A probabilistic optimization approach to deal with uncertainties in model calibration

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***Abstract*—In this paper, we present an approach based on robust probabilistic optimization via simulation to take into account uncertainties in the data used for model calibration. We apply this work to a fishery resource management problem and show that the results obtained can be used in real situation. The model links two time series that are difficult to estimate. During the calibration phase, we are able to identify if the estimates are consistent with each other and to correct them. It reduces uncertainties, improves our knowledge of the system and increases calibration accuracy. We also identify the limits of this approach and its optimal context of use.**

***Index Terms*—model calibration, optimization, uncertainties**

I. Introduction

The French Research Institute for Exploitation of the Sea has published a report [1] showing that overexploitation affects about a quarter of the fish stocks fished in France. As the oceans are the main source of protein of our planet, it is essential to propose effective stock management strategies.

This is the objective of the PO FEDER MoonFish project[1] on the scale of Corsica, a territory where fishing is still mainly coastal and artisanal. Four main areas (Bastia, Balagne, Bonifacio, Ajaccio) share more than 1000Km of coastline, with 42 ports and anchorage points for approximately 200 boats (49 in Bastia, 23 in Balagne, 44 in Bonifacio and 76 in Ajaccio) and 300 fishermen. Computer tools for planning and decision support allow us to study the evolution of stocks and identify strategies to help decision-makers.

However, the beginning of any study on fishing strategies is to know the population dynamics of the species being exploited. It is the model calibration phase. This phase consists of moving from a theoretical, mathematical model to a one adapted to a real situation. We are going to look for the values of the generic parameters in order to correspond to the observed reality. This can be done automatically, with optimization, or manually with expertise. That is to say, experts in the studied domain will estimate themselves the values for the parameters [2], potentially through real experiments and measurements. They can also carry out a simulation with a set of parameters which seems coherent, observe the results and adapt them until satisfaction. In marine ecology, the ecopath with ecosim software is a reference and the model proposed is entirely based on an expert calibration approach [3]. The automatic methods are mainly based on optimization and a set of real data. The goal is to optimize the model parameters, perform simulations and measure the quality of the results by comparing them to real data. However, the two approaches are not incompatible and it is often possible to combine expert knowledge and optimization to improve results [4] or to ensure the physical consistency (validation) of the proposed solutions [5].

On the other hand, some models can have an infinite number of equilibrium points by compensation between the parameters. This is called the equifinality problem [6] [7]. This problem is all the more important when the data are imprecise time series as we will illustrate later in this document.

So, a part of optimization problems in scientific computing have multi-solution nature, there is more than one combination of the decision variables that can optimize the objective value and find the best one is a challenge. The works presented in this article deal to propose and test an approach based on robust optimization via multiple simulations in order to take into account uncertainties in the input data and correct them when it is possible. We apply it to a real world problematic in an environment where data are always under uncertainties and can never be considered truly reliable. We at least need to consider a margin of error in the estimation or use probability laws.

This article begin with a background section to define the optimization, model types and show some relative works on model calibration. We then present a preliminary work, classical in model calibration, but which presents some limitations in our case. Thus we propose an approach to overcome the identified problems and show its results.

II. Background

A. Optimization

In order to ensure the preservation of endangered stocks at minimum cost to fishermen, methods must be developed and the problem formally defined with: (1) objective functions: mathematical equations, simulation results, fuzzy verbal description, etc.; (2) constraints to be respected.

Optimization is the process of automatically search the values of a set of parameters to get the best possible results

[1] https://moonfish.universita.corsica/

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on the different objectives and satisfying the constraints. Optimization methods can be deterministic or stochastic. When the problem complexity is too high, we favor stochastic approximation methods such as metaheuristics. These are extremely versatile optimization algorithms that can easily be adapted to a very large number of problems. They allow acceptable solutions to be found in a limited time, but cannot guarantee to find the optimal one. On the other hand, they are subject to a problem illustrated by the "no free lunch theorem" [8]: it is very difficult to determine in advance which metaheuristic will be the most efficient on a given problem. This is why, in the rest of the paper, we will use several different algorithms but only present the results of the best one.

The optimization can be used as a preliminary work to help calibrating models [9]. This phase consists, from real data, to carry out simulations with different sets of parameters in order to find the one, or those, allowing to retrieve the known data. An external expertise can also be used [10] to limit the parameters in coherent values, or to add constraints to ensure the coherence of the mathematical model with the reality of the studied system.

The equifinality problem [7] introduces a notion of uncertainty. Indeed, if we cannot be sure of the accuracy of the calibration data, it may be necessary to move towards methods capable of managing uncertainties such as robust optimization. Many methods exist, but here we will focus on a simulation context. In this paper, we use a so-called direct method which consists by using the uncertain informations directly in the evaluation function and adapting the algorithm to take them into account. Metaheuristics, and more particularly evolutionary algorithms, seem to be especially adapted to obtain robust models capable of taking uncertainties into account [11] [12].

B. Relative works on model calibration via optimization

The success of ecopath with ecosim [13] shows that, in some cases, the expert approach alone is valid. But it also has limitations. For example, [14] requires the use of an optimization method to determine a parameter of a physical model of thermal degradation, as it is not experimentally determinable. Thus, model calibration can often be considered as a global optimization problem [15]. Most of the time, a stochastic optimization method is used. Deterministic methods can be considered but they do not allow to solve complex problems because the cost of calculation becomes too high.

In [16], the authors propose the use of global optimization to calibrate a mathematical model of DNA synthesis. Based on a set of experimental data, they use different types of methods. First manually via expertise to determine a parameter. They then use a local search based on this parameter to successfully improve the expert's accuracy. They then propose the same operation using a global search rather than expert knowledge and obtain better results. Coupling expertise and optimization is therefore not incompatible [17]. According to [4] it should even be encouraged because it can reduce the need for calibration and ensure the physical consistency of the solutions [18].

In some cases, multi-objective optimization methods can be considered [19] but we won't address it in this article because we will always have a single objective.

The use of monte carlo simulation can also be useful to ensure the robustness of the solution [20]. In addition, the use of methods based on the neighborhood [21] can allow uncertainties to be taken into account directly during the calibration phase. It can be very efficient on complex models. However, neighborhood measurement can be difficult to define.

In marine biology, accurate data acquisition is very difficult. In the context of Corsican exploitation, where a large number of species are concerned, it is totally impossible to acquire accurate data for each one. Uncertainty must therefore be taken into account right from the model calibration phase. So the model must also be adapted to these problems. We know that it will be impossible for us to use a complex model due to a lack of knowledge about the system. So using a simple model with a fast calculation time can make it easier for us to deal with uncertainties.

C. Fishery models

Fishery models are based on biological models of population growth. We find on one side the global models [22] and on the other side the structural models that distinguish individuals in class of age, size or weight classes.

Structural models offer high precision for efficient management. Nevertheless, they require a large amount of population and farm data to be calibrated.

Global models, which consider the population as a whole with a general biomass, have the advantage of being usable and configurable with a small amount of data. By having knowledge of catches and fishing effort[2] applied by the exploitation, the parameters can be deduced. A particular notion of these models is to consider that without exploitation, the population tends to equilibrate. On the other hand, the loss of precision avoids any regulation in terms of the weight or size of individuals.

Most of the works focuse on a particular species with an industrial type of exploitation. This type of study is not possible in this case. Fishing on the Corsican coast is artisanal and with small boats exploiting many species. This type of exploitation makes it difficult to obtain accurate data on a particular species, which is why we identifyed that it is preferable to move towards a global type model.

III. Preliminary works

A. Graham-schaefer model

We choosed the Graham-Schaefer global model [23], a population dynamic model based on the stock production model introduced by [24]. In a fishery context, it is based on the following equations :

$$B(t+1) = B(t) + r(1 - \frac{B(t)}{k})B(t) - C(t) \qquad (1)$$

[2]Indicator quantifying how intensively fishing has been carried out

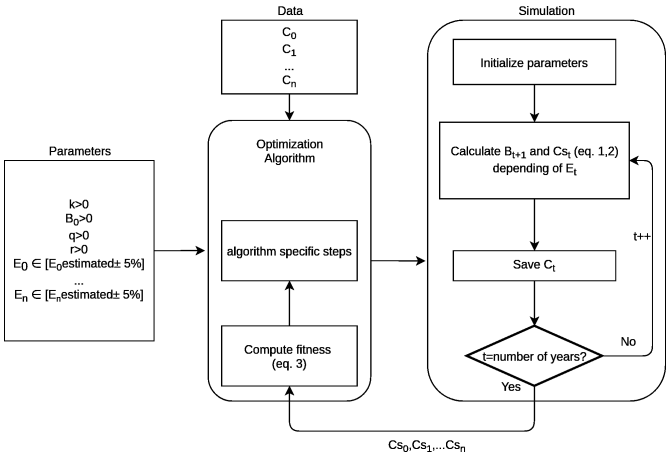

Fig. 1. Problem with accurate knowledge

$$C(t) = qE(t)B(t) \tag{2}$$

With:

- k : biomass at equilibrium (in mass);
- r : the growth rate per unit of time;
- q : caturability per unit of effort;
- $B(t)$: the biomass at time t (in mass);
- $E(t)$: the fishing effort apply from time t to $t+1$

The simplicity of this model allows us to calibrate it even when a little amount of data is available. Indeed, for any pair of time series $(C(t), E(t))$ coherent between them, there is an infinity set of parameters allowing to find these data. The model being simple, the simulation time is very short which is also an advantage in situation of evaluation via multiple simulations.

B. Model calibration

Based on two datasets for each species:

- catches estimations, $C(t)$, during 58 years presented in [25]
- and estimations of fishing effort associated to these catches defined by value intervals

Our goal is to find the parameters set of the Graham-Schaefer model allowing, via simulation, to find back the known catches using the estimate efforts.

Thus, at each iteration and for each potential solution, a simulation of the fishery is conducted using known fishing efforts. This will determine catches associated with the proposed population dynamics. The efficiency of the proposed solution is then estimated by calculating the quadratic error committed, i.e. the difference between estimated and simulated catches.

$$f(x) = \sum_{i=0}^{nbYears} [C_i - Cs_i]^2 \tag{3}$$

We have defined several configurations of this problem:

- 10 or 58 years of data
- a level of knowledge of the fishing effort: perfect; accurate (limits of $\pm 5\%$ of the true value); no knowledge.

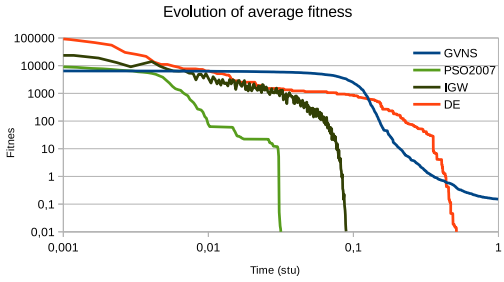

Fig. 2. Evolution of average fitness on 100 replications of the problems with 58 years with perfect knowledge

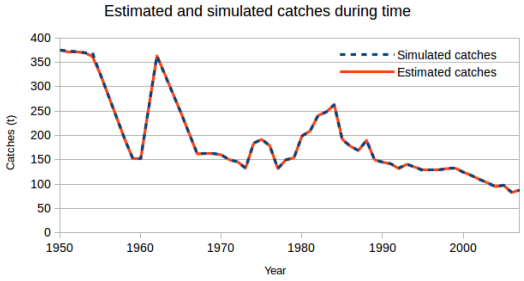

Fig. 3. Calibration results for consistent data estimations

On each one, we tested 6 algorithms from the literature: General Variable Neighborhood Search algorithm [26] [27] (GVNS); Ant Bee Colony [28] (ABC); Differential Evolution [29] (DE); Particule Swarm Optimization [30] (PSO2007), Improved Grey Wolf [31] (IGW); Whale Optimizatoin Algorithm [32] (WOA).

For each, we used the same parameters as in the associated publication. In addition, we limit the computing time to 1 Standard Time Unit [33] (STU) which is equivalent to 7s on 1 thread of a 4GHz Intel I7 processor.

Figure 1 represents the optimization process on the problem with accurate knowledge. Without knowledge, we set $E_t > 0 \; \forall \; t$. With perfect knowledge, the E set is fixed and managed by the simulation.

The results are presented in the table I where NA means Not Applicable. They allow us to conclude that assuming perfect knowledge, PSO2007 is the algorithm to use. Indeed, even if other algorithms have close average performances, its convergence time is optimal as shown in the figure 2. Finally, still according to the table I, if we know that the data are inaccurate, GVNS should be used. We can also note that the DE presents competitive results up to 10 years of simulation.

Figure 3 shown the simulated and real catches curves are superimposed, so the calibration could not be better. However, a problem arises, these results can be found with a large number of parameter sets.

To illustrate this, we have carried out 2000 calibrations on fully simulated data for which we know the result to be obtained during the calibration phase. For each one, we use

		GNVS		ABC		DE		PSO2007		IGW		WOA	
years	knowledge	mean	t (tsu)	mean	t (tsu)	mean	t (tsu)	mean	t (tsu)	mean	t (tsu)	mean	t (tsu)
10	perfect	2,68E-2	7,20E-1	1,23E-3	6,80E-1	2,45E-6	2,40E-1	8,98E-2	9,40E-3	4,68E-4	2,60E-2	5,27E-2	3,90E-1
10	accurate	4,18E-5	1,40E-1	1,13E-5	4,20E-1	4,39E-2	7,10E-1	9,60E-7	2,76E-1	1,22E-4	2,50E-1	7,60E-1	8,20E-1
10	none	1,00E-8	8,60E-2	1,81E-3	5,70E-1	3,83E-1	8,30E-1	NA	NA	7,41E-1	8,60E-1	NA	NA
58	perfect	NA	NA	NA	NA	7,70E-7	6,90E-1	8,30E-7	1,10E-2	2,74E-3	8,60E-2	NA	NA
58	accurate	2,50E-5	4,40E-2	2,46E+0	8,90E-1	NA	NA	NA	NA	2,75E+0	7,90E-1	NA	NA
58	none	9,98E-3	9,20E-2	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA

TABLE I
MEANS FITNESS AND CONVERGENCE TIME FOR EACH ALGORITHM ON EVERY PROBLEMS

the same catches and efforts data, then we made a multivariate kernel density estimate following the Silverman rule of thumb [34] to have a representation of the density of the solution space.

In figure 4, each point represents a perfect solution to the calibration problem. The color represents the density of the solutions in space. The darker the color, the denser the area. Conversely, the closer the color is to yellow, the lower the density is. We deliberately removed a parameter in order to be able to make a graphic representation.

The first test, figure 4(a), with almost perfect knowledge of efforts (5% maximum variation) and catches presents a set of points relatively close to each other. On the other hand, when knowledge is relatively low, figure 4(b), the results are much more chaotic and it is impossible to determine which solution to use.

Our work therefore consists of proposing an approach to calibrate the model by taking into account the confidence rate given to each year of data.

IV. APPROACH AND RESULTS

A. Formal description of the approach

We start from two time series denoted $C(t)$ and $E(t)$ such that $\forall t, C(t) \sim P_{C_t}(x), E(t) \sim P_{E_t}(x), \forall x \in R^+$ with P a known probability distribution of some kind, potentially different for each data. Any P is discretized into value intervals for which we calculate the probability of drawing a value in this interval. The width required for each of these intervals can be determined through sensitivity analysis. Moreover, via simulation, for a known E series, we can calculate $C(t)$ corresponding to $\forall t$ (see algorithm 1 line 8). Thus, we can compute the probability $f(C, E)$ (line 10 and 15) that a set of value (C, E) corresponds to reality :

$$f(C,E) = \prod_t min(P_{C_t}(C(t)), P_{E_t}(E(t))) \tag{4}$$

By simulating all possible scenarios for the E series (lines 5 to 13), we can calculate the probability that the proposed solution is valid regardless actual time series (line 15) :

$$F(q,r,k,B0) = \sum_{i=0}^{nSim} f(C_i, E_i) \tag{5}$$

Moreover, if the two time series are consistent with each other, simulating all possible scenarios according to $E(t) \sim P_{E_t}(x)$ should allow us to find P_{C_t} in the case of a perfect solution. Otherwise, $\forall x \in P_{C_t}, \sum P_{C_t} computed(x) = F \Rightarrow \frac{P_{C_t} computed(x)}{F} = P_{C_t} estimates(x)$. Significant differences between $P_{C_t} estimatee$ and $\frac{P_{C_t} computed}{F}$ will then be sign of inconsistency between time series and thus of estimation error over the year t.

This approach is highly parallelizable on GPU which allows us to easily explore all possible scenarios. In case it is impossible to simulate all the scenarios, a significant set can be used. Our goal will be to find $(q, r, k, B0)$ maximizing F, thus obtaining the most coherent solution with respect to our data. At the output of each simulation we obtain a set of final probabilized biomass values that can be used as an input for a future robust optimization process. This allows us to know the evolution of the stock in the best and worst case but also in the most probable set of cases.

To validate our approach, the next two sections first focus on an arbitrarily defined theoretical case study that is consistent with reality.

Algorithm 1 Compute fitness

Require: $P_{C_t} P_{E_t} \forall t$, $(q, r, k, B0)$, n number of years for each simulation, $nsimu$ the total number of simulation, $E[nsimu][n]$ the effort to apply for each year and simulation, $Bfinal[nsimu]$ set to store the final biomass of each simulation

1: Each GPU thread:
2: **for** $j = threadIndex; j < nsimulation; j+ = threadStride$ **do**
3: B=B0
4: proba[j]=1
5: **for** $i = 0; i < n; i++$ **do**
6: $c = q * B * E[j][i]$
7: $B = B + r * (1 - B/k) * B - c$
8: $proba[j] = proba[j] * min(P_{C_i}(c), P_{E_i}(E[j][i]))$
9: **end for**
10: Bfinal[j]=B
11: **end for**
12: Thread synchronization
13: $fitness = \sum_{i=0}^{nsimu} proba[i]$

B. Application on consistent estimations

To illustrate our approach, we decided to start from theoretical data that we generated by simulating the evolution of a random species. Thus, a first test on perfect estimates will allow us to validate the coherence of the approach.

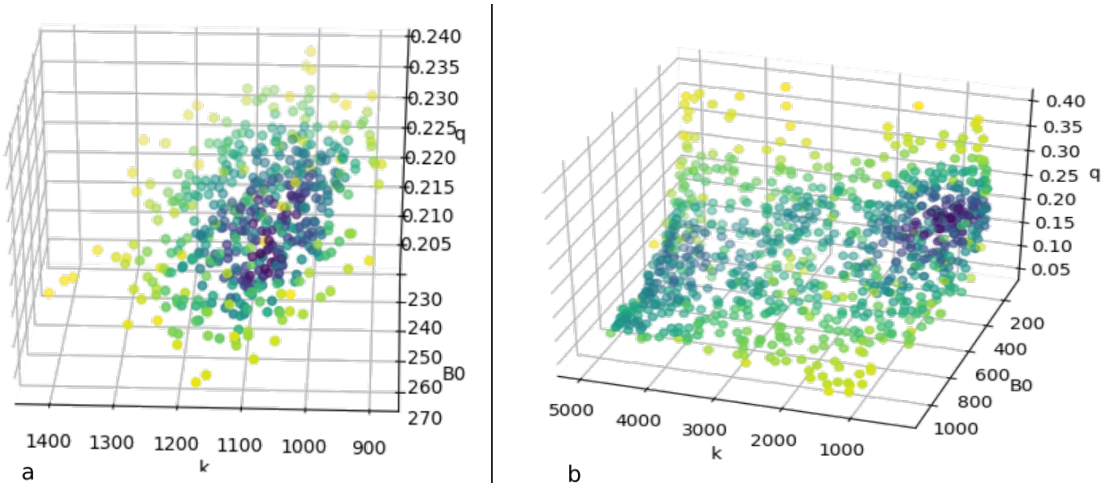

Fig. 4. Kernel Density Estimation on 2 tests. (a) accurate knowledge about real catches and fishing efforts. (b) Large value intervals for the fishing effort dataset

For this, we start from an arbitrary scenario that could happen in practice:

- 10 years of efforts and catches estimations
- 6 of these, yr_i, are very reliable
- the 4 others, ye_i, are estimates that follow a normal distribution, centered on the real value and which we have varied σ during different tests.
- effort and catch estimates are consistent with each other.

For reliable years, we consider that $E(t)$ is perfectly accurate and that the estimate of $C(t)$ does not differ by more than 20

As before, it is possible that the parameters compensate each other and therefore there may be several solutions. We have therefore chosen a multimodal optimization algorithm allowing us to propose several solutions for final expertise and validation.

We use the Dual Strategy Differential Evolution (DSDE) algorithm presented in [35]. A solution is only composed of the parameters $(q, r, k, B0)$ of the Graham-Schaeffer model and is evaluated following the algorithm 1.

The table II shows the results obtained according to the variability of the probability laws. Note that the more precise the effort estimates are (low σ_E), the better the results. On the other hand, a higher precision on C than on E gives relatively poor estimates. However, this result can easily be explained. Indeed, as we explore in functions of E, if E covers a large range of values while C covers a small range, a large number of scenarios will have inconsistent C values and thus $f(C, E) = 0$. However, the proposed solution is not necessarily to be rejected and this may help to identify years of data requiring re-estimation, or even correction (section IV-C).

The figure 5 shows the distribution of the final solutions in the space composed of the parameters (q, r, B), the parameter k has been removed to allow a graphical representation. We obtain a set of quasi-equivalent fitness solutions. The relatively small number and their dispersion can easily allow an expert

σ_C	σ_E	Fmean	σ_C	σ_E	Fmean
C(t)/5	E(t)/5	0.874579	C(t)/15	E(t)/5	0.015499
C(t)/5	E(t)/10	0.965582	C(t)/15	E(t)/10	0.208958
C(t)/10	E(t)/5	0.075843	C(t)/15	E(t)/15	0.893316
C(t)/10	E(t)/10	0.857864	C(t)/15	E(t)/20	0.979369
C(t)/10	E(t)/15	0.991102	C(t)/15	E(t)/25	0.996413

TABLE II
RESULTS DEPENDING OF THE VARIABILITY OF P_{C_t} ET P_{E_t}

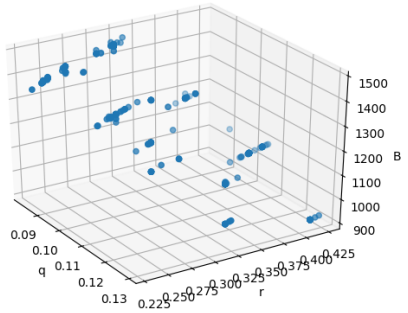

Fig. 5. Solutions of the calibration with perfect estimations of the probability laws

to analyze the results and direct us to the most biologically consistent solution.

In addition, the figure 6 represents the evolution of biomass over time for all the coherent simulated scenarios of one of the proposed solutions. The final biomass varies by about 10% between the different scenarios. This value may differ depending on the data and the variability of the estimates but it is fairly representative of them. Moreover, for each of these values we know the probability that it is correct. We can therefore easily use it in a future robust optimization aimed at improving operating strategies.

Finally, the figure 7 shows the probability laws P_{C_t} esti-

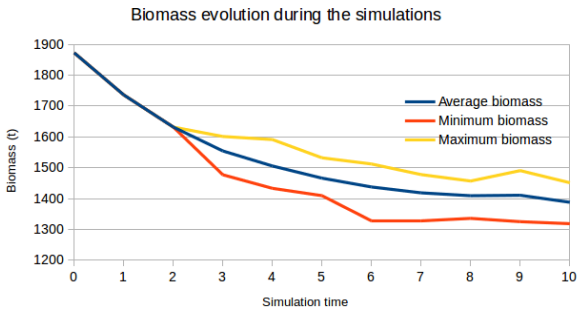

Fig. 6. Biomass evolution between time for each simulation

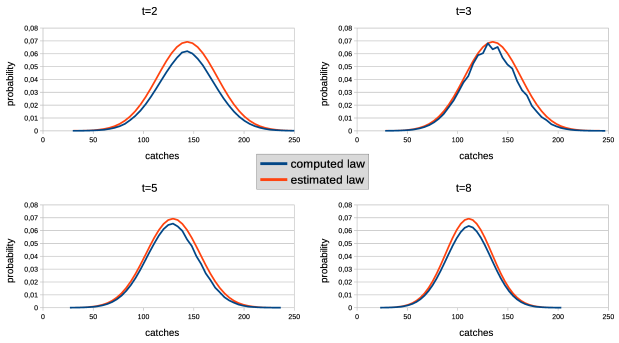

Fig. 7. Comparison between estimated and computed probability law with perfect estimations

mated (in red) and obtained via simulation in blue for the 4 unreliable years (respectively t=2, 3, 5, 8). As we expected in the case of perfectly consistent estimates, we find almost perfectly the estimated distributions.

We will now build on these initial results to identify and correct inconsistencies in the data.

C. Identification and correction of inconsistent data

We start again from the previous scenario on which we have made the following modifications:

- Among ye, the first catch estimated is centered on the right value, the 3 others are overestimated. The user doesn't know this.
- As effort estimates are more easily feasible, they will be more reliable than catch estimates.

The overestimates range from $\sigma(t)/4$ *to* $2*\sigma(t)$ covering a range of variability from very low to very high. Surprisingly, the variability of the overestimate has little impact on the results over this range. Beyond this upper limit, the estimated probabilities become so low that the success of the proposed approach becomes very random.

The goal here will be to modify the estimated P_{C_t} farthest from the computed $Pcomputed_{C_t}$ probability distribution in order to get as close as possible to a coherent solution. Here we will let the algorithm 2 run automatically. In real situation, it can obviously be used to spot potential errors and let an expert update the laws of probability himself.

We start (line 1) by calculating the set of solutions following the method defined above. For each year of simulation, we update $Pcomputed_{C_t}$ (lines 2 to 6). Thereafter, if the laws of probability allow it, we calculate the parameters corresponding to $Pcomputed_{C_t}$. A calculation of relative distance between the estimated and calculated parameters then makes it possible to identify the year $ymax$ for which the estimate is the worst (line 7 to 11), a sign of an estimation error. These parameters are finally modified in the direction of those of $Pcomputed_{C_t}$ (line 12). Note that a bad estimate can easily impact the probability laws of other years, so it is important to modify only one per iteration. In the case where the probability laws do not allow a quick calculation of the parameters governing it, these steps can be replaced by a calculation of the distance between the different values of the discretization intervals and then a direct update of these values.

Figure 8 shows a diagram of the complete system including algorithm 1 and 2.

Algorithm 2 improvement of inconsistent data

Require: $P_{C_t} P_{E_t} \forall t$

1: Use DSDE with the compute fitness algorithm (algorithm 1) and keep $fitness$, $proba$ and C sets of the best solution
2: **for** $j = 0; j < nsimulation; j++$ **do**
3: **for** $i = 0; i < n; i++$ **do**
4: $Pcomputed_{C_i}(C_j(i)) += proba[j]/fitness$
5: **end for**
6: **end for**
7: **for** $i = 0; i < n; i++$ **do**
8: Compute parameters of the probability law $Pcomputed_{C_i}$ (μ, σ for our normal law)
9: Compute relative distance between estimated and computed parameters
10: Keep $ymax$ the year with the maximum difference
11: **end for**
12: Modify the $P_{C_{ymax}}$ parameters in the sens of $Pcomputed_{C_{ymax}}$
13: Loop on first step until a stop criterion is reached

The figure 9 shows the results of this algorithm for the different years of unreliable estimates with:

- In yellow, what we have called perfect law, which is the law of probability that we used in the previous application and that should be found.
- In red, the probability law $Pcomputed_{C_t}$ at the first iteration of the algorithm
- In blue, the probability distribution $Pcomputed_{C_t}$ after 50 iterations.

We notice that at the beginning, even for $t = 2$, the only year for which we kept a correct estimate, the initial $Pcomputed_{C_t}$ expectation is slightly out of line. This difference is even greater for the other years. After 50 iterations on the other hand, most of the errors are corrected and we find almost perfect probability laws.

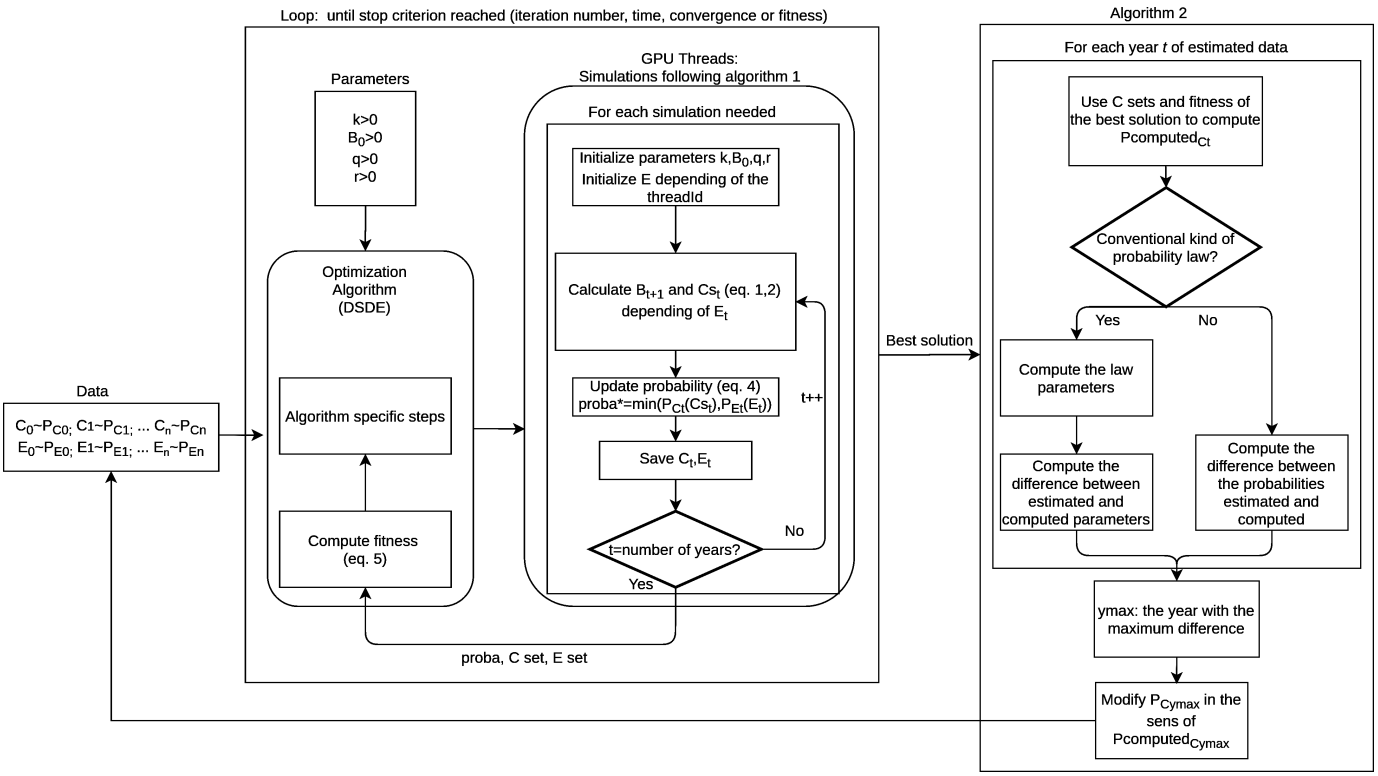

Fig. 8. Complete system diagram

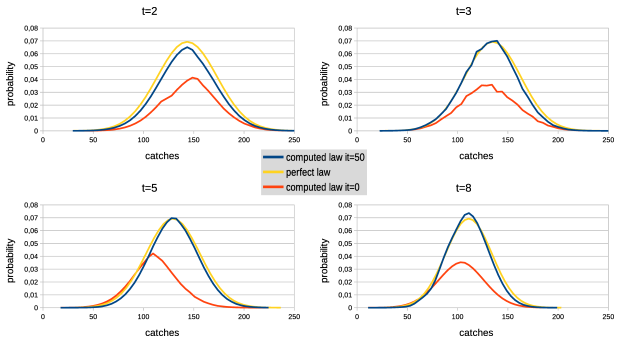

Fig. 9. Comparison between estimated and computed probability law with wrong estimations

V. Conclusion, Limitations and Perspectives

In this paper we have proposed several model calibration methods by first showing the inefficiency of a classical approach in imprecise data situations. To overcome this, we have proposed a robust probabilistic approach that allows us to propose reliable solutions for as many scenarios as possible. It also allows us to identify certain inconsistencies in the input data and to correct them.

Thus, this approach seems very useful for studying phenomena such as marine biology, where data are scarce, hence imprecise estimates but rapid simulations.

However, it has certain limitations. Indeed, in the case where the bad estimates are not all in the same direction (overestimation or underestimation), it can happen that the algorithm never finds a good result. The intervention of an expert is then absolutely necessary to modify the data himself according to the detected inconsistent years.

Moreover, this implies that at least the effort estimates should be consistent. The algorithm only identifies inconsistencies in the (C, E) pair, but consistency between time series does not guarantee that they are correct. An expertise is then essential before concluding anything.

The set of final biomass values obtained makes it possible to limit this parameter, which is difficult to estimate otherwise, to a relatively small number of parameters. This can finally serve as an input for a future robust optimization process using the fuzzy set formed by the parameters determined via optimization and their associated probability of likelihood.

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