Adaptive sequential space-filling design for
geostatistical simulations

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Abstract

Proper uncertainty quantification requires the construction of a large set of alternative Earth models. To overcome computational time, distance-based techniques have been recently used in the context of uncertainty quantification. However, they rely on the construction of hundreds of models, prior to the study. One difficulty is that there is no information \textit{a priori} on the number of models that needs to be generated for accurate uncertainty quantification. This number will depend on the complexity of the test case and the response studied.

In this paper, we present a new workflow for uncertainty quantification which aims at constructing models in an adaptive, intelligent manner. Starting with a few initial models, the method defines locations where new models should be constructed, in order to sample efficiently the space of uncertainty. The procedure is iterated until the uncertainty is stabilized, thus implicitly determining the required number of models.

Preliminary results are presented on two different test cases, one of them having uncertainty in the input parameters. Results show that the proposed method results in a more accurate uncertainty quantification than the random generation of a set of models of similar size.

1. Introduction

Over the last few years we have developed and applied new distance-based methods to the areas of uncertainty quantification, model selection and data conditioning. The main advantage of such methods is that the modeling is linked to the purpose of the application through the definition of a distance between any two
models. By introducing an application-tailored distance, the objective of the study is incorporated into the modeling process, thereby potentially enhancing the efficacy of the overall workflow.

Distance-based methods require a large initial ensemble of models to be constructed. There is no simple rule on how many models are required and the answer is often dependant on the complexity of the problem which may not be known up front. Constructing directly hundreds of models can be infeasible due to computational or logistical limitations. In order to reduce the time required and generate only the number of models necessary for the task at hand (which is unknown \textit{a priori}), we propose to generate models adaptively.

This paper addresses some preliminary ideas on the adaptive generation of models for uncertainty quantification. Starting with an initial ensemble containing a small number of models, we propose to generate sequentially new models to enrich the prior uncertainty model. The new models are created such that they cover the space of uncertainty. This iterative procedure is performed until the uncertainty estimation has stabilized, thus implicitly determining the required number of models.

The paper proceeds as follow. We start by giving a brief discussion on distance-based methods, with emphasis on their use in uncertainty quantification. Then, we present the workflow proposed in this paper – the adaptive enrichment of the space of prior models. A simple example is used to illustrate the concepts of the method. Then, a more complex illustrative example is shown to demonstrate the applicability of the proposed workflow. We end the paper with some concluding remarks.

\section{Distance-based methods - Review}

The key concept in distance based modeling is to define a ‘distance’ between (reservoir) models. The distance reflects how similar models are in terms of their output target response. Once such a distance is defined, well-known statistical tools can be employed for novel workflows and analysis of results.

The definition of the (dissimilarity) distance is the critical task in distance-based modeling. The distance is the vehicle to incorporate the metric of interest, namely one that is related to the application. The better this distance is correlated to the difference in target output response (for example, cumulative oil production), the more effective the distance approach will be. In addition, the distance should be sufficiently rapid to compute such that tens or hundreds of distances can be evaluated in one application. Examples of such distances are the Hausdorff distance (purely geometric), connectivity or streamline-based distances (dynamic distances).

The definition of a distance between any two models intrinsically introduces a metric space. Projections of the metric space can be done using a well-known statistical tool called Multi-Dimensional Scaling (MDS). The role of MDS is to convert the dissimilarity distances into Euclidean distance, and to map models into a

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low dimensional space (usually less than 5-10D). MDS is also a useful visualization and diagnostic tool for model uncertainty. Note that the resulting MDS space is a “fit-for-purpose” space: points close to each other have similar properties (in terms of output target response). The use of this low-dimensional, fit-for-purpose space has shown much promise for uncertainty quantification and model selection by using clustering methods.

For uncertainty quantification, previous work using distance-based methods (Scheidt and Caers, 2009a and 2009b) starts with a fixed (and large) ensemble of models (Figure 1a). It is assumed that this set provides a realistic representation of uncertainty. A fast proxy is used in order to compute the distance between all the models. MDS is subsequently applied (Figure 1b) and clustering methods (kernel k-means) are then applied to select a few representative models (Figure 1c). Full-physics flow simulations are then performed on the centroids of each cluster. Uncertainty quantification is evaluated by computing the P10, P50 and P90 quantiles of the response from the few full-physics simulations only (Figure 1d). Finally, a bootstrap procedure (Scheidt and Caers, 2010) can be employed to verify if enough simulations where performed during the selection method.

![Figure 1: Uncertainty quantification workflow: (a) distance calculation between models, (b) MDS representation, (c) clustering to select a few representative models for evaluation (d) P10/P50/P90 quantile estimation](image)

Although this method has proven to be successful, a few drawbacks exist. First, it is not known a priori how many models are required for accurate uncertainty quantification. The number of models is dependent upon the particular application.
and its complexity and is difficult to know prior to the study. Secondly, it is difficult to determine how many models should be selected during the clustering procedure for full-physics flow simulations. The bootstrap procedure is designed to aid in determining the correct number of models to select, but the procedure can be difficult to implement. Finally, a good distance measure must be employed, which can be sometimes challenging to obtain.

In this paper, we proceed differently. We propose to start with only a few initial models and then generate additional models. The purpose is to avoid generating needlessly large numbers of models, but only a limited number of models for uncertainty quantification. We propose to construct new models in an intelligent manner in order to reduce the total number of models required, while at the same time keeping the uncertainty of a large set of models. The new models will be generated where (locations in MDS space) and when they are needed. Finally, because the number of models to be constructed is small, we propose to use full flow simulations to calculate the distance.

There are several advantages to the proposed method compared to the original method proposed by Scheidt and Caers (2009). First, such an iterative procedure provides the user a gauge as to whether a sufficient number of models have been evaluated. Second, only the “required” number of models is generated: the procedure continues until a sufficient number of models have been created. Finally, no proxy distance is needed; full-physics flow simulations are always employed. This latter point has a double advantage: there is no need to find a good distance, and the user does not have to determine how many models should be evaluated using a full simulation.

The following section describes the methodology proposed by using a simple illustrative example.

3. **Adaptive construction of new models**

Adaptive sampling strategies with experimental design have been recently used for uncertainty quantification and history matching in petroleum applications (Scheidt et al., 2007, Junker et al. 2006, Busby 2009). They consist of iteratively generating new models by varying the input parameter values in order to improve the quality of prediction of the proxy model constructed. However, these methods have several limitations. First, uncertainty assessment is dependant on the quality of the proxy. Second, smoothness of the response is required in order to fit the proxy model to the simulation data. The implication is that spatial uncertainty is difficult to account for with proxy models, and one finds that in most studies, only a single geostatistical realization is employed. Third, the proxy fits only a single response at a single time (eg. cumulative oil production after 10 years). Thus the adaptive design is optimized for the single response, and may not be the optimal design for other responses (or times) of interest. Finally, proxy models are applicable principally for continuous
parameters; the method has difficulties dealing with discrete variables (like facies proportion cubes).

Following the same motivation, in this paper, we propose to generate a few initial models, and then create additional models based on criteria that are presented below. Since initially only a few models are generated and evaluated, the uncertainty represented by these few randomly sampled models will have high variance (but will still be unbiased since random sampling is employed). The objective then is to adaptively add new models to the initial ensemble, which will provide a more accurate evaluation of uncertainty. The procedure is summarized as follows:

1. Generate an initial set of models and evaluate the quantiles for this set of models (Section 3.1)
2. Create a probability density map (pdf) in MDS space for each different prior model and define a location where new models should be created (see Section 3.2)
3. Construct new models using the post-image problem (Park, 2011) that will map in the desired location (see Section 3.3)
4. Accept or reject the created models to avoid bias in the new uncertainty model (see Section 3.4)
5. Re-evaluate the quantiles. If they are stabilized, stop. Otherwise, return to step 2.

Each step in this procedure will be described in further detail below.

### 3.1. Creation of an initial set of models

Many essential features of the workflow proposed in this paper will be illustrated using a simple example involving one training image (TI) representing channels, shown in Figure 2a. The reservoir contains one injection well, and one production well, both producing at fixed rate values. First, a few models (10 in this case) are generated from the prior (Figure 2b) using the multipoint geostatistical algorithm snesim (Strebelle, 2002). The objective of the study is to assess uncertainty on the water production rate, at the producing well. The standard distance-based procedure is then applied, which consists of defining a distance between any two models and then applying Multi-Dimensional Scaling (MDS) to visualize the locations of the models in a low dimensional space (Figure 2c). The distance is defined as the difference in water production at the producing well between two models, obtained by full-physics simulation.
Figure 2: Test Case: (a) Training image, (b) a few realizations and (c) the resulting MDS map.

Once a projection of the MDS space is available, an initial representation of the space of uncertainty is obtained and an initial estimation of the uncertainty in water production can be computed. In this paper, we use the P25-P75 interval to measure uncertainty. For this example, we generate and evaluate 120 models in order to provide a reference uncertainty. As we can see in Figure 3, the P25-P75 interval of uncertainty is poorly estimated by using only the 10 initial models (dotted line), compared to the reference (black line) generated with 120 models.

Figure 3: P25-P75 interval of uncertainty. Note how poorly the estimation of P25 is, especially for the water breakthrough time.

Ignoring the 120-model reference, we assume that starting with so few models results in a very strong variance in the uncertainty estimation. As a consequence, more models should be added to the initial ensemble. The workflow aims to construct new models not randomly, but in an intelligent manner given the prior information provided by the 10 runs. However, generating models in a sequential fashion may induce bias in the uncertainty statement, so bias corrections will need to be employed.

### 3.2. Location of the new models to be constructed

The crucial point in the methodology is to define where new samples should be added. Since the objective is to evaluate accurately uncertainty represented by an
exhaustive reference case, we would like to add models that have different output responses from the initial models (10 in our example). In other words, our sample of models should cover all possible outcomes of the response.

Two criteria are employed to choose a location where new models should be constructed. First, in order to remain consistent with the prior, i.e. not introduce any bias, the location should be taken inside or near the initial cloud of points. This can be done by computing the probability density (pdf) of the initial locations of points and selecting candidate points following this prior pdf. Second, the goal is to sample models that have a response that is different compared to the initial models. Indeed, sampling models with responses similar to the initial set will not provide us with more information about the uncertainty space. Such a goal can be obtained by selecting, among the candidate points, locations far from existing points. Details will be given next.

The probability density map of the set of initial points provides an initial guess of the uncertainty space. In order to compute this probability density map, we use a kernel smoothing technique, which is described in the next section.

3.2.1. Creation of the prior density - adaptive kernel density estimation

The traditional way to compute a probability density for a given set of point is to use kernel smoothing. Kernel smoothing (Bowman and Azzalini, 1997) is a spatial method that generates a map of density values. The density at each location reflects the concentration of points in the surrounding area. An important advantage of kernel smoothing is that it does not require any parametric assumptions about the probability density function. One important parameter to define in kernel smoothing method is the bandwidth for the kernel (Gaussian) smoothing. The bandwidth can be difficult to select, and its value is generally a compromise between acceptable smoothness of the curve and fidelity to the data. The choice of the bandwidth has an impact on the overall appearance of the resulting smooth curve, much more so than the choice of the kernel function which is generally held to be of secondary importance.

Experience has shown that using a univariate bandwidth is not appropriate when creating density maps. This can be seen in Figure 4b, where the “V”-shape of the points is not preserved by the univariate density expression. Multivariate versions of variable bandwidth kernel density estimators can lead to improvement over kernel density estimators using global bandwidth choices (Terrell and Scott, 1992). These estimators (sometimes referred as adaptive kernel smoothing) are more flexible and better able to model complex (multimodal) densities. In this work, we employ a sample point estimator, which places a kernel at each data point, but these kernels have their own size and orientation. The bandwidth matrix is defined as the covariance of the location of k closest points to the current data point. An illustration of the benefits of using an adaptive kernel smoothing strategy is shown in Figure 4.
Figure 4: Examples of univariate and multivariate kernel smoothing. (a) and (c) show the shape of the kernel at each test points for respectively the case of univariate and multivariate bandwidth. (b) and (d) represent the resulting probability density map.

3.2.2. Selection of a location to sample in prior space

As stated earlier, the locations for the new points to be constructed should be in the initial cloud of models, i.e. follow the probability density obtained by adaptive kernel smoothing. To ensure this condition, we propose to generate a series of candidate points, sampled from the probability density of the initial models. In addition, not all sampled points in this series will be of interest, especially areas close to an existing model location. In order to sample different values of response output functions, we propose to use a minimax criterion to select new locations. We proceed as follow:

1. Compute the probability density of the points using an adaptive kernel smoothing algorithm (contours, Figure 5a.)
2. Generate a series of candidate points (black ‘+’, Figure 5a) following the pdf obtained in Step 1 using a Metropolis sampling algorithm (Metropolis and Ulam, 1949; Hastings, 1970)

3. Compute the distance of each candidate point to the closest existing point and sort the resulting distances from maximum to minimum

4. Select the first candidate point and accept/reject this point depending on the pdf value at this location. If the point is rejected, move on to the next candidate point.

Once a location in the MDS space is defined (‘X’, Figure 5a.), the next step is to construct an Earth model that will map close to this location. The problem of constructing new models in a particular location of the MDS space is the same as the post-image problem (Park, 2011).

### 3.3. Construction of new models – The Post-Image formulation

Park (2011) proposed a distance-based method for dynamic data integration. The idea is to compute a distance between any two models as well as between each model and the dynamic data. This allows representing the location of the “true” data ($x^{true}$) in the MDS space, even though the “true” model is unknown. By using the locations of the models (given by MDS) instead of the models themselves, the objective function can be expressed in a simpler and much less costly manner: generate new realizations such that their location $x$ in MDS space verifies $d(x, x^{true}) \sim 0$. This is the same objective that is stated in Section 3.2 above.

Note that the post-image formulation results in a non-linear combination of existing models. In case of facies models, the post-image solution results in a continuous model. This solution is used as a soft data (probability cube) in the initialization of the probability perturbation method (PPM, Caers 2003). Park (2011) showed the benefits of using the post-image solution as an initialization of the PPM, the convergence rate of the PPM is faster, mainly because a better initial point is used. For more details about the post-image, please refer to Park, 2011.

Going back to the example, Figure 5b shows the locations of the new points generated by PPM (gray squares). In this case, six new models were generated. Note that the PPM did not converge exactly to the model at the given location (red X) before stopping. This is due to the fact that we are interested in sampling a particular area, not to match exactly a desired location.
3.4. Accounting for the bias: importance sampling with rejection control

Before going into more details, some notations should be introduced. Let’s denote:

- \( f(x) \) the probability density function of the current models at a location \( x \). It is obtained by adaptive kernel smoothing, using all the models of the current set.
- \( f^*(x) \) the probability density function of the new models generated by PPM at a location \( x \). It is obtained using adaptive kernel smoothing with all the newly created models.

In an ideal situation, new samples from \( f(x) \) should be generated in order to improve the accuracy of the uncertainty assessment. However, instead of uniformly sampling from \( f(x) \), the new models are obtained from an iterative procedure (PPM), thus from a biased distribution \( f^*(x) \). This might affect the quantile estimation, because many new models (sometimes close to each other) might be constructed during PPM.

Importance sampling techniques attempt to compensate for such bias by...
introducing a weighting term in the probability of acceptance of a new model \( m \), weights being given by the ratio of the priors \( f(x)/f^*(x) \), where \( x \) represents the location of a model \( m \). To adjust samples, we can apply a technique called rejection control (RC, Yuan and Druzdzel, 2007, Liu et al., 1988). The principle of importance sampling with rejection control is the following, for any \( c_r > 0 \):

1. For each of the \( N_{PPM} \) model generated by PPM, compute:
   \[
   w_i = f(x_i)/f^*(x_i), i = 1, \ldots, N_{PPM}
   \]

2. Draw \( U_i \) from a uniform distribution on \([0,1]\)

3. Accept the model \( m_i \) if
   \[
   U_i \leq \min\left\{1, \frac{w_i}{c_r}\right\}, i = 1, \ldots, N_{PPM}
   \]

Instead of setting a rejection threshold \( c_r \) in advance, we sort the sample weights \( w_i \) and let \( c_r = w_{\alpha} \), where \( \alpha \) is a chosen percentile, as proposed in Yuan and Druzdzel (2007).

By accepting/rejecting samples using importance sampling with rejection control, we correct the bias that might be introduced using PPM.

In the example problem, the application of such a procedure allows for the selection of four models out of the six models that were generated. When adding these four models to our initial set of 10, we obtain a new P25-P75 interval of uncertainty based on 14 models, as shown in Figure 6b. We can see that adding four new points to the initial set of models has some impact on the quantiles values. Since changes have occurred to the interval of uncertainty, we decide to repeat the procedure and add new points.

![Figure 6: (a) Importance Sampling results: in grey are the models rejected and in magenta the model accepted for uncertainty quantification (b) Resulting P25-P75 quantile interval](image)
The procedure described earlier is then repeated incorporating the additional points that were created and selected. A new estimation of the probability density of the current models is computed, and new candidate points are generated in order to define a new location. Results of the successive iterations are illustrated on Figures 7, 8 and 9. Note that for each iteration, we show the probability density maps obtained by kernel smoothing (contour plots), the metropolis samples (‘+’) and the chosen location (‘X’). In addition, all the models generated by the PPM are presented by squares; in gray are those not selected by the importance sampling procedure and in magenta are those retained.

The different steps of the second iteration are shown in Figure 7. Note that in the previous iteration, a location on the left side of the map was selected. In order to enrich the uncertainty space for both late and early water arrival, we propose to only sample the right side of the map for the second iteration to ensure that a location on the right side is chosen. In this case, the use of PPM requires seven simulations before reaching the desired area. The application of the importance sampling allows for the selection of five models. Looking at the uncertainty, we can see moderate changes; the differences are observed in the later times (> 4000 days).

For the third iteration, the selected location is at the far bottom right side of the MDS map. This is quite challenging, as it is an “extreme” point that is difficult to obtain with the post-image procedure. Again, seven models were required for the PPM to converge to a reasonable location. Only one model was rejected using the importance sampling procedure. The resulting P25-P75 interval can be evaluated, using the additional six models. Looking at the uncertainty, we can see that the estimated P25-P75 interval has improved significantly, particularly the P25 quantile.
Figure 8: Iteration #3: (a) PDF obtained by kernel smoothing, selected location (‘X’), (b) New models generated by PPM, (c) Quantiles after addition of the new models.

Figure 9 illustrates the fourth iteration. In the previous iteration, points in the right part of the map were added. In order to compensate for the addition of those points, only the left part of the plot is now available for the candidate points.

Figure 9: Iteration #4: (a) PDF obtained by kernel smoothing, selected location (‘X’), (b) New models generated by PPM, (c) Quantiles after addition of the new models.

In this particular case, the initial model of the PPM (as given by the post-image solution) was very accurate, allowing the PPM to converge in the desired area with only two simulations. Those two models were accepted in the importance sampling procedure. Note that the quantiles have stabilized; not many changes are observed between the 3rd and 4th iterations. As a consequence, we consider that an accurate estimation of uncertainty is reached and the process is stopped.

Finally, we propose to compare the previous results with a random generation of models. In the example, the quantiles were calculated using a total of 27 models (accepted in the importance sampling step). However, 32 simulations were performed in total in order to obtain those results. As a consequence, we will generate randomly multiple sets of 32 models and evaluate the P25-P75 interval. Note that in order to take into account the randomness of the procedure, we generate ten different sets of 32 models. Figure 10 shows the estimated quantile intervals.
obtained by the ten sets of random models (gray), the reference (120 models, in black) and for the adaptive generation of models (red – dashed lines).

![Graph showing water production over time for different model generation methods.](image)

**Figure 10**: Comparison of the P25-P75 interval with random generation of the same number of models.

We observe that the quantile intervals obtained by random generation of models are more uncertain, with large fluctuations. By using a random procedure, one might be very lucky and obtain a good estimation of the uncertainty, or an extremely bad estimation of uncertainty is also possible. Note also that in the case of a random procedure, the number of models to generate is not known \textit{a priori}.

4. Extension of the methodology for cases with multiple training images

To illustrate the generality of the approach, consider a second example, which has uncertainty in the input parameters. The example is similar to what was shown in the first example, except that this second case has four different training images, reflecting uncertainty in the channel orientation and width. Let’s denote \((T_1, T_2, T_3, T_4)\) the four alternative training images, which are illustrated in Figure 11.

![Four alternative training images representing uncertainty in channel orientation and width.](image)

**Figure 11**: Four alternative training images representing uncertainty in channel orientation and width.
Different prior probabilities were attributed to each training image, denoted \( p_1, p_2, p_3, \) and \( p_4 \) respectively. For this case, \( p_1 = p_2 = 0.2 \) and \( p_3 = p_4 = 0.3 \). 400 prior models were generated to provide a reference uncertainty space, with respectively 80 models for \( T_1 \) and \( T_2 \) and 120 models for \( T_3 \) and \( T_4 \).

An initial set of 10 models was constructed \( (n_1 = n_2 = 2 \) models for \( T_1 \) and \( T_2 \); \( n_3 = n_4 = 3 \) models for \( T_3 \) and \( T_4 \), where \( n_j \) denotes the number of models generated using \( T_j, j = 1, \ldots, 4 \)). The resulting MDS representations for the exhaustive set of 400 models and the initial set are shown in Figure 12. We can also observe the P25-P75 uncertainty interval resulting from both sets. We can clearly see a considerable underestimation in the uncertainty interval for the subset of models.

![MDS representations](image)

**Figure 12:** The top two plots show the MDS representations of the exhaustive set of models and the initial set of models. The bottom plot shows the estimation of the P25-P75 quantile intervals for both sets.

The presence of uncertainty in the input parameters as well as the different prior probabilities for each scenario (TI) introduces an additional difficulty compared to the previously illustrated example. Indeed, when adding new models to the initial set, the prior probabilities of each TI should be preserved. We will see later how this affects the workflow.
In order for the post-image solution to be employed for the generation of new models, the use of a unique training image is required. As a consequence, one single training image is used for each iteration.

In contrast with the first example, the first step in this example is to select the training image. The training image is chosen randomly, according to the prior probabilities of each training image. Once a training image is selected, the same workflow as before is employed, using only the models derived from the selected training image.

Returning to the 2\textsuperscript{nd} illustrative example, the 4\textsuperscript{th} training image ($T_4$) is selected. Subsequently, the exact same procedure is applied as in the 1\textsuperscript{st} example, using realizations constructed only from $T_4$. The results are presented in Figure 13. First, the probability density function associated with $T_4$ is estimated using adaptive kernel smoothing (represented as contours). Then, candidate points (black ”+”) were generated by sampling the pdf using a Metropolis sampling algorithm, and finally an area is defined using the minimax criterion (described in Section 3.2.2). The location of the new models to be constructed is shown by the cross.

![Figure 13: Iteration #1: (a) PDF obtained by kernel smoothing, selected location (purple cross), (b) New models generated by PPM, (c) Quantiles after addition of the new models.](image)

For the initial iteration, seven models are generated during the PPM procedure to create a model in the desired location (Figure 13b). The next step is to apply the importance sampling procedure with rejection control in order to correct for any bias introduced by the use of PPM. During this step, we propose to add an additional criterion to the method described in Section 3.4 for accepting/rejecting models, in order to preserve as much as possible the prior probabilities of each training image.

**Extension of importance sampling procedure**

We have seen before that a model $m_i$ is accepted depending on the probability $\min\left\{1, \frac{W_i}{c_i}\right\}$, $i = 1, \ldots, N_{PPM}$, $N_{PPM}$ being the number of models created by PPM, at
the current iteration. The problem now is that PPM generated a new set of models from one single training image, therefore introducing a bias in the proportion of models sampled from each training image. In order to correct for this in the importance sampling, we propose to multiply $w_i/c_r$ by the ratio of the prior probability of the training image used ($p_j$) and its current probability ($p_j^{\text{curr}}$). As a consequence, the procedure becomes:

1. For each model generated, compute: $w_i = f(x_i)/f^*(x_i), i = 1, \ldots, N_{\text{PPM}}$

2. Compute the “current” probability of the selected training image $T_j$:
   
   $$p_j^{\text{curr}} = n_j/N,$$
   
   with $n_j$ being the current number of points accepted from the training image $T_j$ and $N$ the total number of models for all training images.

3. Draw $U_i$ from a uniform distribution on $[0,1]$

4. Accept the model $m_i$ if $U_i \leq \min\left\{1, \frac{w_i}{c_r} \times \frac{p_j}{p_j^{\text{curr}}}\right\}, i = 1, \ldots, N_{\text{PPM}}$

5. If the model $m_i$ is accepted, increase $n_j$ and $N$ by 1

Following the procedure above, if the current probability of a training image is larger than its prior probability then it will be penalized and the chance of accepting the model is decreased. Contrarily, if the current probability of a training image is smaller than its prior probability then the chance of accepting the model is increased.

Returning to the illustrative example, five out the seven models were accepted by rejection control. Using those five additional models, a new estimation of the uncertainty interval is evaluated (see Figure 12c). We can observe a drastic change in the quantiles; they have shifted towards lower water production. This can be explained by the fact that all the new models are located on the right of the MDS map, where models with late water arrival are found. By sampling other training images in the next iterations, this bias will be accounted for (by sampling in the left part of the map). This is to ensure that the prior probabilities are preserved as much as possible.

**Accounting for prior probabilities**

Now that new models have been added for one particular training image, the prior probabilities of each training images have changed. Let’s denote $p_1^*, p_2^*, p_3^*$ and $p_4^*$ the observed probabilities at the current iteration. For this particular case, $p_4^* > p_4$ (there are too many samples from $T_4$). As a consequence, for the next iteration, the
selection of the next training image should account for this difference: $T_1$, $T_2$ or $T_3$ should be preferably selected. We therefore propose to select the next training image based on “corrected” probabilities: $p_i^c = p_i - \left(p_i^* - p_i\right)$. In this manner, scenarios that have a higher current probability than the prior probability will be penalized, whereas scenarios that have a lower current probability than the prior probability will be preferred.

In the illustrative example, for the second iteration, the second training image ($T_2$) is selected. The location selected by the proposed procedure is at the far left of the map (red “X” in Figure 13a). In order to obtain a model in the desired area, five models were generated using PPM (red squares in Figure 13b). Among them, four were retained in the rejection sampling step. Looking at the estimated quantiles (Figure 13c), we can see that they have improved significantly, showing a much larger uncertainty.

Figure 13: Iteration #2: (a) PDF obtained by kernel smoothing, selected location (red cross), (b) New models generated by PPM, (c) Quantiles after addition of the new models.

Going to the 3rd iteration, the 3rd training image ($T_3$) was selected. The procedure described above was applied, the results are shown in Figure 14. Two models were generated using PPM, neither being rejected by the importance sampling procedure. Adding the two models selected, a new estimation of the quantiles reveals slight changes, even though only two models were added.

Figure 14: Iteration #3: (a) PDF obtained by kernel smoothing, selected location (green cross), (b) New models generated by PPM, (c) Quantiles after addition of the new models.
In the 4th iteration, $T_i$ is selected, which is vastly under-sampled compared to the other training images. The results are shown in Figure 15. Few simulations (two) are needed to sample the desired area. Note though that adding only two models to the current set of model has a significant impact on the P75 quantile, which has improved compared to the reference.

![Figure 15: Iteration #4](image)

Figure 15: Iteration #4: (a) PDF obtained by kernel smoothing, selected location (blue cross), (b) New models generated by PPM, (c) Quantiles after addition of the new models.

In the 5th iteration, the same training image as previously was chosen. The results are displayed in Figure 16. This is because only two models were added in the previous iteration, and thus $T_i$ remains under-sampled. Three models were generated by PPM before converging, one of them being subsequently rejected during the importance sampling step. Finally, we can see that the quantiles did not move by adding the new models. Thus, we therefore conclude that a sufficient number of samples has been obtained, and stop the process after the 5th iteration.

![Figure 16: Iteration #5](image)

Figure 16: Iteration #5: (a) PDF obtained by kernel smoothing, selected location (blue cross), (b) New models generated by PPM, (c) Quantiles after addition of the new models.

As in the example before, a comparison with random generation of models is performed. For this example, even though only 25 models were employed to estimate the uncertainty interval, a total of 29 models were created and simulated. As before, we generate 10 sets of random models. In order to preserve as much as possible the prior probabilities, 6 models for $T_i$ and $T_2$ were generated and 9 models for $T_3$ and $T_4$. 

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(which gives 30 models in total). The resulting uncertainty for each set is shown in gray in Figure 17.

![Figure 17: Comparison of the P25-P75 interval with random generation of the same number of models.](image)

We observe that the quantile intervals obtained by random generation of models are not very precise, especially for the P25 quantile, which shows significant variation (in terms of arrival time as well as production).

5. Discussions/Conclusions

This paper presents some preliminary ideas and results to adaptively construct new models to estimate response uncertainty. The proposed workflow relies on distance-based methods, which have been successful in previous applications for uncertainty quantification. Starting with a few initial models, the workflow aims at constructing new models in an intelligent manner for the purpose of uncertainty quantification. By doing so, the total number of models to be constructed does not need to be known \textit{a priori}. In addition, the number of models can be reduced compared to previous distance-based methods (which require generating a large initial set of models), for an accurate estimation of uncertainty. The proposed workflow can be applied in the context of spatial uncertainty (multiple training images for example) and with multiple responses (or time-depend responses), through the definition of a distance function. As a result the workflow is more general than methods that require proxy models.

We applied the proposed methodology in two examples and we show that in both cases, the adaptive generation of models can be successfully applied for uncertainty quantification. In both cases, the proposed method outperforms a random generation of the same amount of models.

As stated earlier, this paper only presents preliminary work. We are currently
investigating alternative procedures which may improve the workflow. For example, experience has shown that the location area to sample has a very significant impact on the quantile estimates. One does not want to over/under sample one side of the MDS map, or preferentially one TI. It is important to ensure that models are equally built in each side of the map (in other words for both extremes values of the response). In the first illustrative example, a user-specific procedure was applied to ensure that the extremes were sampled. An alternative procedure to achieve such a goal is to apply kriging on the rank of the current models, and use the kriging value and the kriging variance to obtain a new location to sample.

Other ways of improvement of the method could be to use a proxy model during the PPM procedure, in order to limit the time required to generate new models in the desired area. Concerning the stopping criteria, additional constraints should be considered. For example, if only one or two models are added in the current iteration, the impact on the quantiles could be null, without necessary meaning that the process should stop.

References


Scheidt, C., and Caers, J. (2009a): Representing spatial uncertainty using distances and
kernels. Math. Geosci. 41(4), 397–419


