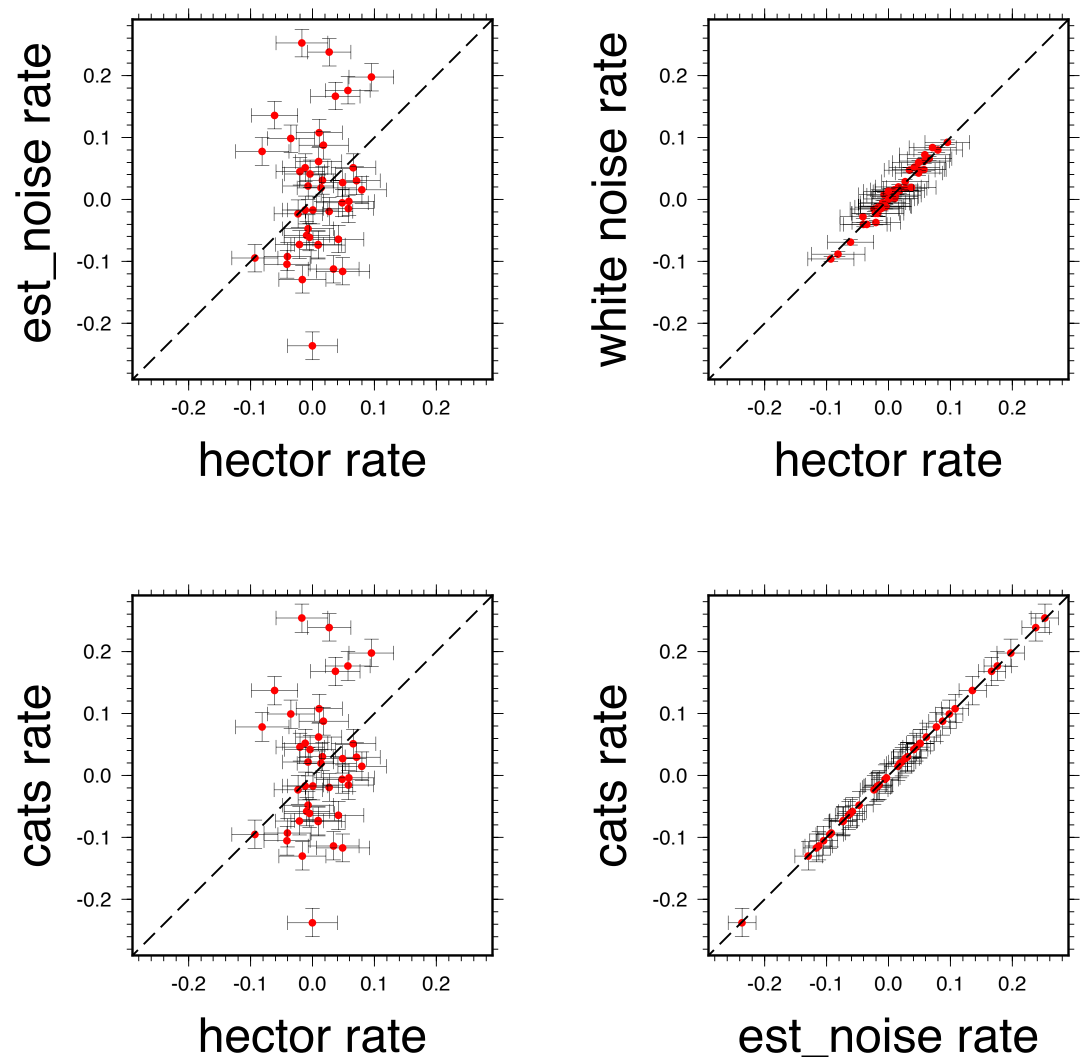

Figure 3: Scatter plots between rates estimated by est_noise, hector, and cats for 42 simulations of 10 year long time series with a power law amplitude and index of 2.7 and 2.5 and **GM of 1.4 cycles/yr**

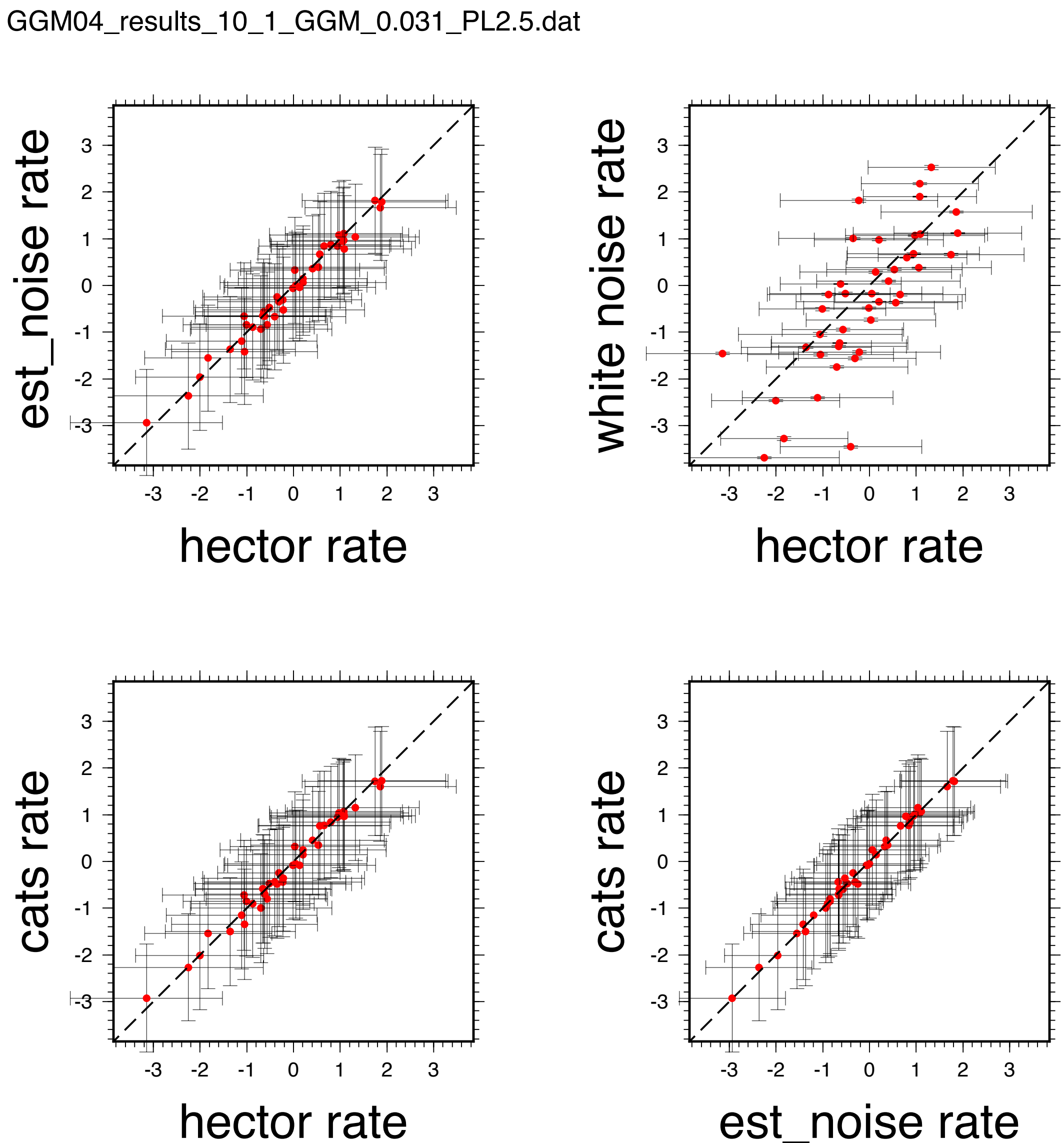

Figure 4: Scatter plots between rates estimated by est_noise, hector, and cats for 42 simulations of 10 year long time series with a power law amplitude and index of 2.7 and 2.5 and **GM of 0.03 cycles/yr**. With a low value of GM frequency, this set of simulations is closer to power-law noise with an index of 2.5

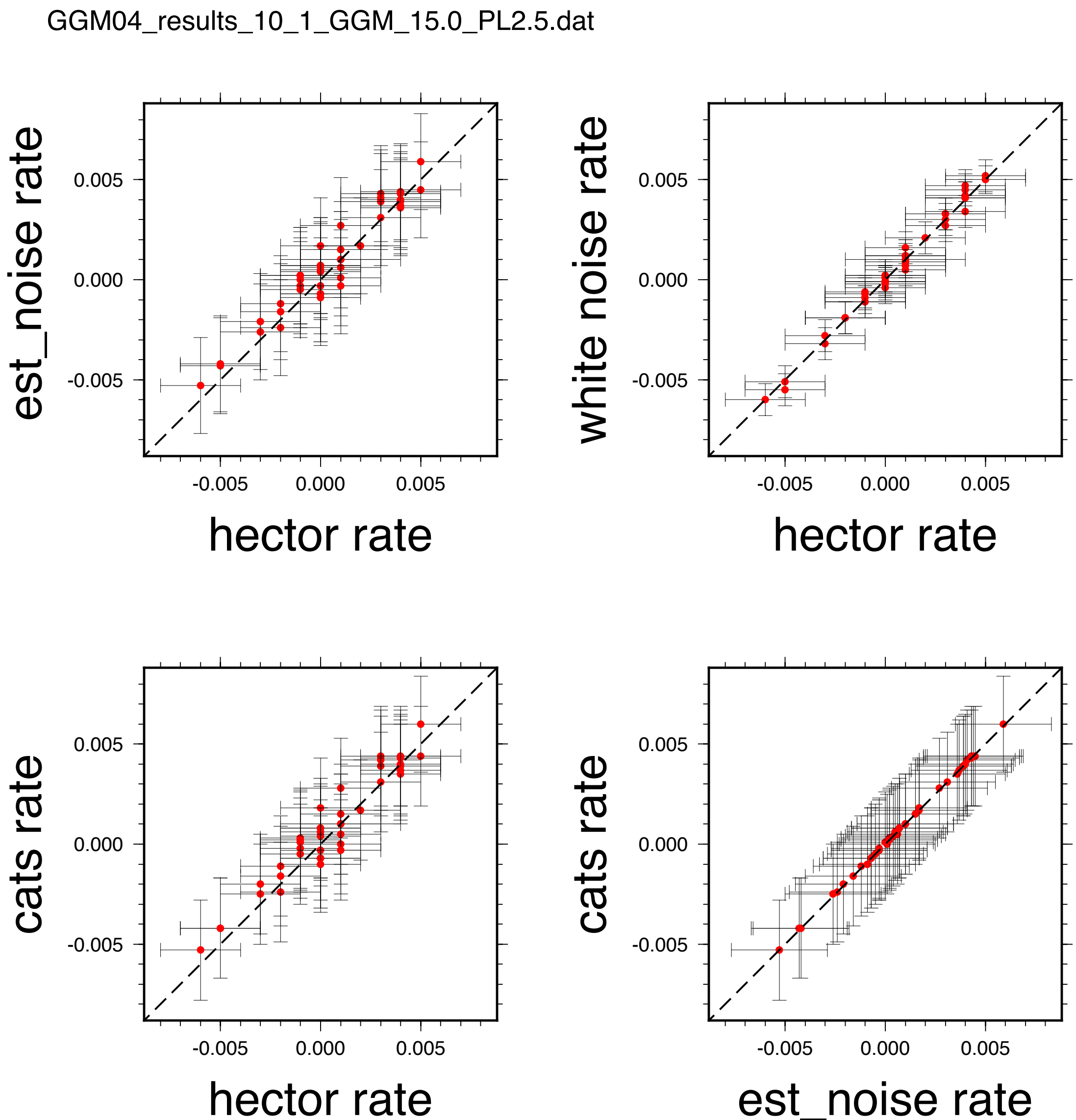

Figure 5: Scatter plots between rates estimated by est_noise, hector, and cats for 42 simulations of 10 year long time series with a power law amplitude and index of 2.7 and 2.5 and **GM of 15 cycles/yr**. With a high value of GM frequency, this set of simulations becomes closer to white noise. Note that the step-wise estimates of rates for hector is due to the limited resolution provided in hector's output.

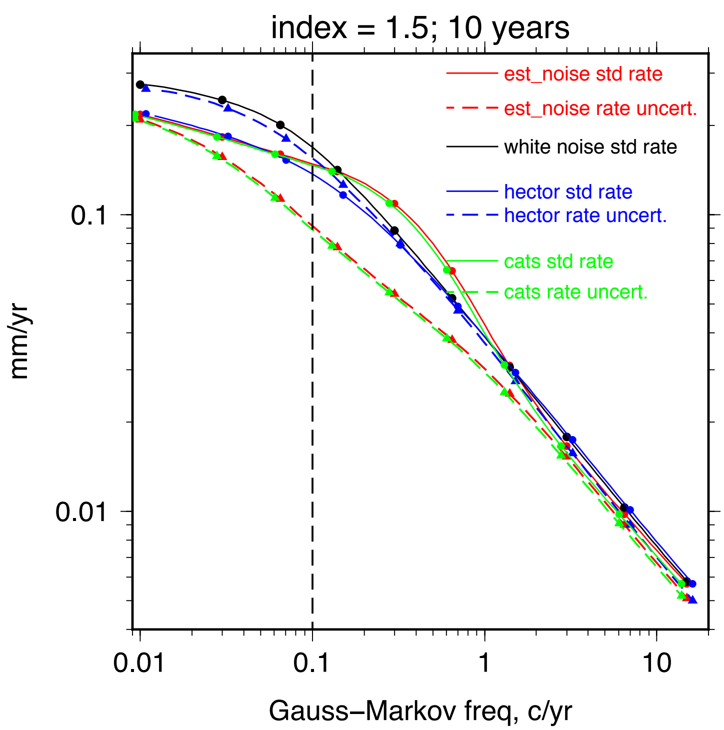

Figure 6: Comparison of standard deviation in rates and rate uncertainties from est_noise, hector, and cats from simulations of generalized, Gauss-Markov noise for a variety of cut-off frequencies, f_o, for power-law index of 1.5 and 10 year long time-series.

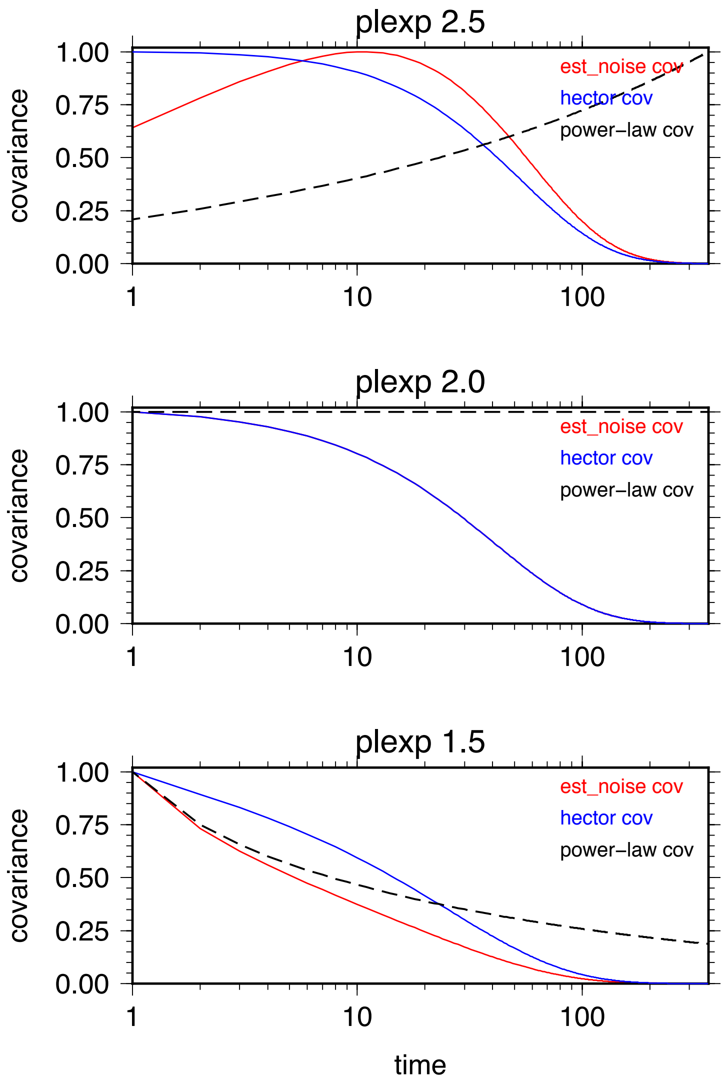

Figure 7: Plots of the first row of the covariance matrix used by est_noise for GGM (red), hector for GGM (blue), and est_noise for power-law noise (dashed black) for difference values of power law indices, 2.5, 2.0, and 1.5. Covariances have been normalized by their maximum value such that the plotted results never exceed 1.0. For all of the GGM covariances, $f_o = 1.4$ cycles/yr.

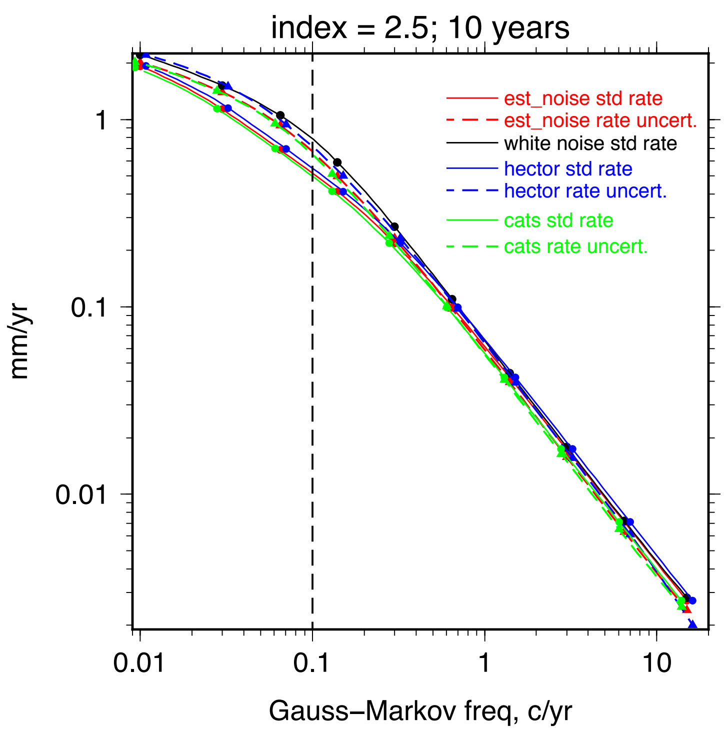

Figure 8: Comparison of standard deviation in rates and rate uncertainties from **work-around** for est_noise and cats with hector for simulations of generalized, Gauss-Markov noise for a variety of cut-off frequencies, f_o, for power-law index of 2.5 and 10 year long time-series.

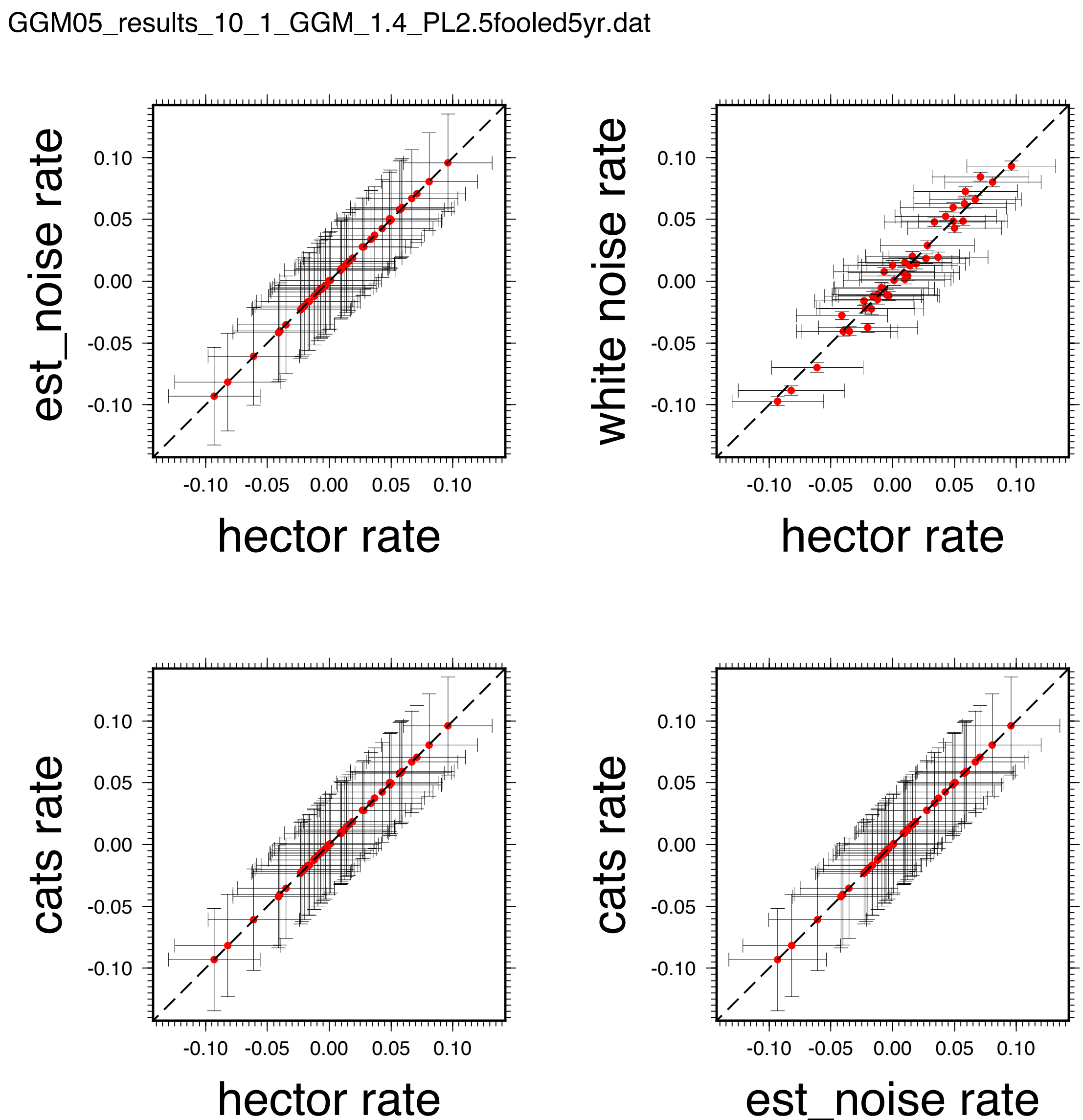

Figure 9: Scatter plots between rates estimated by est_noise, hector, and cats for 42 simulations of 10 year long time series with a power law amplitude and index of 2.7 and 2.5 and **GM of 1.4 cycles/yr**. Note, for est_noise and cats, a work-around described in the text has been employed.

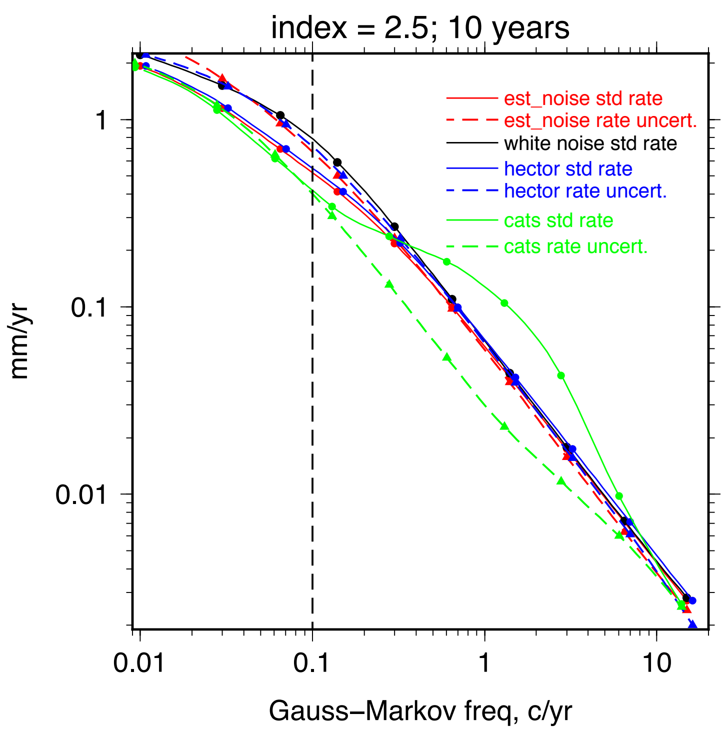

Figure 10: Comparison of standard deviation in rates and rate uncertainties from the **fixed version** for est_noise and cats (unmodified) with hector for simulations of generalized, Gauss-Markov noise for a variety of cut-off frequencies, f_o, for power-law index of 2.5 and 10 year long time-series.

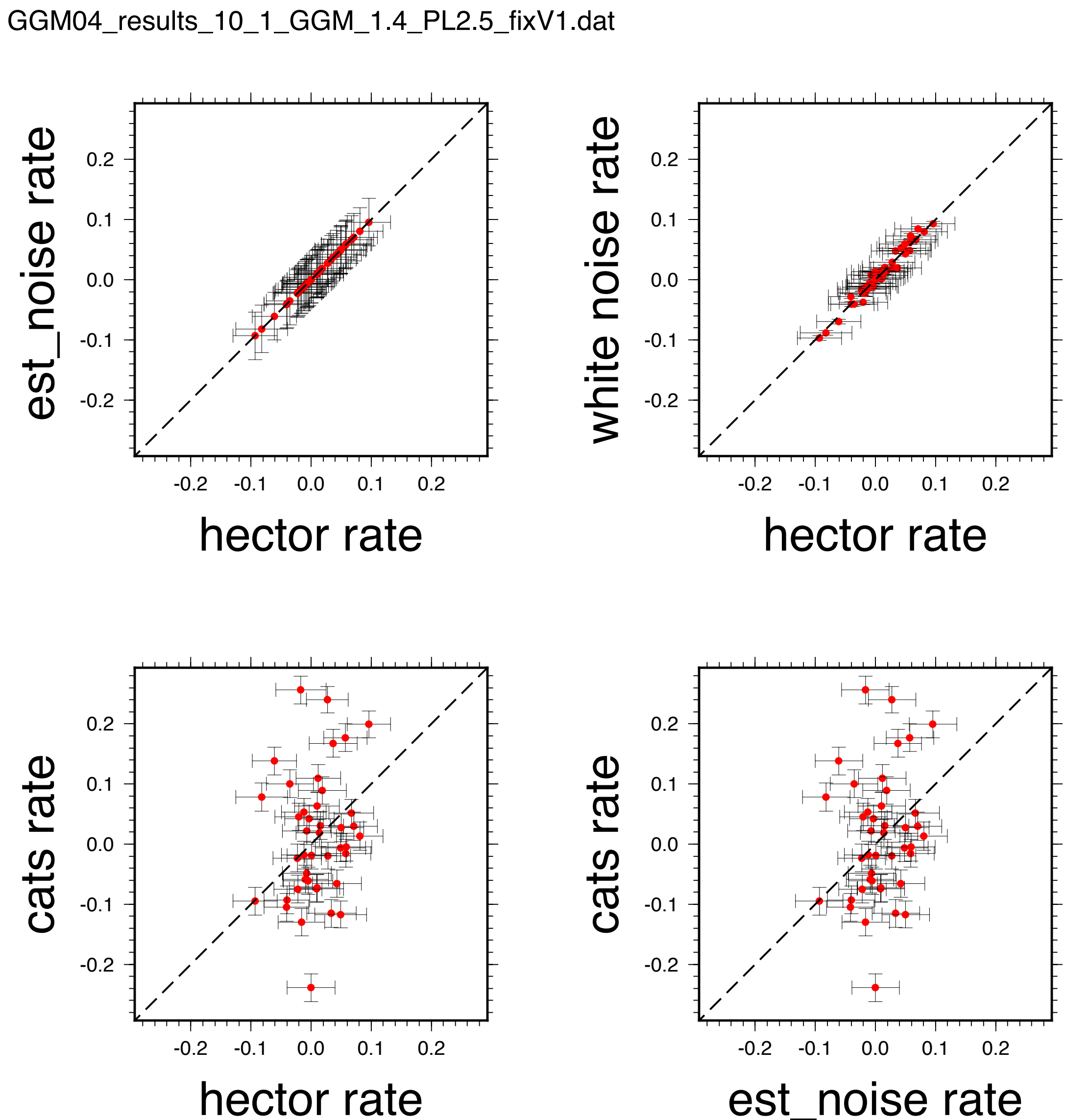

Figure 11: Scatter plots between rates estimated by est_noise, hector, and cats for 42 simulations of 10 year long time series with a power law amplitude and index of 2.7 and 2.5 and **GM of 1.4 cycles/yr**. Note, for est_noise uses the *fixed* version.