1 Response to Reviewer 1

In the following, we denote comments by the reviewer in **bold** and our own reponses in standard fonts.

The manuscript proposes to automatically derive model structures using Gene Expression Programming (GEP) introduced by Ferreira (2001). The authors apply GEP to different components of terrestrial CO2 fluxes measured in an 80 year old deciduous oak plantation in the Alice Holt forest in SE England. The goal is to compare automatically derived model structures with predictions by other machine learning methods and from other published models of ecosystem respiration. The paper is in the scope of the journal and the topic could be interesting for a broad audience of geoscientists. In the present form, I cannot recommend publishing and ask the authors to thoroughly review their manuscript taking the below mentioned points into account. Additionally, the manuscript would benefit from a proofreading by a native speaker.

We would like to thank the reviewer for the evaluation and detailed comments on our manuscript. We further provide responses for the posed questions and details on how we revised the manuscript. Please note that our UK based co-authors had revised the original paper, and have been involved as well in the submission of the revised manuscript.

We would like to mention that all page and line numbers for specifying changes in the manuscript are given based on the difference mark-up file. **Major comments**

1. **The goals stated in the introduction are scattered over page 3 (ll. 34, ll. 2325, ll. 2830). Please state them clearly at the end of the introduction.**

    - The section was re-organized as suggested by the reviewer in the revised manuscript. The goals of this study are now concisely stated (p4 ll 11-19).

2. **GEP is the key part of the manuscript. It is not a standard modelling framework and needs a clear introduction. In the present form, Section 2.1 is difficult to understand for someone not familiar with GEP. Please define clearly what is a gene, a chromosome and an expression tree and how they are related. Use examples for illustration. The original paper by Ferreira (2001) is written for a broad readership and can serve as an**

example. How are the mathematical statements coded in chromosomes evaluated to generate predictions?

- Thank you for pointing this out here. We included a figure explaining the most important processes of the GEP evolution in the revised version of the manuscript (Fig. 3).

  We described more carefully what we understand here as "gene", "chromosome" and an "expression tree" and added the definitions in the **glossary**. We agree that this is absolutely key to the readers (Section 2.1).

3. **The use of the fitness measures is inconsistent throughout the manuscript. In section 2.2 you derive a composite fitness measure CEM and state that this is your final normalized form of the fitness function (eq. 2.3). However, later in the results you report MEF or MEF+NP (that was never property introduced). Explain clearly which function was used to measure the fitness. Also p. 8 l. 45 shows that CEM is apparently not your final fitness function.**

   - We apologize that we have not been sufficiently clear in our descriptions: CEM=MEF+NP+SE (modelling efficiency +number of parameters+ signal complexity measure) is the final fitness function used for optimizing the solutions for all GEP results presented in this paper. The MEF values are reported for quantifying the model-data misfit which is more natural to "read".

     More explanations on MEF+NP were added to the revised manuscript as well. This function is a fitness function similar to CEM, but where the entropy component is missing. This function was introduced in the manuscript in order to better illustrate the effect of each fitness function component for the final GEP solutions performance (p 9 ll 11-15).

4. **What were the functions that were coded in GEP and could thus form algebraic expressions? How did you chose them?**

   - Usually in genetic programming type of approaches, the identification of input functions depends on the type of problem which we try to solve. If we tackle symbolic regressions, as is the case here, most often a set of primitive functions is proposed, such as addition, multiplication, exponential and so on. More complex functions could increase

model complexity too much and risk over fitting. We added a more detailed explanation in the revised manuscript (p 5 ll 18-23).

5. **Section 3.1.1: You state the the machine learning methods (Artificial Neural Networks, Support Vector Machines, Random Forests and Kernel Ridge Regression) were used without tuning the hyperparameters. I have a serious objection here. While some of the hyperparameters could be safely set to default values, others have to be tuned and do affect the performance of those models (e.g. the C2 cost parameter of Support Vector Machines). I recommend that you consult the technical literature here and tune hyperparameters for a fair comparison. A good point to start is the book by Kuhn and Johnson (2013).**

   - *W*e are sorry for the confusion here: we wrote that "All the runs were performed with default settings" e.g. regarding the choice of their Kernels. But we did, of course allow the hyper parameters to vary and adjusted them in a cross-validation approach as described in Camps-Valls2012.

     The only approach run with default settings was the RF approach from the Matlab statistics toolbox implementation.

     The paragraph should say:

     "The toolboxes and settings used for generating the predictions of the ANN and KRR methods are described by Tramontana2016 and found in the "simpleR" regression toolbox Lazaro-Gredilla2014, the predictions of the SVM were obtained by using the "LIBSVM" library Chang2011 from the "simpleR" regression toolbox where the regularization term, the insensitivity tube (tolerated error) and a kernel length scale are automatically adjusted. Lastly, the RF predictions were given by the Matlab statistics toolbox implementation running with default settings. "

     Was corrected in the manuscript (p 8 ll 20-25).

6. **Which predictors did you use for the machine learning methods on the artificial data?**

   - Thank you for pointing this aspect out. All the machine learning methods (GEP, KRR, ANN, SVM and RF) learn based on the same input data set for all artificial problems, which contains 3 candidate variables

(x_1, x_2 and x_3), which means that all methods are allowed to perform a feature selection as well. We apologize that this was no made clear in the manuscript but we have now corrected that p7 l25-26.

7. **p. 9 l. 2932 You state that you log-transformed the fluxes before modelling and back-transformed the model structures. Did you also back-transform the predictions? At least in standard regression, back-transformations need particular attention. When back-transforming from the log transformation, the variance of the residuals has to be considered in order to avoid a bias. Please explain what and how you back-transformed. How did you take care of a possible bias?**

   - For the GEP solutions, we trained on log-transformed target data. That gave us a set of solutions. But of course, in order to obtain the initial fluxes an exponential function was applied to these solutions. From the exponential functions we obtained predictions which are further compared with the original target data and MEF values were reported. So, yes - we back-transformed the resulting structures.
   - For the remaining machine learning approaches (ANN, SVM, RF and KRR) the exponential is applied directly to the predictions obtained after learning from the log-transformed target and the resulting predicted fluxes are compared with the original target by means of MEF.
   - We don't exactly understand the issue of the bias - it would actually matter during the optimization as the cost-function deals with the log-transformed data. But after back transforming, the data are in original space and the evaluation with the MEF should be fine. This means also that the model selection should be unbiassed.

8. **Fig 8 shows a lot of dynamics in residuals from the GEP approach. Because you are dealing with time series, reporting MEF only is not satisfactory. A more in depth comparison of the different models at different time scales is appropriate (e.g. Mahecha et al., 2010). Which temporal patterns can be well reproduced by the different models?**

   - We agree that reporting only MEF values is a bit superficial. However, Figure 13 reveals that model-data miss-match is not only an issue of a certain fast time scale, but clearly also occurs on seasonal time scales.

The Mahecha2010 approach is very useful if we would be able to additionally deal with e.g. trends etc. But for this kind of analysis the time-series are simply too short. These aspects and more are discussed in section 5.4.

9. **From Fig 10 we learn that the machine learning algorithms performed better than GEP. In Section 5.2 you state that GEP underestimates high fluxes as do the published semi-empirical models. So what is the advantage of using a GEP approach? What can we learn from it? I suggest that you restructure your discussion such that this aspect becomes really clear. In the present form Section 5.2 is somehow lost.**

    - Thank you for pointing this out. Indeed, this discussion is at the heart of our philosophical approach: We argue that if GEP identifies structurally very different models that, however, yield equivalent model performance, it puts at question the validity of the conventional semi-empirical models. GEP models reveal that certain dynamics that are typically unconsidered in approaches of this kind, for instance the exponential influence of SWC to respiration components or the seasonal influence of GPP. This section of the discussion was restructured in the revised manuscript for increased clarification of where we see the added value of such an approach (section 5.2, p 19 ll 4-16).

Detailed comments

- **p. 3 l. 14 Explain briefly symbolic regression here and in more details in the method section (p. 4 ll. 9ff). C3**

  A symbolic regression is a type of regression where not only the parameters of a known (linear) function are optimized based on data, but where the functional form itself is also constructed based on data as a combination of basic linear and non-linear mathematical functions. Further expanded in the method section.

- **p. 4 l. 1417 You state that the variables and functions are subsequently mapped to a set of characters, then that the mapping process generates sets of strings. . . And then in the next sentence the mapped letters are randomly combined . . . . This is confusing. State clearly what is the alphabet used to map functions and variables. They cannot be randomly combined: a binary function has to have two inputs, for example, and**

this is taken care of in the coding sequence. The initial chromosomes are generated randomly, however, the genes must be valid mathematical expressions.

The input variables and functions are indeed mapped to characters that are combined into strings which encode the mathematical expressions. The validity of encoded mathematical expression is insured by the internal translation language and by the equation: tail=head*2+1. Thus although each of the sections, head and tail are generated based on random selection from the input characters sets (functions+variables sets for head and variables for tail), there are still rules that insure validity of mathematical expressions (except for cases where a solution can only be deemed invalid by evaluating the expression, such as division by 0, etc)

- **p. 4 l. 32 explain individual.**

  The individual is a component of the evolution population which encodes a specific mathematical expression. It is the same as chromosome. Added better definition in glossary.

- **p. 5 l. 1 How is the hyper-parameter tuned?**

  The hyper-parameter has either some commonly used default values in the community, especially for the genetic operators rations, or some values that have been empirically established with experience, depending on the problem we are looking at.

- **p. 5 l. 89 How is the population diversity related to stochastic bias?**

  Once diversity is insured in the evolution population, we can be more confident that a certain solution does not appear just by chance, as it would have to be good enough to beat a larger pool of solutions.

- **p. 6 l. 2 and eq. 2.2 inconsistent names: SE or S[P]?**

  SE is the name we use for the Shannon entropy. S[P] is changed as well to SE in the manuscript.

- **Give more details on the calculation of the permutation entropy (Bandt and Pompe, 2002). A reader not familiar with the method should be able to understand what you calculated.**

  In short, the calculation of an entropy as a measure for randomness from a time series (e.g. Shannon's entropy) requires to determine a probability

distribution that underlies the time series (or dynamical system), which is usually done by a partitioning step (also called phase space reconstruction in other contexts). This is a fundamental step in the methodology, and various methods have been used to arrive at this probability distribution, for instance frequency or histogram-based measures, procedures based on amplitude statistics, or symbolic dynamics (see e.g Kowalski et al 2011 for an overview). In recent years, the Bandt Pompe approach has become popular, because it directly takes sequences in time into account: The technique hence divides the time series into ordinal sequences (i.e. ordinal patterns, or symbolic sequences), and then computes entropy measures directly from the probability distribution of these ordinal patterns Bandt2002. This approach has a number of advantages, namely that it is robust to noise (no sensitivity to numeric outliers) and to trends or drift in the data, it is an (almost) non-parametric method and no prior assumptions about the data are needed (the only parameter that has to be specified is the embedding dimension, i.e. window length), and allows to disentangle various possible states of the system that are then encoded in the probability distribution (see e.g. Zanin2012 for a review of the method and applications). We described the method in more detail, and give a few examples of its application in the revised manuscript (p 8 l 26– p 9 l 3).

- **Eq. 2.3. I dont understand the last term in your derivation of CEM. Why 1 SE? The permutation entropy varies between 0 and log(n!), n being the order of permutation (n = 4 in your case). Did you normalise SE by its maximum?**

  SE is indeed normalized by its maximum; hence SE varies between 0 and 1, where 1 indicates no correlated structure in the residuals. Furthermore, the best CEM value can take, and towards which the optimized values tend to is 0.

- **Is CEM maximized or minimized?**

  Throughout the entire paper, the optimization is done by minimization of the fitness function value.

- **p. 6 l. 22 Why are model parameters constant values? This term for an entity being optimized is confusing.**

GEP as a method does not offer a specific optimization of parameters, as it evolves entire mathematical formulations. So until there is a special treatment in terms of optimisation for the parameters, they are considered constants. Once a final solution is reached, a specific optimization algorithm is used for

- **p. 7 l. 26 and Tab1: You never explained head and tail of genes.**

  We apologise for the slip. Added to glossary.

- **p. 9 l. 25 Explain briefly how the Singular Spectrum Analysis works and give references to the original publications (Broomhead and King, 1986, for example).**

  The SSA method is a very useful tool used mainly in time series analysis with the purpose of decomposing an original time series into the sum of its components, such as trends, seasonality and high frequency components. More details and the references are added to the revised manuscript (p 13 ll 16-18).

- **p. 10 l. 12 I dont understand how your split you data in training and test data sets. According to p. 8 l. 21 you have two years of hourly observations. So what are the 500 target time steps and why are there 613 time steps in total? How did you calculate the subsets?**

  Thank you for pointing this aspect out. It seems that we have not been clear enough in the description. Data is available with hourly resolution, however, we use daily means for model constructions. So for two years, we should have 732 data points, but after filtering we are left with a gapped set of 613 observations. Those 613 d.p. are split into two sets of 500 and 113 d.p 50 times. For each of this split we then learn a model and the best over-all at validation is finally selected and presented in the results section. Section is revised for clarity.

- **p. 12 l. 2022 What do you mean by a component of Reco not seen in the training procedure? Which components were not modelled?**

  Each component was separately modelled and a solution is built with GEP. Then, the parameters of each of these solutions are re-calibrated using CMA-ES for the rest of the components for a fair comparison of modelling capacity.

- **p. 14 l. 10 Which water reservoir do you refer to? Soil water? Then reservoir is misleading.**

  Indeed we refer to soil water. We apologize for the confusion and water reservoir has been changed to soil water in throughout the revised manuscript.

- **p. 16 l. 13 You state that GEP is not prone to overfitting. How did you analyse this?**

  This was concluded for the results of the increase of signal to noise ratio exercise, as the MEF values of the solutions reconstructed when compared to original, noise free data do not change significantly with addition of noise.

- What are the error bars in Fig3(a), (b) and fig4 (c)? The error bars are the standard errors of the mean MEF values at validation computed over the 10 validation sets (p11 ll8-10). Unfortunately, not visible enough at the scale of the plot. For that, two tables with the concrete values given in the plots was added to the supplementary material of the revised manuscript.

- **Fig3(c) is not necessary.**

  Removed from manuscript as suggested.

- **Fig12 is never discussed in the text.**

  The figure is mentioned in p. 15 l 5. However we agree that it needs more clarification in the manuscript.

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1 Response to Reviewer 2

In the following, we denote comments by the reviewer in **bold** and our own reponses in standard fonts.

Review of Reverse engineering model structures for soil and ecosystem respiration: the potential of gene expression programming

We would like to thank the reviewer for the evaluation and detailed comments on our manuscript. We further provide responses for the posed questions and details on how we revised the manuscript.

Please note that all page and line numbers for specifying changes in the manuscript are given based on the difference mark-up file.

In this manuscript Ilie et al. explore the use of gene expression programming (GEP) to select empirical models for soil and ecosystem respiration. The authors make a case that GEP is a technique for reverse engineering model structures by elucidating underlying mechanisms, rather than depending on hypothesis-driven experiments to identify these mechanisms.

- Indeed, this is our main motivation. But clearly also other methods for reverse engineering may be usable.

I have several concerns about the conceptual framework the authors used to present GEP. I am convinced that GEP is an interesting and worthwhile approach to automate model selection. However, I think it is over-reaching to suggest that GEP can reverse engineer model development. It seems to me that the value of GEP is simply to automate the process of exploring a large number of regression models. I am not convinced that GEP reorganizes the model development process, because regression already is often the first step in model development.

- Thank you for challenging our fundamental ideas. The motivation of this work was indeed to automatize model development. And we believe that a GEP type of approach can help in such an endeavour. But we also agree that GEP is basically doing a selection after rejecting a large number of potential regression models. And this is still very different from classical model building. Although the analyst still has a crucial role in identifying plausible models, and controlling/selecting the parameters of the GEP approach, the cost function and driving variables; the algorithm can assist the analyst by identifying model structures that can be deemed *plausible* in the

first place given the signals present in the data. The proposal of the regression model structure is not made directly by the analyst and rather by the algorithm. The points discussed here were added to the revised manuscript (p 3 ll 18-26.).

Further, I find that the claim that GEP minimizes human influence and perception bias to be strong, as the authors seemingly arbitrarily select the driving variables for the model, regardless of how the model's functional form is derived. From other work we know that selecting a single soil temperature at 5 cm soil depth can give a very different model from selecting a temperature from 15 cm soil depth (Graf et al., Biogeosciences doi:10.5194/bg-5-1175-2008). Similarly selecting to use VWC rather than a parameter like matric potential could be the difference between being able to predict rapid increases in flux with rainfall and not.

- We have provided an initial series of candidate predictors among and GEP automatically does a feature selection. Hence the model development remains a more objective approach. Moreover, GEP is meant to select not only the driver but also the model. Therefore, GEP should be able to deal with cases as the one suggested by the reviewer: different T_{soil} measurement depth can lead to different models. And this was clearly illustrated in the analysis with artificial data. Nevertheless, we agree with the fundamental argument of the reviewer, namely that the initial selection of variables is done by humans and by the availability of data (because we will never have "perfect" driving variables...), but this plagues all types of modelling approaches, not only reverse (p 3 ll 18-22).

In the end, the functions selected by GEP suffer from the same problems as previously used formulae shown in Table 2. All of these functions tend to underestimate large fluxes (hot spots and hot moments). While the form of the functions may hold-up from training datasets to prediction datasets, the specific parametrizations often do not. I believe the authors have done a good job discussing limitations of GEP, and empirical approaches in general, in section 5.1.1. We know biogeochemical fluxes integrate multiple pools, reservoir dynamics and lags, and these are difficult to detect using semi-empirical models. The largest gains recently in representing soil respiration have come from simulating enzyme kinetics and solute diffusion (e.g. DAMM model) as well as simulating microbial growth dynamics. These advances have come from implementing expert knowledge, not from expediting regression model selection.

- We agree that we cannot show yet or beat expert knowledge as encoded e.g. in the DAMM model. Still, we believe that our paper is a first step in this direction. And therefore it is important to showcase this opportunity to the relevant scientific community. The field of reverse engineering is young and cannot look back to half a century of experimental and conceptual work aiming at understanding soil respiration modelling.

Overall I would recommend that this manuscript be rejected in the current form, and the authors re-evaluate the presentation of the GEP method both in terms of creating certainty within the biogeosciences community that the approach is effective and accessible, as well as readily applicable to field data as was demonstrated with the data from Alice Holt.

- We do believe that our model approach is readily applicable and a novel tool offering the same accuracy as classical semi-empirical models but crucial with new opportunities of interpretation.

As was mentioned, I believe the GEP method has considerable potential, but as the manuscript is currently written my concern is that it will pass unnoticed by the community as a whole due to poor accessibility rather than scientific merit.

- We disagree with this comment, aligning with the other reviewer and also with the overall statement of the strong potential of this novel approach. However, the important step is to get this approach integrated into the modelling community (which is rather small) and allow it to be tested and modified. We do believe that a more general approach and presentation actually will promote its wider usage.

General Comments:

1. **I do not agree with Figure 1, that model development starts with expert knowledge. Expert knowledge does not come about on its own, but comes from observations, and regressions are critical to making sense of observations. By helping to identify which variables among a large number of potential explanatory variables correlate to a phenomenon, regression-type analyses lead to the second step in the scientific process: manipulative experiments to confirm hypothesized cause-and-effect relationships. Demonstrating cause-and-effect relationships limits the number of processes that need to be represented in models. I am not convinced that GEP provides a short-cut to this process.**

- We thank the reviewer for his valuable point-of view. Maybe the question is rather what one would call "expert knowledge"? We do see observation as one key element of expert knowledge (Fig 1 now includes " including observations") , leading to a first empirically driven (i.e. regression style) approach to model formulation. Yet, once a model could not be immediately rejected it is propagated and used time and again and refined with including more processes etc. This is a tedious process. And here we see that GEP offers a considerable potential indeed. Maybe we have overstated the value of GEP in the manuscript and we revised it accordingly (p3 ll 19-26), but once again - our motivation was thinking and exploring methods that elegantly bypass this approach. For instance, several of the co-authors have worked on the (Migliavacca et al 2011) paper to build a better model for ecosystem respiration in deciduous forests and come to the conclusion that this should be a job realized by a computer. Figure 1 was changed in the manuscript in order to capture and illustrate the points discussed here as well.

2. **Section 3.1 and 4.1, which outline artificial experiments with the GEP method could be strengthened considerably if the authors were to use a simple, mechanistic model of soil or ecosystem respiration rather than a seemingly random set of algebraic expressions. Using such a respiration model would allow the authors to attempt to recover the model basis functions and, if successful, enhance the readers confidence with respect to the data from the site at Alice Holt.**

   - In this sections we mean to show the capacity of GEP to reconstruct functions from relatively simple example in order to shortly explore the effects of increasing non-linearity and number of variables. As ecological models tend to be more complex and the increase in non-linearity and complexity would no be so clear we chose to stick to some known genetic programming benchmark functions.

     Nevertheless we agree with the reviewer that adding a known ecological respiration model structure in the set of functions to be reconstructed would give more confidence in the application of GEP to ecological modelling. Thus the Q_{10} model is added to the GEP benchmark function set. (p 4 l 25 and p 10 ll 27-28).

3. **I am concerned about the evaluations of GEP presented in Figs. 3 and 4. Fig 3 compares alternate machine learning techniques by comparing the MEF of the final model selected by each approach. It seems to me also important to compare the actual model structures, not just the fitness score. Did all the techniques recover the original models? If not, is variation in the MEF meaningful?**

    - In this study, GEP is the only approach which gives a readable model structure back. SVM, ANN, RF and KRR lack that property. Thus the comparison is done on the accuracy of predictions, by comparing the modelling scores and residuals.

4. **Figure 4c suggests that GEP was only able to recover about 30-55% of the correct number of parameters. If so, it seems GEP did NOT do a good job of recovering the original models.**

    - We agree that at first glance, it would seem bad that the model retrieval with GEP based on the 3 different fitness functions gives a lower number of parameters than the initial number. However considering the high values of MEF when validating against original data, MEF$>$ 0.96, we can draw the conclusion that the GEP performed a feature selection, eliminating "low impact" parameters and returned a more simple equivalent solution.

5. **Another major concern is the exercise shown in figure 7. The authors have examined whether summing predicted component fluxes gives predicted total fluxes that resemble observations. This is an interesting idea, but ultimately not that useful for two reasons:**

    (a) The observed fluxes were not independently measured, e.g. Rauto was not measured independently, but was calculated by measuring the total flux (Rsoil) minus RH. I think you want to test whether all the variability simulated for the components can explain the variability observed for the total flux, but you dont have a measure of the component fluxes independent from the total flux.

    (b) We would like to see that the predictions for total flux are no worse than the predictions for the component fluxes. But in several cases the prediction for component fluxes are pretty poor. E.g. Predictions for RECO wont turn out any better than predictions for Rabove, which themselves were poor. Thats not so interesting.

(a) We agree that because of learning from derived fluxes, it would be hard make a clear statement regarding the capacity of GEP to learn the variability of the studied sum and component fluxes.

(b) We believe that nevertheless the exercise is useful as it shows that when we use GEP to learn models for each of the flux, sometimes the low-complexity pressure in the fitness functions make that the final solution has a lower number of parameters and a slightly lower modelling capacity as well. However we see that when we sum up the models of the component fluxes and compare the predictions of these derived models with the original data, although the models have become more complex, the model performance is not significantly improved. This give us more confidence to state that the more simple models retrieved by GEP in the first place have a sufficient capacity to capture the meaningful information present in the data as well.

6. **The manuscript is figure heavy, consider condensing figures or removing. For example can Figures 5 and 9 be combined in an effective way? Are there other figures that may be unnecessary to the reader if they were described in the text or in a table?**

   - Although we agree that the manuscript contains many figures, we believe most are necessary (or at least helpful) for reflecting the full picture presented in the text.

Specific comments:

- **Abstract is long, introduces a lot of terminology. Consider distilling to the most important take-homes, and make more approachable for a general audience.**

  The abstract was be shortened and simplified as suggested.

- **p.3 l. 8. The rationale for reordering should also be to try more options, things that people might miss**

  We would like to thank the reviewer for pointing this out. We agree that the increase in the option pool is a large aspect of our approach and somehow we believed that it would be self-explanatory, however it makes sense to state clearly as well. The aspect is added to the manuscript (p 3 l 13-15).

- **p. 3. L. 30. Why would we expect the functions to be portable across scales? Provide an ecological justification, otherwise this is not an interesting or useful exercise.**

  We believe that this would be more of a wider discussion of the way in which scaling of ecological models is at all interesting and relevant (Urban 2005).

  What we started exploring here is whether a larger grain model would be capable to capture some very strongly influential divers, even by losing specific information and if such processes indeed appear across scales.

- **p. 3. L. 22-35. When reading initially I found it difficult to understand what hypotheses the authors were testing. I think all of this information is there but needs to be re-organized to make it stand out to the reader.**

  Hypotheses and scope of the paper have been re-organized for clarity as it was suggested by other referee as well (p4 ll 11-19).

- **p.4 ll. 5.No need to introduce the conclusions. Consider shortening this to reduce repetition.**

  Thank you for you suggestion. Paragraph removed.

- **2.1 This section was not clearly written, I suggest more careful editing by co-authors. Please avoid including extra words in parantheses, they add complexity without clarity.**

  Section 2.1 was re-written for more flow clarity in the revised manuscript as suggested.

- **p.4 ll.15. Is the process of mapping operations to strings relevant to model fitting? I dont think so. Either this is excessive detail about the internal workings of GEP, or you need to explain how this is relevant.**

  The process is relevant as it is one of the characteristics of the GEP approach. We apologize for not making this clear in the manuscript already, however this aspect and the effects of mapping have been explained in more detail in the method section (2.1) of the revised manuscript (p 5 ll 24-27).

- **p. 4. L. 20, what do you mean by solution The final selected model? Or the respiration predicted by that model? Genes and chromosomes should be presented in quotations initially.**

Solution is the final selected model structure. Quotations are added as suggested.

- **p. 4 l. 30 I think you can shorten this paragraph to one sentence, simply state that in each generation, the best variants of a chromosome are determined by a fitness function described below.**

  The paragraph could be shortened, however the suggested line is not accurate as in a generation, there is only a variant for each chromosome , and the fitness function determines the ranking of all chromosomes in that generation.

- **p. 4 l. 32, what is an individual? Do chromosomes make up individuals?** An individual is a chromosome that encodes a mathematical formulation, made up by a set of strings called genes.

- **p. 5, l. 1 What is a hyper-parameter? Again, please try to avoid parenthetical phrases in this paragraph.**

  A hyper-parameter is a set of parameters which need to be set for the runs of a certain approach. Definition is added to glossary and further parentheses are avoided.

- **p. 5, ll. 12 upon request rather than on demand.**

  Changed as suggested.

- **p. 5, l. 11-14 most of this information doesnt appear useful, for example, does it actually matter that the cluster had 51 nodes? If someone ran it on a cluster with 12 nodes would it also work but be slower? Either explain the relevance of these details or remove them.**

  The description of the system on which all experiments should be relevant as the results might be influenced by the hardware set-up, due to the initialization of the random seed, speed of solution return and so on. Nevertheless, all non-necessary specification are removed.

- **p. 5, ll. 31 Consider omitting derived from information-theoretic considerations.**

  Thank you for the suggestion. Omitted.

- **p. 6, ll. 20-25. I didnt understand the reason for this additional optimization. This sounds very much like ordinary regression model selection; does this undermine the unique value of GEP?** The original GEP gives a solution in the form of a general mathematical structure. For accurate scaling a further parameter optimization would be recommended. The value of GEP lays in the capacity of constructing the structure based on the on information found in the input data.

- **p. 6, ll. 27 Scaling noise with signal amplitude: This is good to include! This has been shown for soil respiration too (Lavoie et al. 2015, JGR-Biogeosciences, doi: 10.1002/2014JG002773)**

  Thank you for providing the reference. Added to paragraph.

- **Section 3.2.1 The first two paragraphs are repetitive in describing computation of GPP.Consider omitting or shortening the section on soil flux measurements, since these methods were reported previously.** Section 3.2.1 re-organized and shortened as suggested.

- **Section 3.2.4 This paragraph can be removed to shorten. Figure 3c, consider omitting. It is repetitive, and the manuscript already has a large number of figures.**

  Figure 3c removed. However we believe that the paragraph is needed for anticipating the comparison done on real observation between established models for terrestrial respiration in the community and the GEP based models.

- **p.12, l. 7 Sentence starting We find that the global modelling performance. . . Please reword, I dont understand this statement.**

  Reworded for clarity as suggested (p 16 ll 1-8).

- **Figure 12, is there a reason that this is presented in a polar plot? It seems on first glance that it could equally be presented as a 4-pane set of cartesian time series plots.**

  By using polar plots, we reveal that the seasonal biases of the studied fluxes and the capacity of the models to capture/or not some of the variations in specific times of the year. But yes, it is a matter of taste as well.

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Reverse engineering model structures for soil and ecosystem respiration: the potential of gene expression programming

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Abstract.

~~Accurate modelling~~

Accurate model representation of land-atmosphere carbon fluxes is essential for ~~future~~ climate projections. However, the exact responses of carbon cycle processes to climatic drivers often remain uncertain. Presently, knowledge derived from experiments, complemented with a steadily evolving body of mechanistic theory provides the main basis for developing ~~the respective~~ such models. The strongly increasing availability of measurements may ~~complicate the traditional hypothesis driven path to developing mechanistic models, but it may~~ facilitate new ways of identifying suitable model structures using machine learning~~as well. Here~~. Here, we explore the potential ~~to derive model formulations automatically from data based on~~ of gene expression programming (GEP) ~~. GEP automatically (re)combines various mathematical operators to model formulations that are further evolved, eventually identifying the most suitable~~ to derive relevant model formulations based solely on the signals present in data by automatically applying various mathematical transformations to potential predictors and repeatedly evolving the resulting model structures. In contrast to most other machine learning regression techniques, the GEP approach generates "readable" models that allow for prediction and possibly for interpretation. Our study is based on two cases: artificially generated data and real observations. Simulations based on artificial data show that GEP is successful in identifying prescribed functions with the prediction capacity of the models comparable to four state-of-the-art machine learning methods (Random Forests, Support Vector Machines, Artificial Neural Networks, and Kernel Ridge Regressions). ~~The case of real observations explores~~ Based on real observations we explore the responses of the different components of terrestrial respiration at an oak forest in south-east England. We find that the GEP retrieved models are often better in prediction than some established res-

piration models. ~~Furthermore, the structure of the GEP models offers new insights to driver selection and interactions. We~~ Based on their structures, we find previously unconsidered exponential dependencies of respiration on seasonal ecosystem carbon assimilation and water dynamics. ~~However, we also~~ We noticed that the GEP models are only partly portable across respiration components; ~~equifinality issues possibly preventing~~ the identification of a "general" terrestrial respiration model possibly prevented by equifinality issues. Overall, GEP is a promising tool ~~to uncover~~ for uncovering new model structures for terrestrial ecology in the data rich era, complementing ~~the traditional approach of model building~~more traditional modelling approaches.

Highlights

- We explore if the process of model building for describing ecosystem CO_2 fluxes can be~~automatized~~, to a large extent, automated .
- We show that Gene Expression Programming combined with parameter optimization can be a useful algorithm to automatically derive models from ecological time series.
- We propose alternative models for the influence of key environmental variables on various respiratory fluxes CO_2 in an oak forest.
- Conventional ecosystem response functions can be revised by new models identified with GEP.

1 Introduction

One prerequisite to understand and anticipate the global consequences of anthropogenic climate change is an accurate quantitative description of the terrestrial carbon cycle (Bonan, 2008; Heimann and Reichstein, 2008; Luo et al., 2015). However, the description of the mechanisms underlying the total terrestrial efflux of CO_2 (Peng et al., 2014a), often referred to as "terrestrial ecosystem respiration" (R_{eco}), varies across the scientific literature and existing global models. This is partly because R_{eco} does not originate from a single process but is the sum of fluxes from different autotrophic and heterotrophic respiration processes that operate across different temporal and spatial scales and compartments (e.g. soil depths). Hence, it is experimentally very difficult to disentangle the main abiotic and biotic factors driving respiratory processes at the ecosystem level (Trumbore, 2006) and to derive suitable models for the individual respiration processes. In the remaining manuscript we use the term "model" as an equivalent of "response functions" i.e. some analytic description of how environmental drivers influence ecosystem fluxes.

Traditionally, respiration models have been based on some theoretical considerations but largely remain empirical in nature (e.g. Reichstein and Beer, 2008; Gilmanov et al., 2010; Hoffmann et al., 2015). Conventional model building (Fig. 1) is primarily hypothesis driven and capitalizes both on some understanding of the system and reported scaled experiments (Migliavacca et al., 2012; Richardson et al., 2008). Gupta et al. (2012) describe this common paradigm of model development as a four step approach involving *a*) observational, *b*) conceptual, *c*) mathematical and, *d*) computational phases (see also e.g. Bennett

et al., 2010; Williams et al., 2009). During the observational phase, the system under scrutiny is monitored and observations are assembled, ideally representing process responses to hypothesized driving variables. Based on these observations, a conceptual model is proposed, which is subsequently guiding the formulations of mathematical representations of the system states and dependencies. The mathematical description then provides the basis for computational models that are used for simulations (Jakeman et al., 2006). Model-data integration may additionally lead to iterative structural revisions or parameter optimizations (Williams et al., 2009). This conventional approach to model development is also characteristic ~~to~~ of different kinds of ecological model building~~of different kind~~, including the development of biogeochemical models (Williams et al., 2009).

~~The fundamental question addressed in this paper is whether models can be constructed more objectively, i.e. reducing the need for human intuition and expert knowledge. Specifically, we~~ We explore the possibility of reverse engineering offering an automated alternative to model development for predicting terrestrial carbon fluxes (Fig. 1). In reverse engineering, the work flow is fundamentally different (Bongard and Lipson, 2007): *a*) database set-up phase, *b*) computational phase, *c*) mathematical phase and a *d*) conceptual phase (Gupta et al., 2012). The rationale behind reordering the key phases is firstly to minimize the human influence and perception biases that might shape the formulation of new hypotheses, and secondly to increase the chance for novel model structures to automatically emerge from the available data and that would not be so obvious from a direct analysis. Reverse engineering is aiming at identifying some mathematical representation of a system that is to a large degree independent from a priori conceptualizations; in the current case, the respiratory response of terrestrial ecosystems to environmental drivers. Reverse engineering leaves the model construction up to an algorithm and is therefore a way to empirically learn from observations with minimal user input. ~~Therefore, reverse engineering is related~~

Of course, expert knowledge still has a large influence on the modelling process, as only a certain set of variables can be measured and even a smaller subset is indeed available for model development, which includes the restriction to a certain plausible number of time lags, and hence full objectivity of automatic model development cannot be truly achieved. Furthermore, expert knowledge comes into play when the algorithm is set for running, by tuning the set of parameters according to the problem needed to be solved and as well during the observation collection and during the final decision on whether the solution returned by the algorithm actually makes sense at all and whether it can be further used. Nevertheless, we believe that by shifting the moment when the analyst make the decision regarding the selected model, a larger degree of objectivity in modelling is achieved.

Reverse engineering is close to machine learning based regression techniques, where various candidate model formulations and specifications are explored in order to minimize the prediction error. The fundamental difference from typical model building is that reverse engineering typically provides a symbolic regression, that is, the resulting structures are ideally directly readable as mathematical functions (i.e. response functions) and can be interpreted. ~~Further, one can scientifically~~ The readable character of the returned solutions allows to consider the applicability of the derived structures in other system domains (Ashworth et al., 2012).

Here, we focus on the “Gene Expression Programming" (GEP, Ferreira, 2001) reverse engineering approach. GEP is an evolutionary algorithm that ~~evolves~~ constructs mathematical response functions. ~~The structural designof GEP allows for its use~~ In its essence, GEP basically converges to a solution after rejecting a large number of potential regression models over a

certain amount of evolutionary steps. Due to its structural design, GEP can be applied in a wide range of empirical modelling problems (Peng et al., 2014b; Khatibi et al., 2013; Traore and Guven, 2013), including (soil) hydrology (Fernando et al., 2009; Hashmi and Shamseldin, 2014). To the best of our knowledge the potential of GEP has not yet been explored for modelling ~~biogeochmical~~ biogeochemical fluxes in terrestrial ecosystems.

We seek to understand as well whether automating model development can provide new insights in understanding the dynamics of terrestrial respiration processes. We ~~investigate if automatically derived model structures differ substantially from models conventionally used in the study of R_{eco} and its components or, if they are consistent with established theory. We~~ base our study on data from a long-term monitoring experiment of R_{eco} components i.e. above ground respiration, root respiration, mycorrhiza respiration, soil autotrophic, and soil heterotrophic respiration. The monitoring was done separately but in a time-synchronized way over two years and is described in detail by Heinemeyer et al. (2012). ~~The~~

The fundamental question addressed in this paper is whether regression models can be constructed more objectively by leaving the task of proposing a final regression model to an algorithm rather than directly to an analyst. The need for human intuition during the actual process of constructing a regression model becomes reduced, and the input of expert knowledge shifts towards identifying input variables, parameters, a suitable cost function and model plausibility.

With the current study we investigate as well if automatically derived model structures differ substantially from models conventionally used in the study of R_{eco} and its components or, if they are consistent with established theory. The separation of R_{eco} into its components also allowed us to test the portability of individual model structures across different respiration components. In this sense, we investigate whether a generic “respiration" response can be derived, or if specific formulations for a range of respiration components are required.

~~Our study is structured as follows: First~~

1.1 Study structure

First, we introduce the GEP methodology and explore its performance for symbolic regression type of problems using an artificial experiment under varying degrees of noise contamination designed to resemble R_{eco}. Second, we apply GEP to model the various respiration observations provided by Heinemeyer et al. (2012). ~~This is an exceptionaldata record, as typically only integrated measurements of either soil (Heinemeyer et al., 2012)~~

The observational record provided by Heinemeyer et al. (2012) is exceptional, because measurements of soil or ecosystem respiration ~~are~~ that are typically only integrated, are here continuously and regularly measured, and the components measured offer a perfect test case for the GEP methodology.

For both the artificial experiment and real world observations, we systematically confront the prediction error of GEP with other state-of-the-art machine learning regression approaches. In addition, we adjust the modelling approach such that the objective function (or fitness function) accounts not only for absolute or relative error, but also reduces structure in the residuals. The discussion focuses on the comparison of the various GEP derived models, their equifinality, and performance compared to widely used literature models. ~~Conclusions and outlook focus on the potential of the discussed GEP approach for the further applications in this branch of research.~~

2 Method

We rely on the GEP method (Ferreira, 2001) which automatically ~~derives model structures from~~ constructs model structures based on a set of given observations. As the models we want to obtain are mathematical structures, their ~~extraction~~ construction can be achieved by solving a symbolic regression (Kotanchek et al., 2013) type of problem. That is, we are not only interested in determining an optimal set of parameters for a known regression, but here, we want to discover the symbolic form of the regression itself by identifying the most important predictors and their functional transformations. The general GEP approach in solving symbolic regressions is presented in the following section and is illustrated in Fig. 2.

2.1 Gene Expression Programming, GEP

~~In GEP the structure building process starts with a set of possible explanatory variables and a set of elementary functions that are given as input (~~The process of finding the most suitable model structure based on signal present in data in GEP starts with an initial generation of n possible model structures (Fig. 3a). These can be called evolution individuals and in GEP, they are known as “chromosomes". The chromosomes are composed of a set number of “genes" that are connected by a binary mathematical operator. Each gene is encoded in a string with a set fixed length that contains specific characters that map to either a set of possible predictors, e.g. ~~$\sin, +, -, \times$~~). ~~The variables and functions are subsequently mapped to a set of characters (e. g. $a, b, c, +, -$) according to an internal coding language called “ Karva language~~ $A = \{a, b\} \rightarrow A_m = \{x_1, x_2\}$ or a set of their possible functional transformations, e.g. $F = \{+, -, L, E\} \rightarrow F_m = \{$addition,substraction,logarithm,exponential$\}$, (see Fig. 3a).

The choice of input functions used for applying mathematical transformations on the predictors depends on the type of problem we try to solve with GEP. When the problem is a symbolic regression type of problem, as here, most often a set of primitive functions is proposed; such as addition, multiplication, exponential and so on. More complex functions could increase model complexity too much and risk over fitting. However if there are already known functional transformations of certain predictors that could be part of the final desired solution, the user can define a new function and introduce it in the set of input functions.

All genes are made up of a “ gene head"~~(Ferreira, 2006). The mapping process generates sets of strings that represent the basis for a manipulative evolutionof operations. The mapped letters are randomly combined into fixed lengthstrings called “genes~~, containing a combination of characters mapping to both predictors and functional transformations and a “ gene tail", with characters that map only to predictors. The gene length is given by $g_l = h_l + t_l$, where $t_l = (f_{max} - 1) \times h_l + 1$, with g_l as gene length, h_l head length, t_l tail length and f_{max} as the maximum parity of a functional transformation.

As in biology evolution, regardless of the actual length, the GEP genes have active sections of variable length called “open reading frames" (~~Fig. **??** of suppl.). The~~ ORF) that can encode various expression trees which can be evaluated into mathematical expressions (Ferreira, 2006). The lengths of the ORFs are determined only after the encoded expression trees are translated using an internal reading language (see Fig. 3b). Ferreira (2001) argues that, the power of GEP lies in its use of

fixed length linear strings for representing expression trees (ET) of varied shapes and sizes ~~,~~ that simplifies the evolutionary process~~of GEP (Ferreira, 2001).~~

~~A set number of genes is aggregated into a chromosome with the help of a binary function (e.g. $+, -, \times$). The resulting chromosomes can be translated into expression trees encoding mathematical structures. The chromosomes are the objects involved in the evolution (extraction) of the final solution . The total sum of combinations of functions and variables, i.e. mathematical structures formed during an evolution time~~ , and helps reach a final solution faster.

The total number of chromosomes generated over each evolution step make up ~~a generation~~the GEP population. The evolution steps are also known as "generations". The maximum number of generations ~~needed to reach~~ allowed to run until reaching a solution is often used as a stopping criterion.

One ~~deciding factors in constructing a model during~~ of the crucial components of model developing within an evolutionary algorithm is the selection process. ~~Since~~ In GEP, the chromosomes can be translated into mathematical expressions that can be evaluated, ~~"fitness values" (i.e. measures of model performance) are assigned to each chromosome during each generation. Depending on the fitness function, the fitness values can be crucial as they give a measure of how distant each of~~ and a distance between the current structure based predictions ~~is from the observations. The fitness measures are assigned to the chromosomes~~ and the original target is computed. The measures are known as "fitness values" and are assigned to all the chromosomes in the population at each generation by means of a ~~fitness function that is optimized~~predefined fitness function. The evolution of the final solution with GEP is done based on optimizing the fitness function values after each generation, usually by minimizing prediction error~~. Based on~~ , but more complex criteria can be taken into account as well.

Once all the fitness values have been computed and assigned, the chromosomes in a generation are sorted ~~and a selection for a new time step generation is made.~~ from best to worst fit.

~~The best chromosome , which is also replicated once for the subsequent generation , and the remaining selected chromosomes can go through a set of genetic manipulations that produce new individuals with new associated fitness measures. The manipulation rate is an important~~ If no stop criteria has been met, preparations for the reproduction of new chromosomes for the next generation are made. The chromosome with the best fitness value is reproduced unchanged in the first position of the new generation. For filling the remaining n-1 positions, chromosomes are selected from the entire population for the new generation with a tournament procedure, n-1 times.

In tournament selection, 2 chromosomes are randomly selected from the entire population and the individual with the better fitness value one goes through.

For insuring that novel material is introduced in the pool of possible model structures, and n-1 newly selected chromosomes are subject to genetic operators, such as: mutation, recombination, transposition and inversion as presented in Fig. 3d, that can fully change the encoded mathematical expressions (see Fig. 3c).

Once the population of chromosomes is ready for the new generation, the evolution procedure is repeated until a stop criterion is reached, such as best fitness achieved, maximum number of unimproved generations is reached, time limit, etc.

The hyper-parameter needed for a GEP run has either components with recommended default values, especially for the genetic operator rates considered when applying the available genetic operators (Ferreira, 2006), or has components for which

the values have been established empirically after experience in working with the GEP approach. The latter typically depend on the requirements of the problem looked to solve.

Such is the case for setting the length the gene head, or the number of genes in a chromosome that can be lower if the interest is in obtaining more compact solutions, with larger values possibly leading to a fast expansion of solution length which can easily over-fit the initial target. When the lengths of the chromosomes are kept too low, the structures in the population can convergence too soon to a unique solution that might lack the ability to capture meaningful signals present in the training data, due to low diversity of the encoded expression trees.

Another important component of the hyper-parameter ~~(Tab. 1) in GEP (as in other genetic programming approaches) since it is decisive in the amount of new individuals created from a generation to the other. For example, if the~~ to set is the mutation rate (one of genetic variation operators) is too large, it can become disruptive and lead to loss of the information acquired along the previous evolutionary time steps and reduce the convergence of the algorithm. Conversely, if the rate is too low, one may not identify new relevant model structures in due time. ~~The process of selection and genetic manipulation is repeated until a stopping criterion is reached (i.e. best fitness achieved, maximum number of unimproved generations is reached, etc.), and a solution in the form of a mathematical structure is returned.~~

The current implementation of the GEP approach does not contain an explicit population diversity management component ~~. However in~~ which could increase the confidence that a certain solution did not just appear by chance, but that it was actually selected over a larger pool of possible model structure types. In order to reduce stochastic bias and avoid getting stuck in local optima ~~and produce over-fit~~ that would produce over-fitted results, we chose ~~a~~ the practical approach of multi-start (multiple runs with the same settings) as proposed by Ferreira (2006).

The version of the GEP method presented in this paper was implemented by the first author in the C++ language and is ~~available on demand~~freely available upon request. All the experiments reported in this work were executed on a cluster ~~containing 51 nodes,~~ running SuSE SLES 11 SP1 and StorNEXT (global file system running on the IO nodes) ~~. In summary~~ and that contains 868 CPU cores, 14.5 TB RAM, 1.2 PB file space. ~~All the nodes are attached via GB LAN and OPENLAVA 3.1 is used as queueing system~~The large performance capacity of the cluster allowed for multiple parallel runs and speed in reaching the final solutions.

2.2 Fitness measure

In our study, the fitness measure is reported in terms of the Nash–Sutcliffe modelling efficiency (MEF) coefficient (Nash and Sutcliffe, 1970; Bennett et al., 2010) which is often used in the context of quantifying the performance of terrestrial biosphere models (Mitchell et al., 2009; Migliavacca et al., 2015). The MEF is computed as

$$\mathrm{MEF} = 1 - \frac{\sum_{i=1}^{n}(o_i - p_i)^2}{\sum_{i=1}^{n}(o_i - \bar{o})^2} \tag{2.1}$$

where o_i is the observed value at step i and p_i is the predicted value at step i and $\bar{o}$ is the mean of observed values. MEF values range between $-\infty$ and 1, where an MEF value of 1 corresponds to the case where the predicted and observed values

are identical. A negative MEF value means that the predictions are worse than the mean of the observations in recreating the observed signal. MEF=0 indicates that the models prediction are as good as a prediction by $\bar{o}$.

During the GEP learning process, however we use the (1-MEF) measure as we want to minimize the fitness function values.

Although the MEF metric offers a straightforward interpretation, it does not take the number of parameters of the models into account. In real-world applications, it might be desirable to derive models with ~~lower number of~~ fewer parameters if those are not (much) worse in terms of prediction capacity than models with higher number of free terms. Thus, we include in our cost (fitness) function a normalized term related to number of parameters (ratio of current number of parameters to ~~maxim~~ maximum number of possible parameters given the GEP run settings).

Moreover, any systematic signature in the model residuals ~~(the differences of model predictions and observations)~~ needs to be reduced as the latter should ideally only represent uncorrelated noise. To meet this criterion, we complement the fitness function with a term related to the information content (entropy) in the residual time series~~, i. e. derived from information-theoretic considerations. .~~ Entropy values would ~~thus~~ be maximized for data without structure (i.e. white noise), and lower entropy values would be obtained for structured data, e.g. correlated stochastic or deterministic processes (Rosso et al., 2007) . The information content in a time series is typically quantified by the Shannon Entropy (SE, C. E. Shannon (1948)) , i.e. a term of the form

$$SSEP(X) \;=\; -\sum_{i=1}^{N} p_i \ln [p_i] \;. \tag{2.2}$$

Here, ~~$P = \{p_i; i = 1, \ldots, N\}$~~ $X = \{p_i; i = 1, \ldots, N\}$ denotes a probability distribution with $\sum_{i=1}^{N} p_i = 1$ and N possible states. To calculate Shannon's entropy measure from a time series, the series thus has to be adequately partitioned into a suitable probability distribution. As our aim is to minimize structure in the residuals, the temporal order becomes important . Here, we extract ordinal patterns from the time series and derive a (discrete) probability distribution through counting the occurrence probabilities of each pattern, following Bandt and Pompe (2002). This approach is fully based on the temporal dynamics in the residuals (i.e. the order within the time series) and largely non-parametric, as only the window length has to be specified. This parameter is set to $n_{demb} = 4$ throughout the paper, following previous work on ecosystem gross primary productivity dynamics (Sippel et al., 2016).

In short, the calculation of an entropy as a measure for randomness from a time series (e.g. Shannon's entropy) requires to determine a probability distribution that underlies the time series (or dynamical system), which is usually done by a partitioning step (also called phase space reconstruction in other contexts). This is a fundamental step in the methodology, and various methods have been used to arrive at this probability distribution, for instance frequency or histogram-based measures, procedures based on amplitude statistics, or symbolic dynamics (see e.g Kowalski et al. (2011) for an overview). In recent years, the Bandt Pompe approach has become popular, because it directly takes sequences in time into account: The technique hence divides the time series into ordinal sequences (i.e. ordinal patterns, or symbolic sequences), and then computes entropy measures directly from the probability distribution of these ordinal patterns (Bandt and Pompe, 2002). This approach has a number of advantages, namely that it is robust to noise (no sensitivity to numeric outliers) and to trends or drift in the data, it

is an (almost) non-parametric method and no prior assumptions about the data are needed (the only parameter that has to be specified is the embedding dimension, i.e. window length), and allows to disentangle various possible states of the system that are then encoded in the probability distribution (see e.g. Zanin et al. (2012) for a review of the method and applications).

The final normalized form the fitness function further used in our work is:

$$\text{CEM} = \sqrt{(1-\text{MEF})^2 + (\frac{P}{P_{max}})^2 + (1-\text{SE})^2} \tag{2.3}$$

$$P_{max} = gN \times hn_g \times l \tag{2.4}$$

where, CEM ~~will stand~~ stands from here on for "complexity corrected efficiency in modelling", P is the number of parameters present in a model structure, P_{max} is the maximum numbers of parameters possible for each individual from a GEP run set-up, ~~gN~~ n_g is the number of genes in a chromosome and ~~hl~~ is the length of a gene~~(Fig. ?? of suppl.).~~ .

For assessing the effect of adding the entropy component for the residuals in the CEM fitness function, we introduce as well the following fitness measure which contains elements regarding only MEF and number of parameters.

$$\text{MEF+NP} = \sqrt{(1-\text{MEF})^2 + (\frac{P}{P_{max}})^2} \tag{2.5}$$

For all experiments reported in this paper, the optimization is done by minimizing the fitness function values. The best value that can be reached for all presented fitness functions is 0.

2.3 Parameter optimization

The GEP algorithm does not have a specific treatment of constants in the building of model formulations but mutations can change both the model structure and constants. However, the scaling of constant values (model parameters) might be a decisive factor in adequately determining the fitness of a formulation. Without this, a model structure might be discarded regardless of potentially being a very powerful candidate. Furthermore, model parameters are often very informative regarding a system's sensitivity to some modifications of the drivers. These aspects have led to the addition of a final parameter optimization step at the end of each GEP run.

In order to obtain an optimal set of parameters for the GEP extracted model structures, an approach that would be applicable in a large set of generated search spaces was necessary. Here we use the "Covariance Matrix Adaptation Evolution Strategy" (CMA-ES~~) (Hansen et al., 2003)~~ , Hansen et al. (2003)) for optimization. The CMA-ES is a stochastic optimization algorithm that seeks to minimize a fitness function by estimating and adapting a covariance matrix according to a sampling from a multivariate normal distribution (Beyer and Schwefel, 2002; Auger and Hansen, 2005). According to Hansen (2006), one of the main arguments in favour of the CMA-ES approach is that it has shown good results even in the case of ill-posed problems (Kabanikhin, 2008), which may very well be the case for some of the GEP structures that are automatically generated.

The CMA-ES version used for the final step of optimization is the Hansen Python implementation found at ~~https://pypi.python.org/pypi/cma.~~ https://pypi.python.org/pypi/cma.

3 Experimental design

For exploring the possibility of using GEP in developing relevant model structures for describing the terrestrial carbon fluxes, two case studies were designed: Firstly, an experiment based on artificially generated data to better understand and present the general properties and capacities of GEP. Secondly, we explored the use of GEP on real measurements of various respiratory flux components monitored continuously over two years in an oak forest (Heinemeyer et al., 2011).

3.1 Artificial experiments

These experiments were designed to explore whether our implementation of the GEP method is suitable for symbolic regression type of problems, and how robust/vulnerable it is across various signal to noise ratios. We explored a set of functions with increasing levels of non-linearity to generate data points.

$$f(x_1) = 2x_1 + 1 \tag{3.1}$$

$$f(x_1) = x_1^2 + 3x_1 + 5 \tag{3.2}$$

$$f(x_1) = e^{x_1} + 1 \tag{3.3}$$

$$f(x_1) = e^{-x_1} - x_1 \tag{3.4}$$

$$f(x_1) = x_1^2 - 4\sin(x_1) \tag{3.5}$$

$$f(x_1) = x_1^3 + 6x_1^2 + 11x_1 - 6 \tag{3.6}$$

$$f(x_1, x_2) = x_2 x_1 \tag{3.7}$$

$$f(x_1, x_2) = x_2 x_1 - 3\cos(x_1) \tag{3.8}$$

$$f(x_1, x_2) = 2x_1^2 + 3x_2^2 \tag{3.9}$$

$$f(x_1, x_2, x_3) = 2x_1^2 + 3x_2^2 + 2\sin(x_3) \tag{3.10}$$

2000 data points were randomly generated with $x_1 \in [1, 20]; x_2 \in [1, 5]; x_3 \in [1, 100]$ and each functional values were computed based on ~~these~~the same initial set of 2000 data points. Out of the 2000 data points, 1000 data points were used for training, while 1000 data points were reserved for validation. The GEP settings used for each of the 20 runs are given in Table 1. If a returned structure was identical to the originally prescribed function or if $(1 - \text{MEF}) \leq 10^{-5}$ at validation, the retrieval of the original structure was considered to be a success. For allowing the approaches to do an automatic feature selection, all 3 variables, x_1, x_2, x_3, were used for learning and validation for all 10 functions in the benchmark set.

For investigating the capacity of GEP to reconstruct a simple model used in the ecology field as well, we introduced as well an artificial test for the "Q_{10}" model that is used in the field for simulating the response of ecosystem respiration to change in air temperature of 10^oC at a reference temperature of 15^oC The formulation we used for the "Q_{10}" model is:

$$R_{eco} = 2^{(0.1T_{air} - 1.5)} \tag{3.11}$$

with R_{eco} as ecosystem respiration flux and T_{air}, the air temperature. Again, we generated 2000 data points for both predictor and target and we used half for training 100 runs and half for validation. The modelling capacity of the best structure in terms of fitness value at validation is reported.

In order to investigate the response of the GEP approach to noise contaminated data, we simulated Gaussian noise that scales with signal amplitude as often observed in the case of terrestrial ecosystem ~~fluxes (Lasslop et al., 2012)~~ (Lasslop et al., 2012) and soil respiration (Lavoie et al., 2015)fluxes. The signal-to-noise ratio (SNR, measured as ratios of standard deviations) was varied between 10 and 1 in six steps.

For each of these functions and SNR levels, we sampled 100 validation data points 10 times. 20 GEP runs were performed ~~and the retrieved~~ on the 1000 training data points and the GEP model structure with the highest ~~MEF values at the validation points~~ mean MEF value over the 10 validation sets was chosen. ~~If a returned structure was identical to the originally prescribed function or if $(1 - MEF) \leq 1e05$ at validation, the retrieval of the original structure was considered to be a success.~~

As the choice of fitness function was crucial for the construction of structures in a GEP type of approach, we also investigated in one experiment the effects of minimizing the CEM values (eq. 2.3) as opposed to using only MEF (eq. 2.1) ~~as acceptance criteria~~or MEF+NP (eq. 2.5) as fitness function.

3.1.1 Alternative Machine Learning Methods

The prediction performance of the best GEP derived models based on the data in section 3.1 was compared with the prediction performance of four commonly used state-of-the-art machine learning methods (~~MLM~~MLM), i.e Artificial Neural Networks, ANN, (Yegnanarayana, 2009), Support vector Machines, SVM (Hearst, 1998), Random Forests, RF (Breiman, 2001) and Kernel Ridge Regressions, KRR (Hoerl and Kennard, 1970). ~~The toolboxes~~

The toolboxes and settings used for generating the predictions ~~of~~ by the ANN and KRR methods are described by ~~Tramontana et al. (2016~~ found in the "simple R" regression toolbox (Lazaro-Gredilla et al., 2014), the predictions of the SVM were obtained by using the ~~LIBSVM package (Chang and Lin, 2011) and~~ "LIBSVM" library (Chang and Lin, 2011) from the "simpleR" regression toolbox where the regularization term, the insensitivity tube (tolerated error) and a kernel length scale are automatically adjusted. Lastly, the RF predictions were ~~given by~~ obtained after running the Matlab statistics toolbox implementation with default settings.

All the present machine learning approaches have been applied on the same training data sets as those used for building the GEP models, and their predicted values were compared with the validation sets used for determining the best GEP solution. ~~All the runs were performed with default settings.~~

3.2 Measured ecosystem CO_2 fluxes

In the second experiment we ~~tried~~ assessed the possibility to reverse engineer model structures R_{eco} and its components based ~~on~~ only on real measured data. Specifically, we explored GEP derived model structures for various components of terrestrial ecosystem respiration fluxes ~~collected~~ measured in an 80 year old deciduous oak plantation in the Alice Holt forest in SE England as described in (Heinemeyer et al., 2012; Wilkinson et al., 2012).

3.2.1 Alice Holt in-situ data

The ~~particular strength of the~~ Alice Holt data set ~~is that component fluxes~~ contains observations of R_{eco} ~~were measured separately. R_{eco}~~ and the total influx of CO_2 to the ecosystem as mediated via photosynthesis (gross primary production, GPP), and various soil respiration components.

R_{eco} and GPP were estimated from eddy covariance measurements of the forest net CO_2 exchange (NEE, Eq. 3.12) ~~, and the various soil respiration components were measured separately for two years with hourly time resolution for total soil respiration (R_{soil}), root respiration (R_{root}), mycorrhiza respiration (R_{myc}), soil autotrophic respiration (R_{soil_a}) and soil heterotrophic respiration (R_{soil_h}) and above ground respiration (R_{above}) estimated by difference (Eq. 3.13). Additionally, we have access to derived measurements of GPP, as well as direct measurements of soil moisture (SWC), air temperature, surface temperature, and soil temperature taken at 2, 10~~ and ~~20 cm depth.~~

~~R_{eco} and GPP~~ were obtained from a micro-meteorological measurement tower at the same site that reports half hourly integrals of ~~net ecosystem exchange (NEE)~~ NEE with the eddy covariance (EC) methodology (Moncrieff et al., 1997). The Reichstein et al. (2005) procedure was used for gap-filling and separation of NEE into GPP and R_{eco}. Given that R_{soil} is a fraction of R_{eco}, above ground respiration can calculated as the difference between R_{eco} and R_{soil}. For an in-depth description of other site conditions and measurements see Heinemeyer et al. (2012).

A multiplexed chamber system was used for ~~measuring~~ separately measuring soil respiration (R_{soil}) and its components, using a continuous sampling method at fixed locations during two years at an hourly resolution. In order to partition the R_{soil} flux into its components, mesh-bags that are not penetrable by roots, but allow for mycorrhizal hyphae development were installed. Deep steel collars were applied to stop both root and mycorrhizae in-growth. As a result, root respiration (R_{root}) is given by the difference of R_{soil} and the respiration recorded in the mesh bag chambers, mycorrhiza respiration (R_{myc}) is given by subtracting the steel collar flux from the mesh bag chamber flux, and the soil heterotrophic respiration (R_{soil_h}) is given by the CO_2 efflux at the steel collar chambers~~and~~ . Lastly, soil autotrophic respiration (R_{soil_a} ~~is~~) is estimated as the sum of R_{myc} and R_{root} (Eq. 3.14 and 3.15) .

The above ground respiration (R_{above}) was given as well and was estimated by difference (Eq. 3.13). Additionally, direct measurements of soil moisture (SWC), air temperature, surface temperature, and soil temperature taken at 2, 10 and 20 cm depth are present in the dataset.

$$R_{eco} = \mathrm{NEE} + GPP \tag{3.12}$$

$$R_{above} = R_{eco} - R_{soil} \tag{3.13}$$

$$R_{soil_a} = R_{root} + R_{myc} \tag{3.14}$$

$$R_{soil} = R_{soil_a} + R_{soil_h} \tag{3.15}$$

The computation of R_{above} as difference between R_{eco} and R_{soil} might be highly uncertain because of the different techniques used to compute the two respiration components, the completely different footprints, and the typical high flux under-

estimation and low flux overestimation of R_{eco} from EC (Wehr et al., 2016). The limitations of the separation of R_{eco} into its components and the uncertainty of the estimates are further discussed by Heinemeyer et al. (2011), Heinemeyer et al. (2012) and Wilkinson et al. (2012).

3.2.2 Data processing

We used the following candidate driver variables: soil volumetric moisture measurements, air temperature (from micro-meteorological station), and temperatures at different soil depths, and GPP. A number of recent studies have shown a tight linkage between GPP and R_{soil}, reflecting dynamics of respiratory substrate supply to roots and mycorrhizal fungi from recently assimilated C in plants. (Moyano et al., 2008; Mahecha et al., 2010; Migliavacca et al., 2011, amongst others). We use GPP obtained from EC measurements at the site, but acknowledge the conceptual problem that R_{eco} and GPP were derived from the same observations of NEE. In order to minimize the potential spurious correlation between R_{eco} and GPP as well as redundancy of possible GPP influence with the meteorological drivers, we considered low-frequency variability of GPP only (i.e. low-pass filtered modes of GPP which corresponds to variability beyond a 60 days periodicity only, see Mahecha et al., 2010). “Singular Spectrum Analysis" (SSA, Broomhead and King (1986)) as described and implemented by Buttlar et al. (2014) was used to obtain a smooth GPP signal. The seasonal cycle was extracted with the SSA method as the assumption is that GPP affects mainly the seasonality of the respiration while the variability at the high frequency is assumed to be more related to meteorological drivers (e.g. temperature, Mahecha et al., 2010). The SSA method is a tool used mainly in time series analysis with the purpose of decomposing a time series signal into its independent sum components, such as trends, seasonality and high frequency components based on a singular value decomposition of trajectory matrices computed after embedding the time series (Buttlar et al., 2014).

To reduce the skewness and the search space that the GEP evolution would have to cover in order to construct valuable solutions (Keene, 1995), we log-transformed the seven target respiration data sets (see Figure 1 in supplemental material) and applied a back-transformation when reporting the respective model structures. The time series used for the candidate drivers remain unchanged.

3.2.3 GEP set-up

For each combination of respiration target and possible drivers, 50 subsets of 500 target time steps each were randomly selected and used for the training of GEP models using the settings found in Table 1. The 50 subsets of the remaining 113 time steps are used for cross-validation and the model with the lowest average validation CEM value is finally selected for each respiration type.

We were particularly interested in determining the general character of each extracted model with respect to the different respiration fractions. We therefore re-optimized the parameters of all extracted model structures when applying one extracted model as the candidate function for a different respiration term. For example, the model formulation extracted for R_{eco} is re-calibrated for all the other types of respiration, creating six parameter sets (one for each respiratory flux) per equation. To

cross-validate parameter sets, we computed performances for each train–validation data set pair and report averaged MEF values.

As in the artificial example, we compared the returned GEP solutions predictions performance with that of other common MLM such as SVN, KRR, ANNs, and RF. All methods were used for generating 50 subsets of 113 prediction values, after training on the 50 subsets of 500 time steps of observations presented in the start of section 3.2.3. Then, a mean MEF value was computed for all methods for all respiration components and the best mean MEF values were reported and compared with those of the GEP extracted models. The comparison is done in terms of MEF as number of model parameters were not available and CEM could not be computed.

3.2.4 GEP in the context of other known ecological models: Real observational data

A comparison was done between the GEP built models and some common literature respiration models with different structures and driving variables that were also optimized using CMA-ES. The optimization was performed for each respiration dataset and its candidate drivers and parameters (Table 2). The structures and prediction performances of the GEP models were then compared with those of the optimized literature models.

4 Results

4.1 Artificial experiments

In the first artificial experiment the GEP approach is used to verify if it can reconstruct prescribed functions. Following the training of the 20 independent GEP runs, the initial functions were successfully reconstructed for all 10 equations defined in section 3.1.

For the Q_{10} model artificial test, the following structure was finally selected:

$$R_{eco} = 0.35 \times 2.5^{(0.01 T_{air})} \tag{4.1}$$

with a validation MEF value > 0.99.

MEF values for the GEP extracted models and for the predictions generated by ANN, RF, KRR and SVM are illustrated in Fig. 4a. These MEF values were obtained through cross validation against independent, yet equally noise contaminated data points (the SNR values are given on the x axis in reverse order for visualizing the increase in noise levels). There is a clear pattern of decreasing MEFs with increasing noise contamination. This was expected, as none of the methods should fit the noise added to the signal.

Figure 4b shows MEF values equivalent to fig. 4a, but applied to noise-free data points of the validation set, in order to compare GEP outputs to the “true" structure underlying the artificial data set. In this set-up, the MEF values remained relatively constant across SNR values above 2. When SNR level was set to 1, predictions for all investigated machine learning methods, except for GEP predictions, show decreased fitness, with MEF values decreasing to a minimum of 0.8.

~~Figure ?? compares the two validation approaches described above - SNR is now represented by a colour code. This figure suggests that we may not expect MEF values of $\gtrapprox$0.9 under real scenarios (where no noise-free validation is possible).~~

In order to verify the effects of changing the fitness function from MEF to CEM, we compare the distributions of MEF values for all runs for all studied SNR. Figure 5 exemplifies outputs for equation 3.10; panel a shows a drop of prediction capacity of the GEP models with noise increase for all types of fitness functions when compared with noise-infused data. This contrasts the reduced MEF assessed against original data, where a slight drop in MEF with noise increase for the MEF optimization structures was seen, and where the CEM optimized structures show stability in MEF with noise. The new CEM leads to a reduced number of returned parameters compared to MEF (Fig.5c), as well.

4.2 Measured ecosystem CO_2 fluxes

Applying GEP on the Alice Holt data set yielded a series of model structures for each respiration type. The returned model structures are illustrated in equations 4.2-4.8.

$$R_{eco} = \log(T_{-10}) \times e^{(\frac{GPP_s}{T_{-10}})} \tag{4.2}$$

$$R_{above} = 0.9SWC^{0.2} \times e^{(0.1GPP_s)} \tag{4.3}$$

$$R_{soil} = e^{(1.2T_{-10}^{0.4}+1.3SWC-3.1)} \tag{4.4}$$

$$R_{root} = e^{(0.9\frac{1.2GPP_s-8.1}{T_{-10}})} \tag{4.5}$$

$$R_{myc} = 1.8T_{-10} \times e^{(1.2T_{-10}^{SWC}-7.4)} \tag{4.6}$$

$$R_{soil_a} = e^{(1.2T_{-10}^{0.5}+2.5SWC-4.9)} \tag{4.7}$$

$$R_{soil_h} = e^{(-0.3+0.6\frac{1.1GPP_s-3.6}{T_{-10}})} \tag{4.8}$$

where, GPP_s is gross primary production that has been smoothed using the SSA method with a 60 day window ; T_{-10} is soil temperature measured at 10 cm depth; and SWC is volumetric soil water content. The corresponding cross-validation MEF values are given in Table 3, indicating a range of capacities for GEP models to represent different respiration types.

Whilst GEP-derived models may differ between respiration types, there are a number of equivalent models for different respiration components. R_{soil} and R_{soil_a} were described by identical model structures (but distinctive parameter values), and R_{root} and R_{soil_h} were described by similar (but not identical) models. Overall, the most common selected drivers were T_{-10}, SWC and GPP.

The highest performance in terms of MEF value was recorded for R_{soil_a} and for R_{soil}, that is 0.82 and 0.81 respectively. The lowest capacity of process representation, with an MEF value of 0.28, was recorded for R_{above} (Table 3), possibly because this specific component would need to include active versus inactive periods determined by dormancy and leaf fall (i.e. seasonality in this deciduous forest). A comparison of the predicted values and observed fluxes for all types of respiration can be seen in Figures 6 and 7. In order to explore the capacity of the GEP models generated for the R_{eco} components to recreate the larger, across compartmental ~~sum~~ summed fluxes, we summed the predictions of the models and ~~compare~~ compared them with

the original fluxes ~~. We find that the global modelling performance~~ (Fig. 8). Based on a modelling performance comparison of the models defined as sum models of the ~~derived models remained in a very small range of the~~ initial ~~trained for the sum fluxes GEP models (Fig. 8), indicating that the larger fluxes actually exhibit sensitivity to some of the non-selected drivers , except~~ GEP models trained on the component fluxes with the original GEP models trained on the summed fluxes, we found no significant differences. However, we found that the total number of parameters is much larger for the sum models. This can be a result of the GEP approach eliminating the "low impact " drivers due to complexity pressure. We can see as well that the sensitivity ~~is present only in a certain compartment.~~ of the sum fluxes to certain drivers can strongly manifest itself only in certain components which is why the drivers only get selected in the models built for those specific components

The residuals depict some remaining patterns (Fig. 9 and Fig. 2 of suppl.) and the null hypothesis of normal distribution was rejected for all seven respiration component residuals at 5% significance level with the one-sample Kolmogorov-Smirnov test. Hence, we might expect additional information that could be extracted from the residuals. In order to check whether the remaining structure was missed in the first training routine because of imposing a multiplicative form in the models by log-transforming the target data, we performed GEP runs on the residuals and combined the models. The improvement in overall modelling performance is minimal, yet model structures become overly complex. The capacity of the GEP approach to retrieve new information from the residuals is illustrated in Fig. 11 in comparison with that of the other MLM presented in section 3.1.1. When correlation values were computed between the candidate drivers and the residuals, no significant linear correlations were found (Fig. 4 of suppl.).

4.2.1 Model transferability

We investigated the capacity of each extracted model structure (equations 4.2-4.8) to represent a component of R_{eco} not seen in the training procedure. This was done by means of new CMA-ES optimization steps. The new prediction performances are illustrated in Tab. 4.

After optimization, none of the structures show an overall best MEF for all the R_{eco} components (i.e. we clearly cannot identify an optimal general model). However, we identify certain model structures that tend to perform overall better than others. This is the case for the R_{myc} model (eq. 4.6). It can also be seen that after the individual model optimizations, the structures for R_{eco} and that for R_{soil_a} have similar prediction capacities.

The prediction capacity of the GEP generated models in the context of other commonly utilized MLMs was assessed as well. KRR, ANN, SVM and, RF were used for generating 113 predicted data points as described in section 3.2 (Fig. 10). The prediction performance of GEP, KRR, ANN, SVM and, RF are shown in Fig. 11. Panel a contains the average MEF values computed for all MLM methods predicted values when compared to the original observations for $R_{eco}, R_{above}, R_{soil}, R_{root}, R_{myc}, R_{soil_a}, R_{soil_h}$. For all other cases, the performance is in the same range for all methods, but the GEP derived models having the lowest mean MEF values. Panel b shows that when all MLM were trained on the residuals obtained from comparing the GEP outputs with the observations, the GEP approach has the lowest capacity of capturing new relevant signals and is strongly outperformed by the rest of the MLM, indicating that amount of information retrievable by GEP with the current fitness and settings is limited and captured already in the first run.

4.2.2 Comparing with literature models

Lastly, the GEP generated models were compared with some of the most commonly used literature models for describing respiration. The resulting MEF values obtained after individual parameter optimization using the CMA-ES procedure for each literature model are given in Tab. 5. The literature model structure that performed best overall in terms of prediction capacity measured as MEF is the $WaterQ_{10}$ model (Fig. 12). Figure 12 shows as well that certain types of respiration are easier to represent by all models, including the models GEP generated, whilst other types of respiration are poorly predicted by all models. Nevertheless, for all respiration types, the highest MEF values are generally recorded by the GEP models.

As the studied literature models performed best in modelling R_{soil}, we focus on contrasting GEP model results to literature model outcomes for this ecosystem respiration component. Of all models included, the GEP model and Q_{10} model including SWC dependency captured seasonal variability best, but no model satisfactorily represented short-term CO_2 flux variations (Fig. 13, panel a). All models show the largest range of residuals for the months May to July in 2008, and June/July in 2009 (Fig. 13, panel b), with the two best-performing models (GEP and $WaterQ_{10}$) having the narrowest range of absolute residuals. Monthly mean average errors (MAE) indicate as well a systematic underestimation of soil CO_2 efflux in the first year (Fig. 3 of suppl.).

5 Discussion

5.1 On the GEP method

In this work, the primary reason for the artificial experiments was obtaining a better understanding of the capacity of GEP to solve symbolic regression types of problems. We put an emphasis on GEP performance in the presence of noise. This aspect was important, given that monitoring data from terrestrial ecosystem CO_2 effluxes are typically contaminated by sometimes substantially large random uncertainties and measurement noise. In the case of NEE flux measurements, Lasslop et al. (2008) and Richardson et al. (2008) show that the measurement error typically scales with the magnitude of the flux, leading us to simulate that type of situation by adding noise that scales with signal to an already known function, equation 3.10. The results show that all the studied methods are stable to presence of noise in the training set. These results increase our confidence in the predictions generated by studied machine learning methods; in particular GEP derived modes can tolerate SNRs of 1. Considering that the SNR in the R_{eco} observations (if noise is only considered as random error) is probably larger than 4 which is where the curve starts decreasing in Fig. 4, the noise presence in the data should not influence the automated model construction process and the real signals should be accurately captured when data uncertainties follow the pattern described here. On the other hand, for R_{soil} and other CO_2 fluxes measured with other techniques the magnitude and the distribution of the uncertainty can be different (Ryan and Law, 2005; Pérez-Priego et al., 2015), and we cannot state what the response of the present MLM is in the presence of different types of uncertainties and measurement noise.

Our findings illustrate that selection of CEM over MEF as a fitness function for optimization has a minor effect on the global mean MEF (Fig. 5a). We also notice that due to ~~the constraints on~~ applying constraints on the presence of structure in the residuals and the length of the parameter vector, the final mean number of parameters is lower when CEM is chosen.

5.1.1 Limitations

One of the critical aspects in our work is that GEP, as implemented here, can only represent and derive "$n \rightarrow 1$" type of response functions. We are not able to generate model structures that encode e.g. system-intrinsic dynamics like feedback loops, which are expected from our current understanding of biogeochemical cycles in terrestrial ecosystems (Ehrenfeld et al., 2005; Friedlingstein et al., 2006). Hence, we believe GEP is suitable to e.g. understand and describe the sensitivities and non-linear responses to changes in hydro-meteorological drivers, but fails to represent more complex carbon or ~~water reservoir~~ soil water dynamics. Pools and pool transfers cannot be introduced currently in the input, unless the ~~depletion~~inflow/~~repletion~~ outflow equations are known and can be included in the set of functions that can participate in the evolution.

Lagged responses can only be detected if the number of lags from a driver is correctly included in the input, which already implies sufficient knowledge of their existence and behaviour. Whilst in the current implementation of the GEP algorithm, shifts in conditions and responses cannot be encoded or detected; these could be addressed with the inclusion of a conditional operator in the set of functions encoded in the GEP evolution individuals.

Nevertheless, it would be fair to mention that the same limitations can affect the results of the other MLM and empirical models presented in this paper.

5.2 The value of GEP for modelling ecosystem respiration fluxes

We automatically generated a series of model structures to describe terrestrial CO_2 respiration fluxes (equations 4.2-4.8) with the GEP approach. Most of these structures (5 out of 7) were of rather low complexity~~i.e. requiring~~, requiring only 4 free parameters ~~(which is certainly an effect of the chosen cost function CEM)~~and allowing for further interpretation. The most complex structure is found for the R_{myc} ~~model~~representation, which is in line with previous findings (Shi et al., 2012). ~~Nevertheless, there is need for more in-depth analysis for determining whether the described processes make actual biological sense and the selected drivers and their interactions represent real processes and responses.~~

Interestingly, the models derived for R_{eco} and R_{soil} are structurally very similar. That is also the case of R_{root} and heterotrophic respiration, where the difference lies in the set of parameters and the added presence of an intercept in the formulation of the R_{soil_h} model. This finding suggests a consistency in the response of the R_{soil} components to their drivers, considering that the separation of the R_{soil} into its components might still lack accuracy (e.g. P. J. Hanson, N. T. Edwards and Andrews, 2000; Kuzyakov, 2006; Subke et al., 2006; Heinemeyer et al., 2011). ~~However, all selected GEP generated models led to an underestimation of the high respiration fluxes (Fig. 7) and typically do not capture the peaks (fast responses). This phenomenon is in some cases a systematic pattern, and sometimes affects only certain times of the year. We suspect that is partly due to surface moisture affecting litter decomposition and fungal activity, as soil moisture was only monitored over the average 8 cm surface but the top few centimetres were most likely the most active and partly due to some potential processes/drivers~~

like lags between GPP and respiration (Hölttä et al., 2011) or phenology (Migliavacca et al., 2015) that were not specifically included in the learning process.

However, semi-empirical models similarly struggle to adequately simulate CO_2 flux peaks and in some cases monthly flux averages (Fig. 13). Structurally, the GEP-derived models share some key features When we compared the GEP-derived models with the community established semi-empirical approaches models from a structural point of view, we found that they shared some key features for temperature dependencies of CO_2 fluxes, which are typically captured by exponential relationships., but reveal some previously unconsidered dynamics as well.

A major difference is that when was in the response of the respiration components to SWC has been chosen as driver, GEP often also identifies some , where the GEP models often chose SWC as one of the drivers. Moreover, the GEP models often contained an exponential dependency, i.e. there are only certain parts of the signal that are strongly sensitive to varying SWC. This We believe that the exponential dependency of terrestrial ecosystem respiration components to SWC is a very intuitive pattern , which that has not yet been reported in the literature, and requires further exploration.

Another difference we found was the strongly seasonal response of the respiration components to GPP, possibly as a proxy to light and vegetation availability which were not included in the set of candidate predictors.

Considering that GEP identified plausible models, that are very different structurally from previously reported semi-empirical models, still yielding equivalent or better modelling performance, the validity of the conventional semi-empirical models can be questioned. Nevertheless, we do believe that there is need for more in-depth analysis for determining whether the GEP described processes make actual biological sense and the selected drivers and their interactions represent true processes and responses.

5.3 Data quality

During our study, it was apparent that the highest MEF values were obtained for all the studied methods in the case of the respiration types that had direct measured observations and were not derived. It might be the case that when fluxes are obtained from derivations, the measurement error will also increase, and the partition of clear signal existing in the observations is not sufficient for constructing a good model with GEP.

5.4 High frequency variability

For some of the modelled respiration components (e. g. R_{eco}) a large amount of high frequency variability present in the observations was lost

All GEP generated models underestimated the high respiration fluxes (Fig. 7) and typically did not capture the fast responses.This phenomenon was in some cases a systematic pattern, and sometimes affected only certain times of the year. Similarly, semi-empirical models struggled to adequately simulate CO_2 flux peaks and in some cases monthly flux averages (Fig. 6). 13).

A more in-depth comparison of all the GEP and conventional respiration models, based on a time-scale dependent assessment of model-data mismatch (Mahecha et al., 2010) could help to further elucidate the problem and clarify some of the strengths and weaknesses of the different modelling approaches, especially when seasonal mismatches appear. Nevertheless, a detailed

time-scale dependent assessment is beyond the scope of this study, and for such an analysis, the current time series are simply too short.

The question is whether the GEP method lacks the ability to build models that correctly represent the processes and their fast dynamic responses, or whether the candidate drivers and the observations used for their representation are simply not sufficient for generating representative models. In the end, the response of R_{soil} and R_{eco} to external drivers might be too complex to describe solely with the currently available measurements and with the selected drivers.

We believe that the consistent underestimation of fast responses was partly due to surface moisture affecting litter decomposition and fungal activity, as soil moisture was only monitored over the average 8 cm surface, with the top few centimetres most likely presenting the highest activity and partly due to some potential processes/drivers like lags between GPP and respiration (Hölttä et al., 2011) or phenology (Migliavacca et al., 2015) that were not specifically included in the learning process.

Another explanation for missing some of the (high flux) variability could be in our choice of fitness function. As we decided to penalize during the learning process for structures with many parameters, it is likely that some structures were eliminated early-on during this process, even though they may be well-suited for describing a given process from a modelling efficiency point of view. However, this is a case of trade-off between a good fit and structural simplicity, and in our approach, we decided that simplicity of structure, i.e. the possibility of interpretation is a very important asset.

We ~~suspected as well that the~~ explored as well the possibility of the underestimation of the carbon flux variability ~~was~~ being caused by the log-transformations ~~we did on~~ applied to the observations. ~~That could have introduced a bias that~~ It could have been the case that the log-transformations excluded interesting components of the model structures by forcing the method to build multiplicative models. ~~However~~Nevertheless, when the GEP was run again on the residuals, without log-transforming, no new meaningful information was retrieved, indicating that multiplicative models were sufficient for reconstructing the ~~studied~~ R_{eco} components present in this study.

5.5 Equifinality

Table 4 shows that when optimizing the parameters for all structures, the prediction performance becomes similar, which leads to the question of equifinality of dynamical systems, where different models that try to capture their structure, might have different formulations, but represent the same response.

A critical question for the applicability of any ecosystem model is whether the model structure is more important than the parametrisation of a given “best" model. For this question to be addressed, however, we need a larger sample of ecosystem types representative for different types of responses where we can explore the importance of the obtained structures and their parameter sets.

5.6 GEP models in the context of other machine learning methods

The comparison of GEP generated models and machine-learning methods showed a narrow range of predicted fluxes (Fig. 11). The analysis of training all the MLM on the GEP residual output showed that the GEP approach is not able to retrieve any new meaningful structural components, but that the remaining MLM are much better at reconstructing the signal left in

the residuals. This indicates that although the GEP is actually a reliable MLM when it comes reconstructing the underlying R_{eco} fluxes and is not prone to over-fitting, it could be that the current set-up of the GEP is not sufficient for an exhaustive description of those fluxes, or that might be overly strict on complexity of models compared to other MLM. The GEP approach has, nevertheless, the benefit of producing mathematical model structures that can be the basis for future interpretation.

6 Conclusions and Outlook

Overall, our results suggest that the GEP approach is a potentially powerful tool of reverse engineering, particularly helpful for building ecological models when there is a minimum of a priori system understanding. We exemplified this conceptually using artificial data, but also show that GEP always yields as good or better results compared to conventionally used models in the case of ecosystem respiration. Based on data from a long-term monitoring site of different respiratory fluxes, and using GEP as a reverse engineering tool, we found new structures for modelling R_{eco} components. The GEP derived models outperform conventionally used models and generally differ by the way temperature and GPP, but also SWC are interpreted, indicating that conventional respiration models might have to be revised. At the same time, we found that when the GEP derived models are mutually compared, there are sufficient structural particularities for each terrestrial respiration type as to not allow for the formulation of a general R_{eco} law. More research is needed on a larger set of sites to identify widely usable models and for their interpretation. A particular matter of concern is the apparent equifinality of selected model structures, indicating that many response functions are yielding predictions of almost similar quality. A study of multiple sites would enable an investigation of whether specific ecosystem types result in similar model structures, or ~~if~~ whether response functions apply across contrasting ecosystem types.

The current study has also revealed methodological aspects that could be improved. In particular, we found the inclusion of a parameter optimization step very helpful to further test the transferability of model structures. But this approach could be potentially integrated into the GEP evolution. More specifically, we think that the next development of GEP could include the parameter optimization as an intermediate step before selection during each evolution generation ~~(?)~~(Ilie et al., under preparation). In this way, a model structure could be chosen according to not only the current state of parameters but also on its potential and convergence to a global solution might be achieved faster.

Code and data availability

All code and data used to produce the results of this paper can be provided upon request by contacting Iulia Ilie or Miguel D. Mahecha.

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Glossary

chromosome individual used in automatically evolving an optimal solution comprised of a set of genes that are connected with a binary operation (e.g. $+ \times -$). 5, 6

CMA-ES covariance matrix adaptation evolutionary strategy. 9

evolution the process of producing an optimal solution by GEP through . 5

expression tree binary tree used to represent algebraic expressions. 6

gene set of characters of fixed length that encodes an expression tree. 5

gene head initial section of the string that comprises a GEP gene, containing a combination of characters that map to predictors and possible functional transformations . 5

gene tail end section of the string that comprises a GEP gene, containing only characters that map to predictors. 5

generation time step of an evolution. 6

genetic operator operator that produces changes in the structure of a chromosome and the expression tree it encodes by altering the strings representing composing genes (e.g. mutation, inversion, recombination, etc.) . 6

genetic operator rate probability of a genetic manipulation to occur during a generation. 6

GEP **g**ene **e**xpression **p**rogramming, machine learning method that evolves chromosome structures with the purpose of minimizing a cost function. 3

hyper-parameter set of parameters which need to be set for the runs of a machine learning approach. 6

ill-posed problem a problem for which the solutions might not be unique or unstable, also known as an inverse problem. 9

individual GEP entity that is a component of a population during a certain step of the evolution process. Also known as chromosome. 6

MLM **m**achine **l**earning **m**ethod that can produce predicted values based on a training set. 11

population total set of chromosomes that participate at a certain step in the evolution of an optimal solution in the GEP approach.. 6

reproduction process of generating new individuals for a new generation starting from the present generation individuals after they go through structure modification and fitness based selection. 6

solution finally selected model structure resulting from a GEP run. 3

Table 1. GEP settings

Parameter	Artificial data	Real observations
Number of chromosomes	2000	2000
Number of genes	3	2
Head length	5	6
Functions	$+, -, /, *, x^y, \sqrt{}, \ln, \exp, \sin, \cos$	$+, -, /, *, x^y, \sqrt{}, \ln, \exp$
Terminals	x_1, x_2, x_3	$GPP_s, T_{Air}, T_{-10}, SWC$
Link function	+	+
Max run time	1200 seconds	1800 seconds
Fitness function	CEM	CEM
Selection method for replication	tournament(Coello and Montes, 2002)	tournament
Mutation probability	0.2	0.2
IS and RIS transpositions probabilities	0.05	0.05
Two-point recombination probability	0.3	0.3
Inversion probability	0.05	0.05
One point recombination probability	0.4	0.4

[0] ~~$a, E_0, \phi_1, \phi_2, \phi_3, \phi_4, R_0, R_2, k, k_2$ and α are model parameters that can be optimized~~

~~Respiration model formulations commonly used in the environmental science community~~ ~~ModelFormulationReferenceArrhenius~~

~~$a \times e^{-E_0/RT}$(Lloyd and Taylor, 1994) Q_{10} $\phi_1 \times \phi_2^{(\frac{T-T_{ref}}{10})}$ (Reichstein and Beer, 2008)~~

~~Water Q_{10} $\phi_1 \times \phi_2^{(\frac{T-T_{ref}}{10})} \times \frac{SWC}{SWC+\phi_3} \times \frac{\phi_4}{SWC+\phi_4}$ (Richardson et al., 2008)~~

~~$LinGPP(R_0 + k_2 GPP) \times e^{E_0(\frac{1}{T_{ref}-T_0} - \frac{1}{T_A-T_0})} \times \frac{\alpha k + SWC(1-\alpha)}{k+SWC(1-\alpha)}$(Migliavacca et al., 2011)~~

~~$ExpGPP[R_0 + R_2(1 - e^{k_2 GPP})] \times e^{E_0(\frac{1}{T_{ref}-T_0} - \frac{1}{T_A-T_0})} \times \frac{\alpha k + SWC(1-\alpha)}{k+SWC(1-\alpha)}$(Migliavacca et al., 2011)~~

~~$addLinGPPR_0 \times e^{E_0(\frac{1}{T_{ref}-T_0} - \frac{1}{T_A-T_0})} \times \frac{\alpha k + SWC(1-\alpha)}{k+SWC(1-\alpha)} + k_2 GPP$(Migliavacca et al., 2011)~~

~~$addExpGPPR_0 \times e^{E_0(\frac{1}{T_{ref}-T_0} - \frac{1}{T_A-T_0})} \times \frac{\alpha k + SWC(1-\alpha)}{k+SWC(1-\alpha)} + R_2(1 - e^{k_2 GPP})$(Migliavacca et al., 2011)~~

Table 2. Respiration model formulations commonly used in the environmental science community

Model	Formulation	Reference
Arrhenius	$a \times e^{-E_0/RT}$	(Lloyd and Taylor, 1994)
Q_{10}	$\phi_1 \times \phi_2^{(\frac{T-T_{ref}}{10})}$	(Reichstein and Beer, 2008)
Water Q_{10}	$\phi_1 \times \phi_2^{(\frac{T-T_{ref}}{10})} \times \frac{SWC}{SWC+\phi_3} \times \frac{\phi_4}{SWC+\phi_4}$	(Richardson et al., 2008)
$LinGPP$	$(R_0 + k_2 GPP) \times e^{E_0(\frac{1}{T_{ref}-T_0} - \frac{1}{T_A-T_0})} \times \frac{\alpha k + SWC(1-\alpha)}{k+SWC(1-\alpha)}$	(Migliavacca et al., 2011)
$ExpGPP$	$[R_0 + R_2(1 - e^{k_2 GPP})] \times e^{E_0(\frac{1}{T_{ref}-T_0} - \frac{1}{T_A-T_0})} \times \frac{\alpha k + SWC(1-\alpha)}{k+SWC(1-\alpha)}$	(Migliavacca et al., 2011)
$addLinGPP$	$R_0 \times e^{E_0(\frac{1}{T_{ref}-T_0} - \frac{1}{T_A-T_0})} \times \frac{\alpha k + SWC(1-\alpha)}{k+SWC(1-\alpha)} + k_2 GPP$	(Migliavacca et al., 2011)
$addExpGPP$	$R_0 \times e^{E_0(\frac{1}{T_{ref}-T_0} - \frac{1}{T_A-T_0})} \times \frac{\alpha k + SWC(1-\alpha)}{k+SWC(1-\alpha)} + R_2(1 - e^{k_2 GPP})$	(Migliavacca et al., 2011)

$a, E_0, \phi_1, \phi_2, \phi_3, \phi_4, R_0, R_2, k, k_2$ and α are model parameters that can be optimized

Table 3. Modelling performance for all extracted model structures after cross validation over 90 cases.

Respiration type	MEF	σMEF	Equation
R_{eco}	0.56	0.14	4.2
R_{above}	0.28	0.13	4.3
R_{soil}	0.81	0.13	4.4
R_{root}	0.59	0.10	4.5
R_{myc}	0.42	0.13	4.6
R_{soil_a}	0.82	0.13	4.7
R_{soil_h}	0.51	0.11	4.8

Table 4. Average validation MEF performance for all extracted model structures when re-optimized against all other respiration CO_2 flux observations.

trained for/ opt. for	R_{eco}	R_{above}	R_{soil}	R_{root}	R_{myc}	R_{soil_a}	R_{soil_h}
R_{eco} (Eq. 4.2)	0.56	0.25	0.77	0.51	-0.06	0.67	0.42
R_{above} (Eq. 4.3)	0.56	0.27	0.69	0.52	0.01	0.62	0.47
R_{soil} (Eq. 4.4)	0.50	0.13	0.81	0.35	0.29	0.82	0.40
R_{root} (Eq. 4.5)	0.34	0.22	0.61	0.57	0.03	0.65	0.51
R_{myc} (Eq. 4.6)	0.54	0.16	0.81	0.50	0.43	0.84	0.51
R_{soil_a} (Eq. 4.7)	0.50	0.13	0.81	0.35	0.29	0.82	0.40
R_{soil_h} (Eq. 4.8)	0.55	0.23	0.76	0.53	-0.03	0.67	0.51

Table 5. Average validation MEF performance for CMA-ES optimized selected literature model formulations when compared with respiration CO_2 flux observations.

Model formulation	R_{eco}	R_{above}	R_{soil}	R_{root}	R_{myc}	R_{soil_a}	R_{soil_h}
Arrhenius	0.41	0.15	0.65	0.50	0.07	0.61	0.38
Q_{10}	0.47	0.19	0.69	0.52	0.09	0.62	0.46
Water Q_{10}	0.50	0.20	0.79	0.55	0.40	0.81	0.43
$LinGPP$	0.55	0.25	0.74	0.57	0.17	0.70	0.49
$ExpGPP$	0.58	0.30	0.76	0.57	0.20	0.72	0.54
$addLinGPP$	0.55	0.27	0.73	0.56	0.12	0.67	0.48
$addExpGPP$	0.56	0.27	0.73	0.54	0.20	0.69	0.49

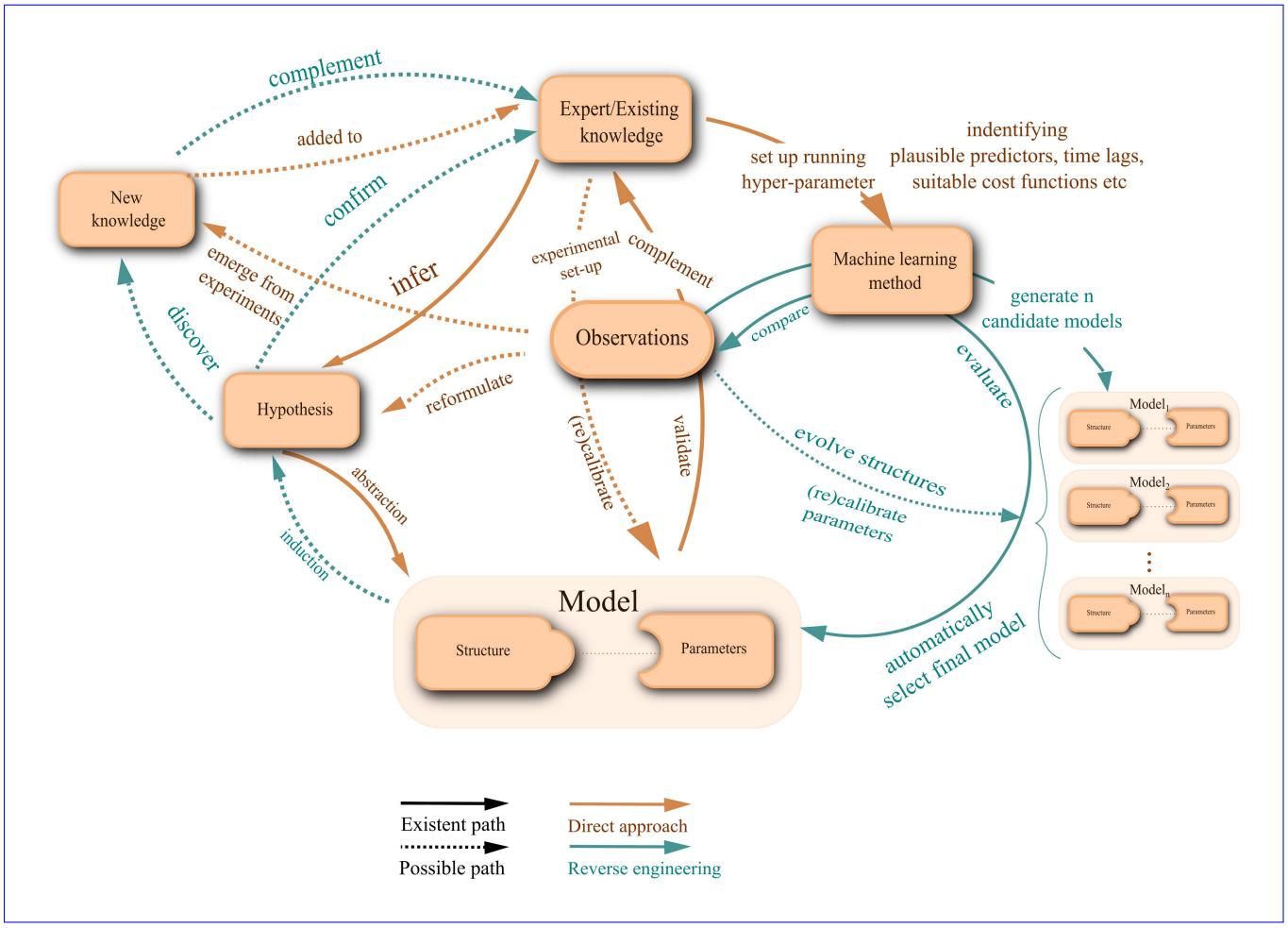


Figure 1. Direct approach and reverse engineering in model development for describing dynamical systems. Existing and possible steps needed in the process of building a model. For the direct approach, the process starts with the building of hypothesis from existing knowledge, the hypothesis is then subject of abstraction and summarized in a mathematical model that has two components: the structure and the parameters. The mathematical model can be translated into a computational form that will generate predictions. Depending on how well the predicted values manage to recreate the available observations, the model's parameters are calibrated or if the general trends are missed, there might be need for structural reformulation. On the other hand, in the reverse engineering approach, a machine learning method is used to generate a set of candidate models that are then compared with the available observations and which according to the prediction capacity may have to go through structural changes by automatic evolution or through a final parameter adaptation. From the set of evolved models, the best model in terms of prediction capacity is chosen and its structure will be the basis for hypothesis building, as an expert would try to explain why a specific structure was automatically evolved and whether the structure of the model can be explained from the studied system intrinsic processes. If that will be the case, and the structure has not emerged randomly, the conclusions can be compared with the existing knowledge which can be ~~either~~ reconfirmed or new aspects of the studied system might be brought into light.

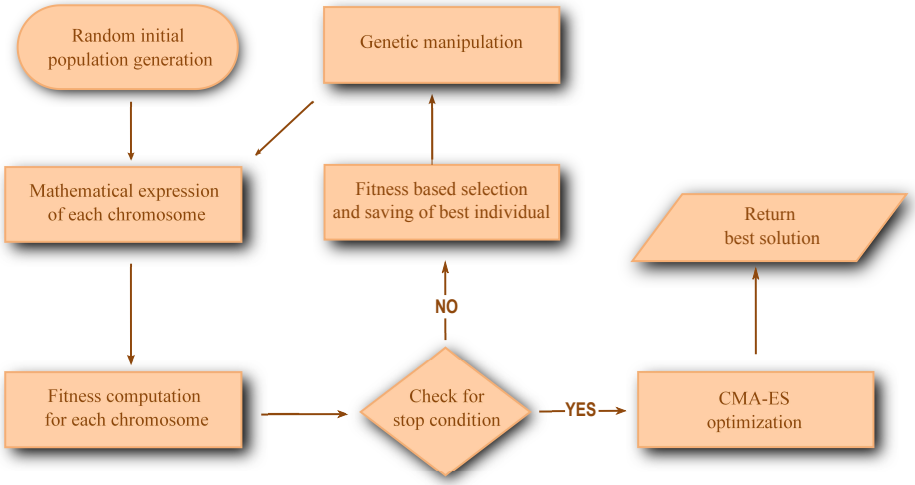


Figure 2. The work flow used in solving symbolic regression problems with GEP.. The process of evolving an optimal solution from observations starts with randomly generating a set number of evolution individuals called chromosomes. The chromosomes are composed of genes that are sets of strings encoding expression trees that can be translated into mathematical expressions in the subsequent step. Following the mathematical expression comes the evaluation of each emerging individual (model) against the target variable values and for each one a fitness values is assigned. If the stopping criterion has not been reached (e.g.. best fitness possible, highest number of generations allowed, convergence etc.) the best individual in terms of fitness is saved and the remaining set of chromosomes are selected for genetic manipulation. When the stop criterion is reached, the parameters of the best chromosome is calibrated against the training data with an optimization approach, the CMA-ES, and the best solution is returned.

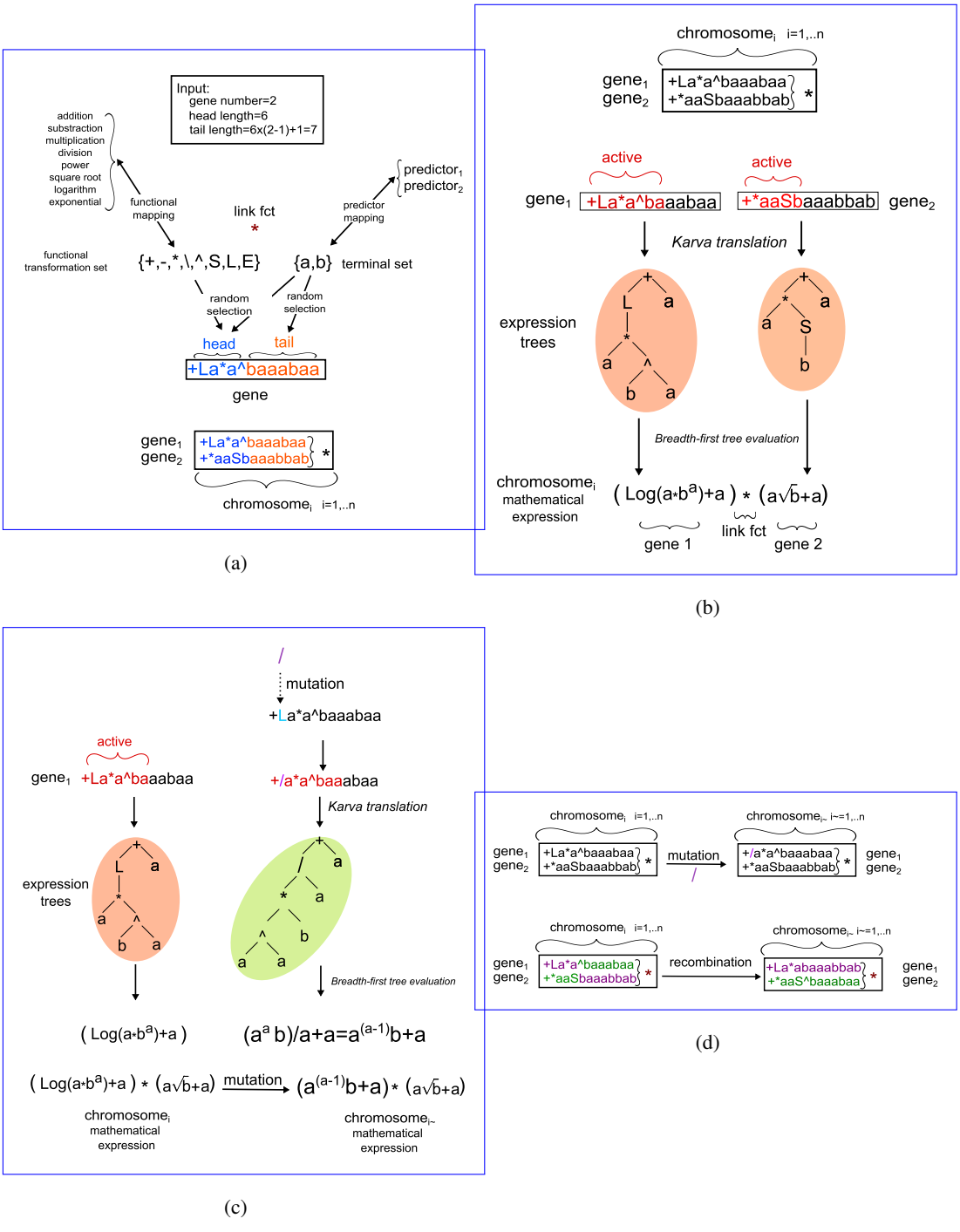
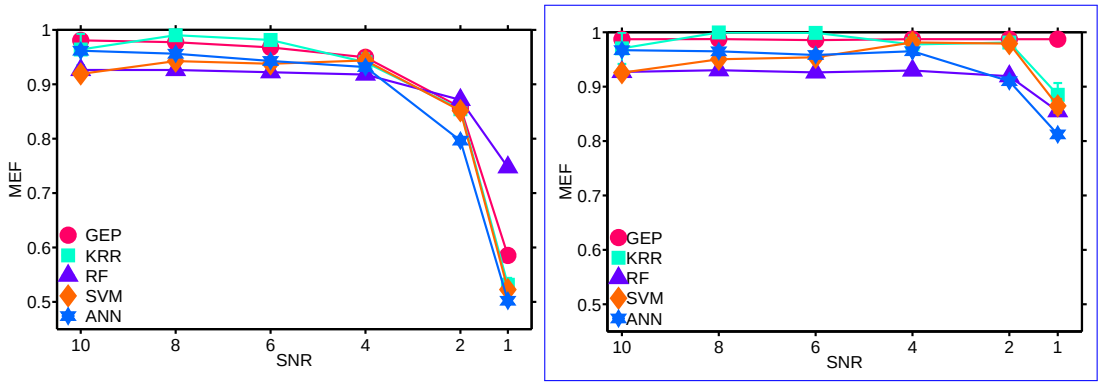


Figure 3. GEP evolution process components.A. Initial random generation of genes for creating chromosomes, the individuals evolved by GEP. **B.**GEP internal translation process from strings to expression trees and mathematical expressions.**C.** Changes made in the mathematical expression when applying the mutation operator on the genes of a GEP individual.**D.** Types of genetic operators for changing the GEP evolution individuals.

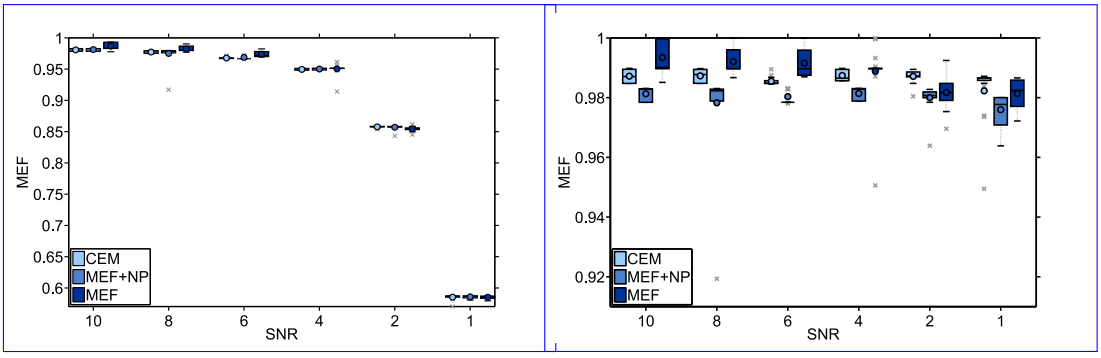


(a) Validating against noise containing datasets.

(b) Validating against noise-free datasets.

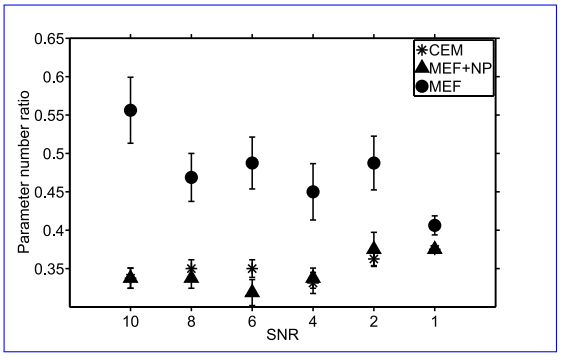
Figure 4. **Effect of adding noise to original signal on prediction capacity for GEP, KRR, RF, SVM and ANN**. The first panel contains the evolution of mean modelling efficiency (MEF) values from 20 independent runs for each increasing level of noise. MEF is computed after learning from a data set of 200 data points and validating against 1000 data points containing noise. The second panel shows the evolution of mean MEF values from 20 independent runs for each increasing level of noise where MEF is computed after learning from a data set of 200 data points and validating against 1000 data points generated from equation 3.10.

~~**Effect of adding noise to original signal on prediction capacity for GEP, KRR, RF, SVM and ANN**. The first panel contains the evolution of mean MEF values from 20 independent runs for each increasing level of noise. MEF is computed after learning from a data set of 200 data points and validating against 1000 data points containing noise. The second panel shows the evolution of mean MEF values from 20 independent runs for each increasing level of noise where MEF is computed after after learning from a data set of 200 data points and validating against 1000 data points generated from equation 3.10. Panel c shows the compared individual MEF evolutions of the studied machine learning methods with noise.~~



(a) Mean MEF when validation against noisy data after 20 GEP runs with different fitness functions.

(b) Mean MEF when validation against noise-free data after 20 GEP runs with different fitness functions.



(c) Ratio of predicted number of parameters to true number of parameters after 20 GEP runs with different fitness functions.

Figure 5. Effects on modelling performance and parameter number caused by choice of fitness function during GEP training for artificial noisy data generated by equation 3.10, where MEF is defined in equation 2.1 and CEM is defined in equation 2.3.

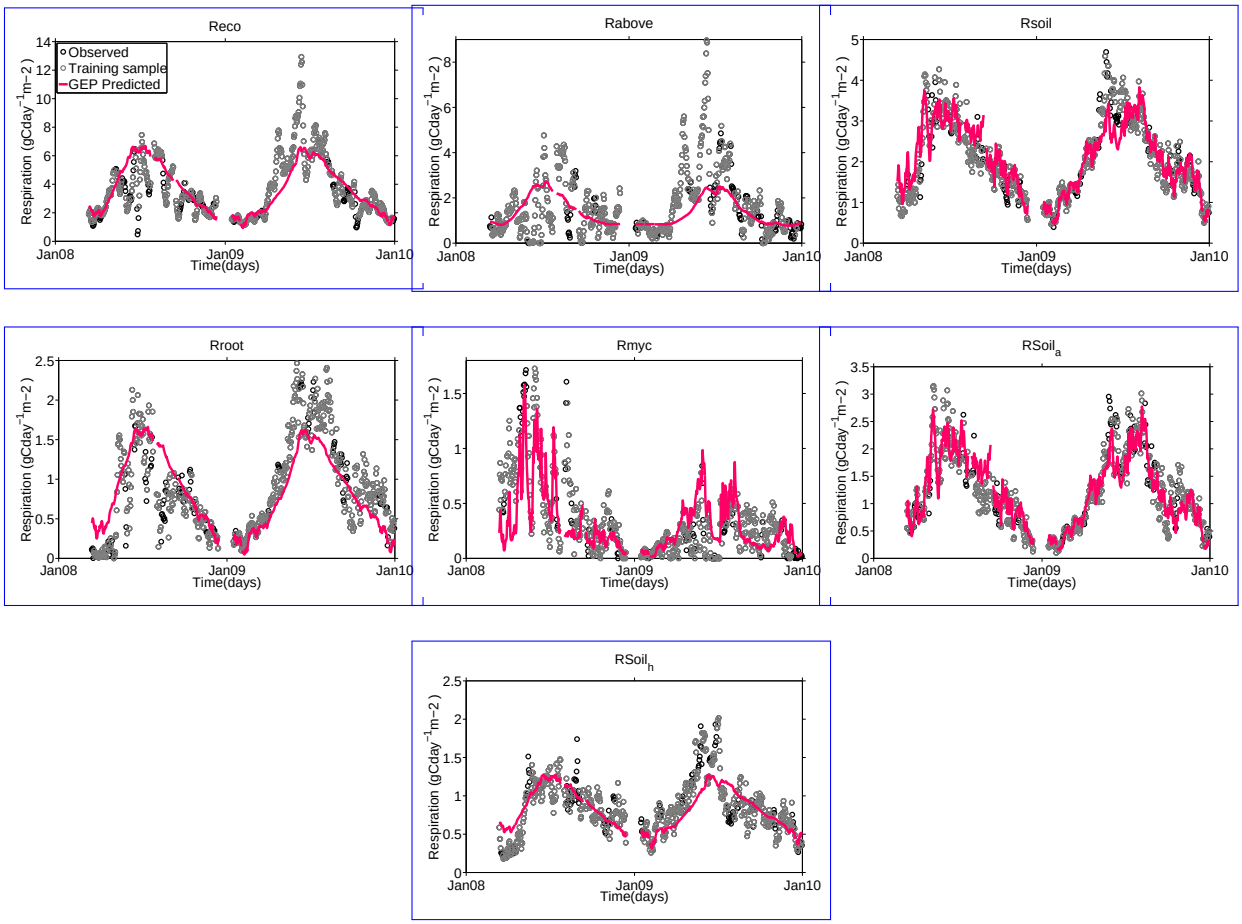


Figure 6. Observed and predicted outgoing CO_2 fluxes. 613 time steps of daily averaged CO_2 ~~effluxesvfor~~ effluxes for two years at the Alice Holt oak forest site. The predicted values are generated with the models extracted by the GEP approach with the settings given in table 1 for the following types of respiration: $R_{eco}, R_{above}, R_{soil}, R_{root}, R_{myc}, R_{soil_a}, R_{soil_h}$. The models are given in equations: 4.2-4.8

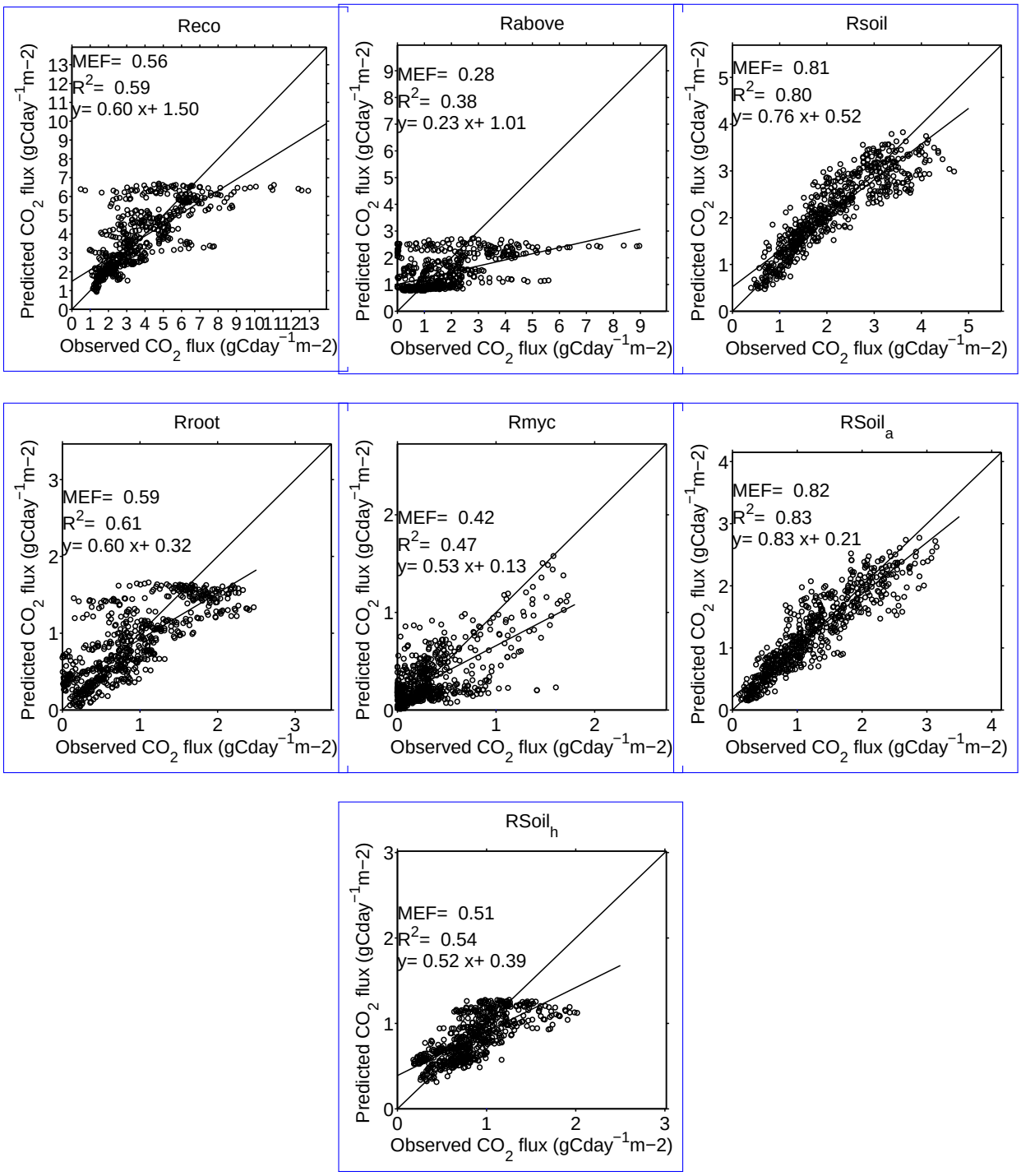


Figure 7. Observed and predicted outgoing CO_2 **fluxes.**613 time steps of daily averaged CO_2 effluxes for two years at the Alice Holt oak forest site. The predicted values are generated with the models extracted by the GEP approach with the settings given in table 1 for the following types of respiration: $R_{eco}, R_{above}, R_{soil}, R_{root}, R_{myc}, R_{soil_a}, R_{soil_h}$. The models are given in equations: 4.2-4.8

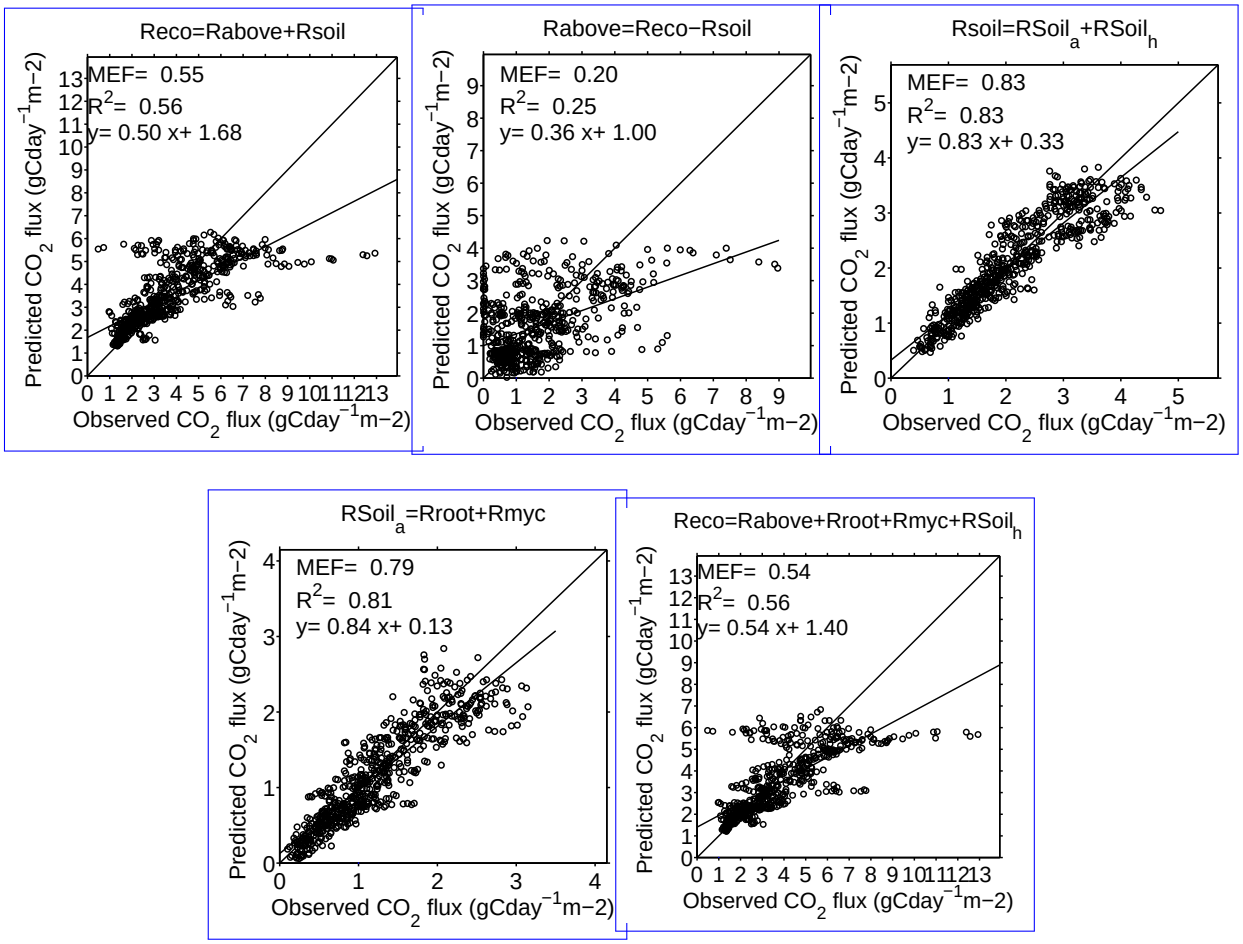


Figure 8. Observed versus predicted R_{eco} components fluxes, where predicted values are computed as derived fluxes.

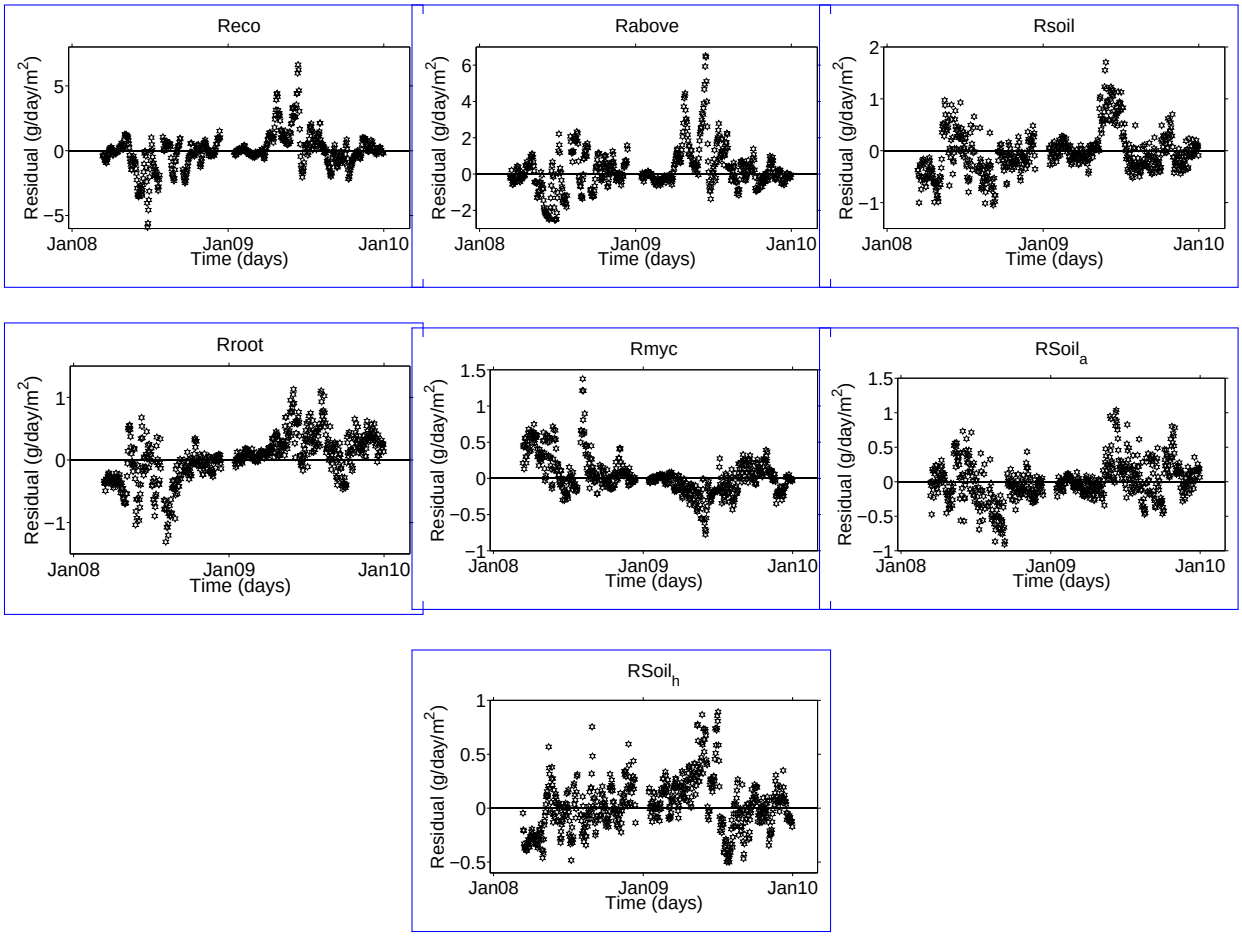


Figure 9. Residuals computed for the GEP models after training on log-transformed data.

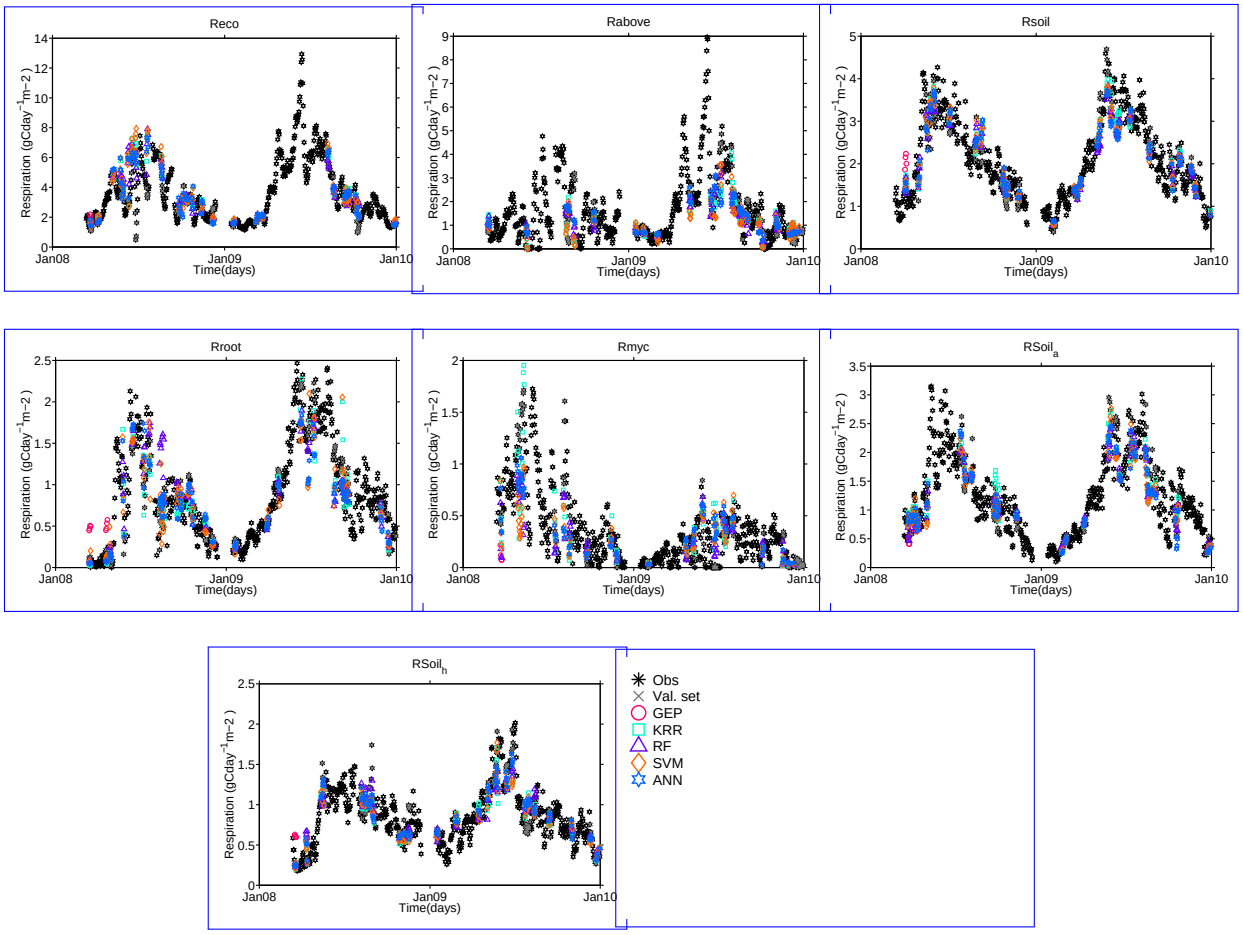


Figure 10. Observed CO_2 fluxes and one set of 113 predicted values given by the some common machine learning methods (MLM) after training on 500 data points.

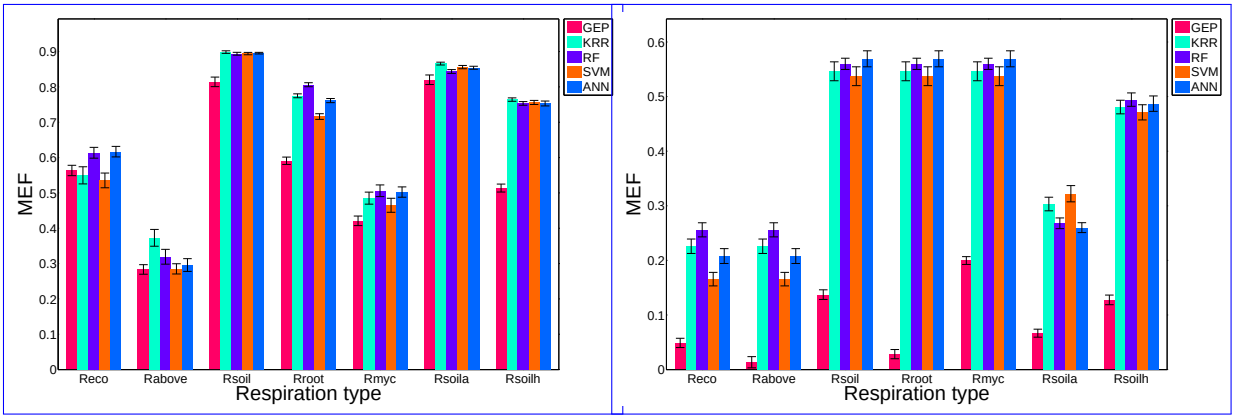


Figure 11. Machine learning methods (MLM) prediction performance for all respirations components (left) and for the residuals (right) resulting from the GEP trained models. The MEF values obtained for validation by all the MLM methods for $R_{eco}, R_{above}, R_{soil}, R_{root}, R_{myc}, R_{soil_a}, R_{soil_h}$

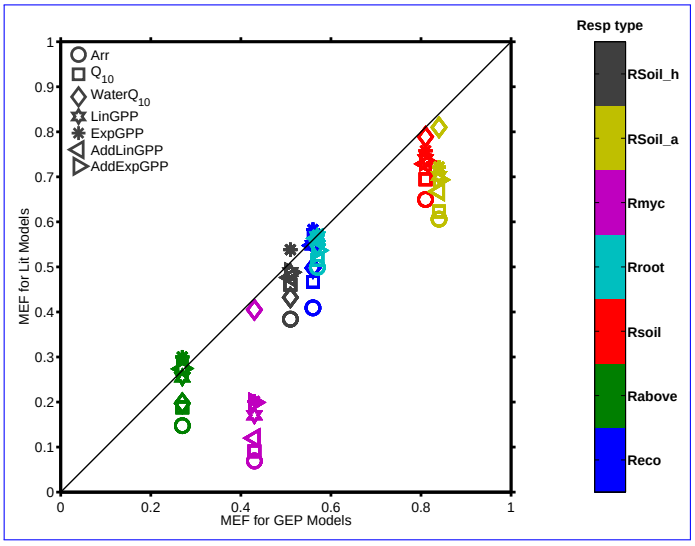


Figure 12. MEF validation values for literature models and for the best GEP model in terms of MEF at each respiration level. Each R_{eco} flux component is shown in a separate colour.

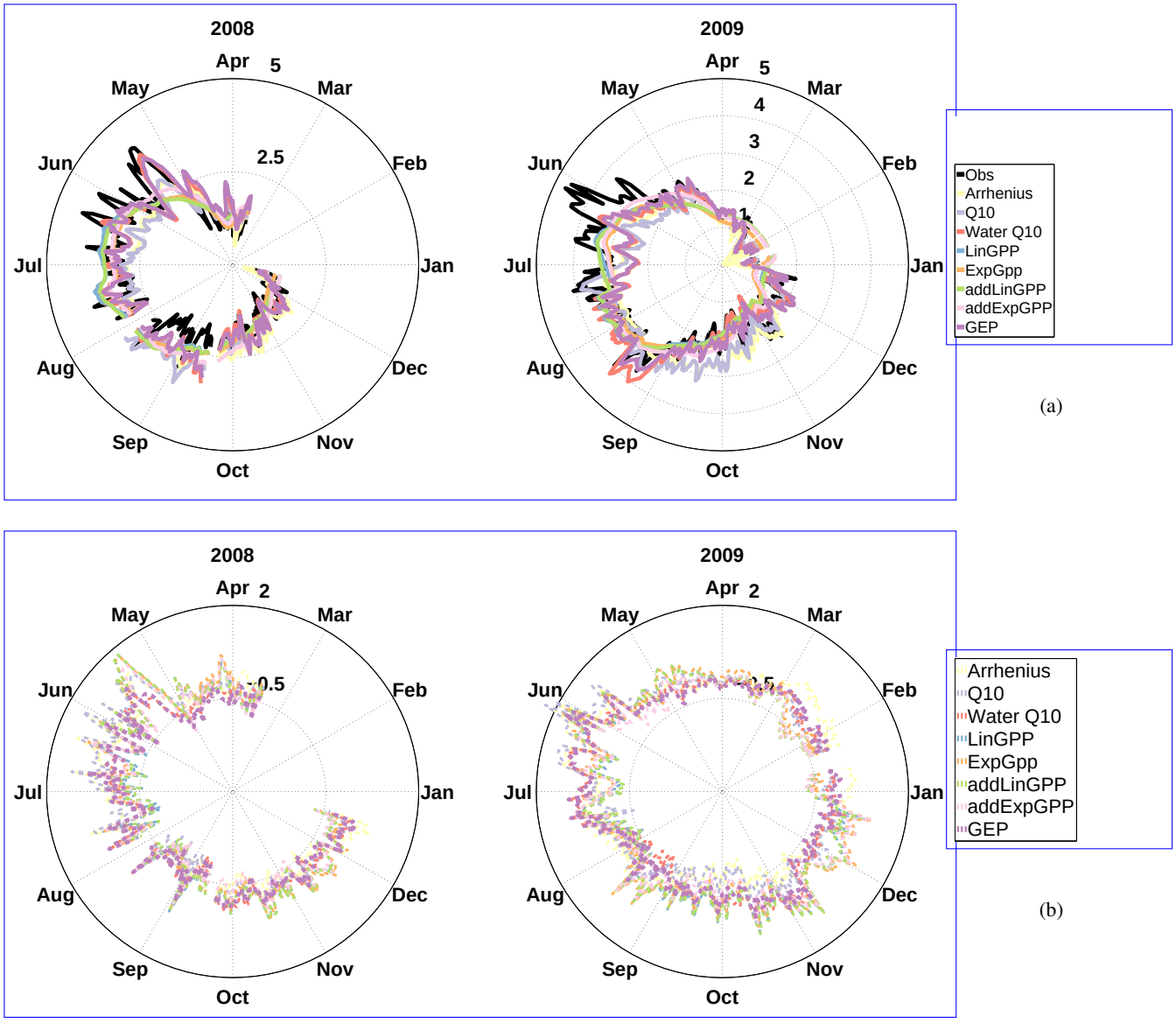


Figure 13. ~~Daily R_{soil} fluxes illustrated in the context of the two studied years and residual values of the total soil daily CO_2 outgoing fluxes as simulated by the investigated literature models and the GEP emerged model.~~ **Daily R_{soil} fluxes (A) illustrated in the context of the two studied years and residual values (B) of the total soil daily CO_2 outgoing fluxes as simulated by the investigated literature models and the GEP emerged model.** The fluxes shown here are the real flux measured at the site and the predicted fluxes generated according to the GEP model and some of the models used in the environmental science community. The center of the plots in the second row is -1. The scale of the fluxes is given in gC/~~day/~~m^2/day.

Supplemental Materials:

Supplemental Materials: Reverse engineering model structures for soil and ecosystem respiration: the potential of gene expression programming

Table 1. ~~The Karva language translation~~ Standard error of ~~a function containing a and b as variables and sin, +, and ∗ as elementary functions. The mathematical structure can be translated into Karva coded genes and~~ the ~~genes expressed into expression trees that can be easily interpreted by machines. The dark coloured section of the gene (string) represents the active component of the gene that is translatable into mathematical expressions, the light coloured section is inactive~~ MEF at validation values for all MLM for different SNR values when the ~~moment~~MEF values are computed against the noisy data.

SNR	GEP	KRR	RF	SVM	ANN
9.82	0.00	0.00	0.02	0.00	0.00
8.18	0.00	0.00	0.02	0.02	0.00
7.01	0.00	0.00	0.02	0.01	0.00
6.14	0.00	0.00	0.02	0.01	0.00
5.45	0.00	0.00	0.02	0.02	0.01
4.46	0.00	0.00	0.02	0.01	0.00
3.27	0.01	0.01	0.02	0.01	0.01
2.73	0.01	0.01	0.02	0.01	0.01
2.34	0.02	0.01	0.02	0.01	0.01
1.96	0.02	0.02	0.02	0.02	0.01
1.75	0.02	0.02	0.02	0.03	0.02
1.40	0.05	0.03	0.02	0.02	0.02
1.23	0.03	0.03	0.02	0.03	0.03
1.09	0.04	0.03	0.03	0.04	0.03
1.00	0.04	0.03	0.02	0.03	0.03

Table 2. Standard error of the MEF at validation values for all MLM for different SNR values when the MEF values are computed against the clear data.

SNR	GEP	KRR	RF	SVM	ANN
9.82	3e-07	4e-05	2e-02	4e-03	4e-03
8.18	3e-07	6e-05	2e-02	2e-02	2e-03
7.01	3e-07	4e-05	2e-02	1e-02	2e-03
6.14	2e-06	7e-05	2e-02	2e-02	2e-03
5.45	2e-06	1e-04	2e-02	2e-02	4e-03
4.46	6e-06	1e-04	2e-02	2e-02	2e-03
3.27	9e-06	2e-03	2e-02	1e-02	3e-03
2.73	4e-05	4e-04	2e-02	1e-02	6e-03
2.34	4e-05	6e-04	2e-02	9e-03	3e-03
1.96	8e-05	1e-03	2e-02	1e-02	3e-03
1.75	2e-04	8e-04	1e-02	1e-02	5e-03
1.40	8e-04	1e-03	1e-02	2e-02	5e-03
1.23	1e-04	2e-03	1e-02	2e-02	4e-03
1.09	4e-03	3e-03	1e-02	2e-02	5e-03
1.00	7e-04	3e-03	1e-02	5e-02	6e-03

GEP models for all log-transformed respirations types time series, before back-transformation.

$$\log(R_{eco}) = \frac{GPP_s}{T_{-10}} + \log(\log(T_{-10})) \tag{1.1}$$

$$\log(R_{above}) = 0.1T_{-10} + 0.4\log(0.8\sqrt{SWC}) \tag{1.2}$$

$$\log(R_{soil}) = 1.2T_{-10}^{0.4} + 1.3SWC - 3.1 \tag{1.3}$$

$$\log(R_{root}) = 0.9\frac{1.2GPP_s - 8.1}{T_{-10}} \tag{1.4}$$

$$\log(R_{myc}) = 1.1\log(1.7T_{-10}) + 1.2T_{-10}^{SWC} - 7.4 \tag{1.5}$$

$$\log(R_{soil_a}) = 1.2T_{-10}^{0.5} + 2.5SWC - 4.9 \tag{1.6}$$

$$\log(R_{soil_h}) = -0.3 + 0.6\frac{1.1GPP_s - 3.6}{T_{-10}} \tag{1.7}$$

Figure 1 in supplemental material illustrates the change in the shape of the PDF estimated for each respiration type after log-transforming. For all time series, the skewness is visibly is reduced.

From Fig. 4 it is worth mentioning the apparent correlation, although weak in terms of R^2 value, of the R_{myc} residuals with GPP_s, even when this was not chosen as a driver, indicating that the relation was not strong enough for an explicit model inclusion but it could show a dependency to a driver for which GPP_s acts as a proxy such as phenology, or substrate availability. Such weak correlations are present as well between R_{soil} and R_{soil_h} residuals and T_{air}.

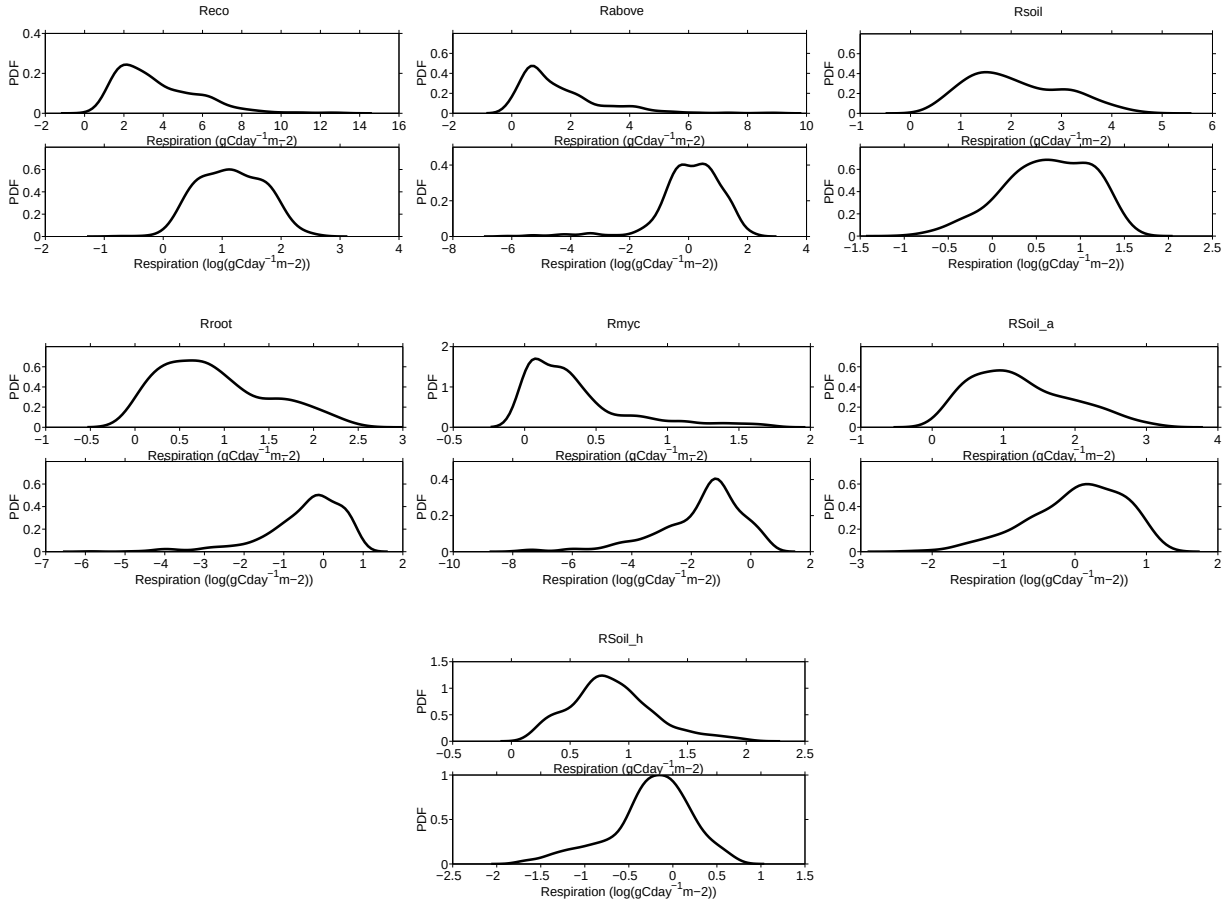


Figure 1. Change in estimated density function of observations before and after log-transforming for all studied respiration types.

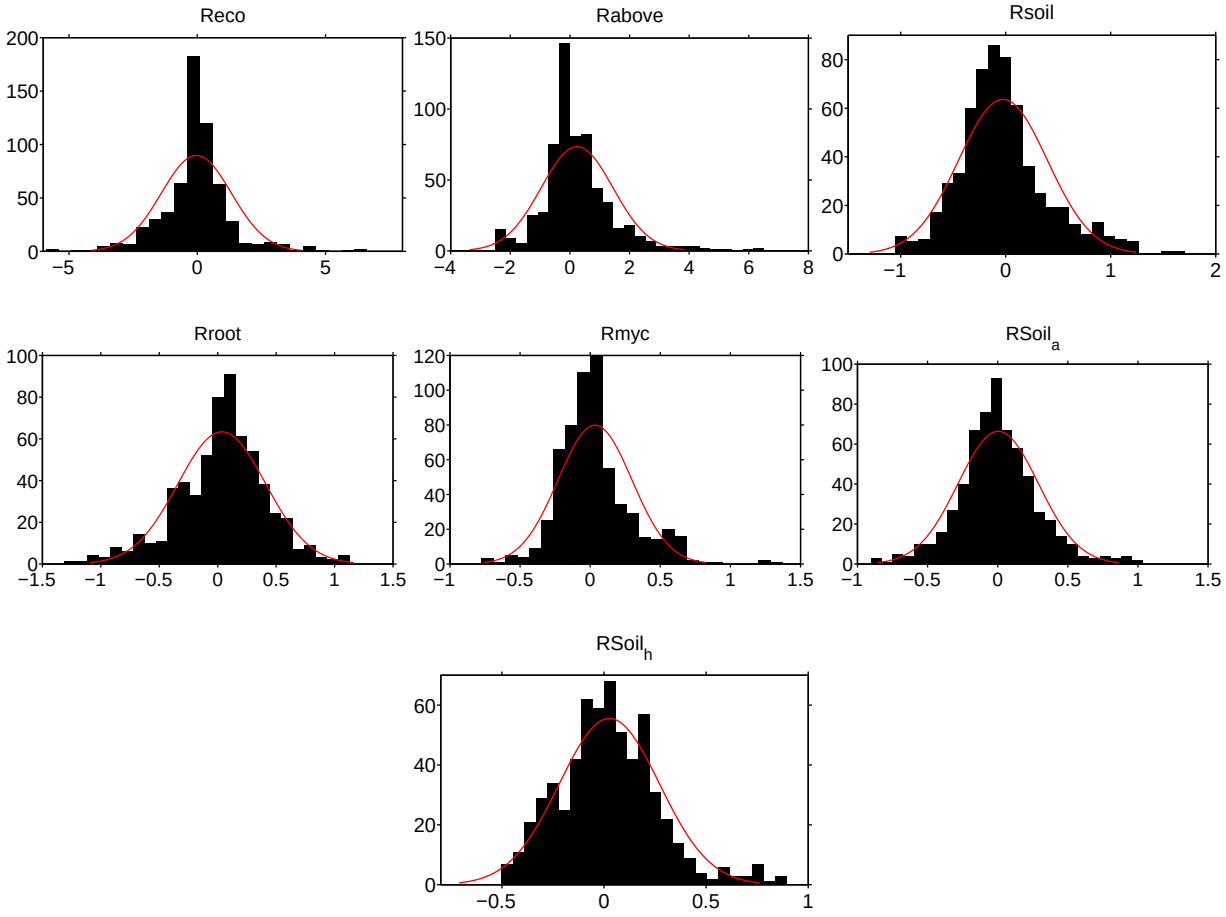


Figure 2. Residuals computed for the GEP models after training on log-transformed data.

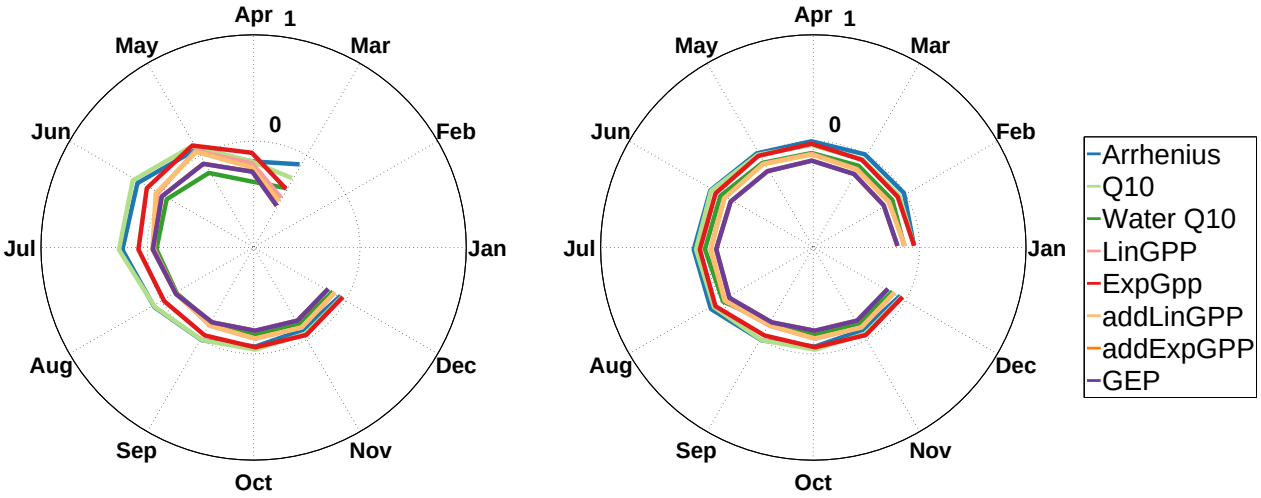


Figure 3. Monthly averaged error values for some literature models for and the GEP generated model for daily soil CO_2 efflux in the two studied years. The center of the plots is -1. The scale of the fluxes is given in $gC/m^2/day$.

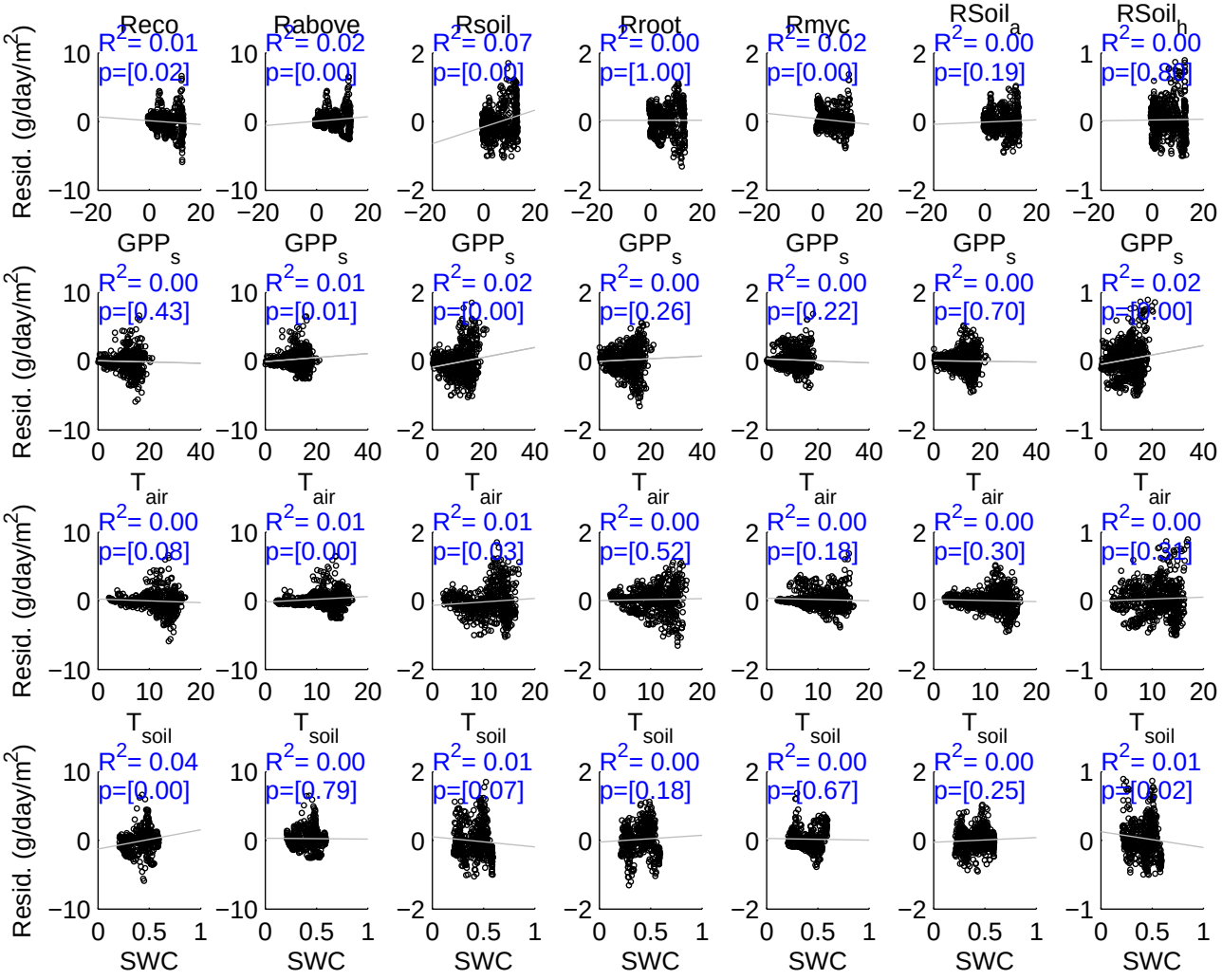


Figure 4. Candidate driver linear correlations with GEP model residuals.