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Stochastic and Robust Multi-Objective Optimal Management of Pumping from Coastal Aquifers Under Parameter Uncertainty

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Abstract Combined simulation-optimization approaches have been used as tools to derive optimal groundwater management strategies to maintain or improve water quality in contaminated or other aquifers. Surrogate models based on neural networks, regression models, support vector machies etc., are used as substitutes for the numerical simulation model in order to reduce the computational burden on the simulation-optimization approach. However, the groundwater flow and transport system itself being characterized by uncertain parameters, using a deterministic surrogate model to substitute it is a gross and unrealistic approximation of the system. Till date, few studies have considered stochastic surrogate modeling to develop groundwater management methodologies. In this study, we utilize genetic programming (GP) based ensemble surrogate models to characterize coastal aquifer water quality responses to pumping, under parameter uncertainty. These surrogates are then coupled with multiple realization optimization for the stochastic and robust optimization of groundwater management in coastal aquifers. The key novelty in the proposed approach is the capability to capture the uncertainty in the physical system, to a certain extent, in the ensemble of surrogate models and using it to constrain the optimization search to derive robust optimal solutions. Uncertainties in hydraulic conductivity and the annual aquifer recharge are incorporated in this study. The

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results obtained indicate that the methodology is capable of developing reliable and robust strategies for groundwater management.

Keywords Saltwater intrusion · Groundwater quality management · Simulation-optimization · Coastal aquifers

1 Introduction

Simulation-optimization models (S/O) are efficient tools for deriving optimal designs and are extensively used to solve complex problems in water resources management. Application in groundwater management includes use of analytical or numerical simulation models coupled with optimization search algorithms to derive optimal groundwater management strategies. Specific applications to coastal aquifer management includes Ayvaz and Karahan (2008); Cheng et al. (2000); Das and Datta (1999a, 1999b, 2000); Dhar and Datta (2009); Datta et al. (2009); Katsifarakis and Petala (2006); Mantoglou (2003); Mantoglou et al. (2004); Park and Aral (2004); Sreekanth and Datta (2010, 2011a, b); Sedki and Ouazar (2011) etc.

In the last two decades surrogate models have been widely used to develop computationally feasible simulation-optimization models as the computational burden involved in using the numerical simulation model with optimization search is huge.

Artificial neural network is the most popularly used surrogate modeling tool in the water resources literature. A number of studies have applied neural network surrogate models for solving optimal groundwater management problems Ranjithan et al. 1993; Bhattacharjya and Datta 2005; Yan and Minsker 2006; Kourakos and Mantoglou 2009; Sreekanth and Datta (2010). Sreekanth and Datta (2010) developed genetic programming based surrogate models for predicting the saltwater intrusion as a result of pumping in coastal aquifers. The advantages of genetic programming compared to neural networks for developing surrogate models were studied and reported.

Despite the wide use of different surrogate modeling approaches for groundwater management, only a few studies have dealt with stochastic surrogate modeling. Aly and Peralta (1999) used neural networks in a stochastic groundwater setting to solve optimal pump-and-treat design problem. Sreekanth and Datta (2011a) demonstrated the application of ensemble surrogate models for the improving the reliability of surrogate modeling in groundwater management using simulation-optimization. The predictive uncertainty of the surrogate models, when used in simulation-optimization framework, leads to erroneous optimal solutions. Ensemble surrogate modeling approach was used to obtain reliable optimal solutions by reducing the predictive uncertainty of surrogates.

The present study extends the ensemble surrogate modeling approach to address uncertainty in the physical system, viz, hydraulic conductivity and aquifer recharge. Multi-objective optimization of pumping management in coastal aquifers to prevent saltwater intrusion considering uncertainty in parameters is accomplished.

2 Optimal Pumping Strategy for Coastal Aquifer

Two conflicting objectives of management are incorporated using a multi-objective optimization formulation. Two sets of pumping wells, viz, production wells and barrier wells are considered for pumping management. The first objective is to maximize the total pumping from the production wells and the second objective is to minimize the total barrier well pumping. The mathematical formulation of the problem is given as follows;

$$Maximize \sum_{p \in PROD} \sum_{t \in T} Q_t^p \tag{1}$$

$$Minimize \sum_{b \in BAR} \sum_{t \in T} q_t^b \tag{2}$$

$$c_i = f_i\left(Q_t^p, q_t^b, \theta\right) \tag{3}$$

$$c_i \leq c_i^{\max} \tag{4}$$

$$Q_{\min} \leq Q_t^p \leq Q_{\max} \tag{5}$$

$$q_{\min} \leq q_t^b \leq q_{\max} \tag{6}$$

where, Q_t^p is the pumping from the p^{th} beneficial pumping well for the t^{th} time period, q_t^b is the pumping from the b^{th} barrier well for the t^{th} time period and c_i is the salinity at the monitoring location i at the end of the management time frame considered in the optimization model, resulting due to the pumping . *PROD* and *BAR* designates respectively, the set of all production wells and barrier wells in the well field. c_i is a function of Q_t^p and q_t^b and also the numerical model parameter set θ. The function f_i represents the numerical simulation model. When the parameter set θ is considered as stochastic, solving this optimization model would imply testing each solution comprising of a set of pumping values against multiple realizations of the uncertain parameter set θ. $Q_{\min}$ and $Q_{\max}$ are respectively the lower and upper limits on the production well pumping and, $q_{\min}$ and $q_{\max}$, the corresponding values for the barrier well pumping.

Due to the computational difficulties in implementing this optimization scheme the ensemble surrogate model is used to replace the simulation model f_i within the optimization model. The ensemble surrogate model based multiple realization optimization implements the reliability concept in the following manner.

$$c_i^r \approx \zeta_i^r\left(Q_t^p, q_t^b, U\right) \tag{7}$$

$$U = \psi(\theta, \omega) \tag{8}$$

$$\beta = {}^{r}/_{R} \tag{9}$$

$$c_i^r \leq c_i^{\max} \ \ \forall r \ \text{ such that } \sum r \geq R\beta \tag{10}$$

The concentration c_i is approximated using c_i^r, which are r different values of concentration at the i^{th} monitoring location, obtained from different surrogates in the ensemble. The functional relationship between the pumping and the resulting salinity level is approximated by r realizations of the salinity obtained from different surrogate models given by ζ_i^r for each location i. The realizations c_i^r are different from each other because of the uncertainty U in the surrogates, which is a function ψ of both numerical model parameters, θ and the surrogate model structure and parameters, ω. Reliability is defined in (9) as the ratio of number of realizations r which satisfies the constraint on the limit of concentration $c_i^{\max}$ to R, the total number of realizations of salinity obtained from the ensemble prediction models. (10) imposes a constraint that all realizations c_i^r which belongs to a set of realizations with a size of at least $r=R\beta$ should satisfy the limit on the concentration given by $c_i^{\max}$. Thus the pareto-optimal front for the multi-objective management problem is derived for a specific reliability level β, which is chosen by the manager depending on how reliable the solutions need to be.

Another variant of the simulation optimization formulation was developed which utilizes only a single surrogate model trained and tested using a bootstrap sample having a higher size than the original data set. The objective is to investigate the possibility of a single surrogate model which can predict the saltwater intrusion process with reasonable accuracy so that optimal solutions for aquifer management may be derived. The mathematical formulation of this coupled simulation-optimization problem is similar to the previous one except that the Eqs. 7–10 is replaced by a single equation given as follows;

$$c_i = \xi\left(Q_t^p, q_t^b\right) \tag{11}$$

3 Ensemble Surrogate Modeling Approach

The coastal aquifer response to pumping in terms of the salinity levels at specified monitoring locations is approximated using genetic programming based surrogates. Input–output patterns of pumping and resulting salinity levels obtained from 3D coupled flow and transport simulation model FEMWATER is used to train the surrogates. Hydraulic conductivity and aquifer recharge were considered as uncertain parameters in the model development. An ensemble of surrogate models was used to implicitly account for the uncertainty in the salinity prediction due to the parameter uncertainty in the model development. The detailed methodology of ensemble surrogate model development is as follows;

3.1 Parameter Uncertainty Characterization and Training Set Generation

In the present study hydraulic conductivity is assumed to be homogeneous but uncertain within a range which is obtained from the values measured in the field. To generate a representative set of hydraulic conductivity realizations Latin-hypercube sampling was performed on a log-normal distribution of hydraulic conductivity. The prescribed distribution that represents the uncertainty in the hydraulic conductivity value was divided into N equi-probable intervals. A single value was selected randomly from each interval.

Similarly Latin-hypercube samples of normally distributed aquifer recharge values were generated to constitute a representative set of probable aquifer recharges. The hydraulic conductivity values and aquifer recharge values are then randomly paired to constitute the random realizations of the uncertain parameter values.

Uniformly distributed Latin hypercube samples of the pumping variables were generated from the variable space bounded by the minimum and maximum rates of pumping possible from the considered pumping locations. One set of values of pumping from the well locations together with the corresponding aquifer response in terms of the salinity levels at the monitoring locations, obtained corresponding to a specific set of the uncertain parameters, form a single pattern of pumping. To generate each input–output pattern, the pumping inputs and the values of the uncertain parameters are chosen at random. Different pumping patterns are input into the simulation model with a random choice of the parameter values to compute the concentration outputs for this combination of pumping and parameter values.

The salinity levels at the monitoring locations were simulated using the 3D density dependent flow and transport model FEMWATER. This results in the generation of a data pool of pumping-salinity patterns corresponding to different realization of the uncertain parameters.

3.2 Bootstrap Sampling

Non-parametric bootstrap method was used to generate different realizations of the original data pool of the pumping-salinity patterns. The key idea is to generate multiple realizations of the data set having different representation of the pumping decision space and uncertain parameters. Bootstrap samples are generated by repeated sampling with replacement from the original data set. This method has been previously used in developing ensemble models by Parasuraman and Elshorbagy (2008) and Sreekanth and Datta (2011a).

The original data pool was divided in to two sets called the original training set (TR) and original testing set (TE) each having a size N. A bootstrap size B is specified so that B different sample sets each of the original training (TR_B) and testing sets (TE_B) are generated after the sampling procedure. Random sampling with replacement from the original training set and testing set were performed to generate the bootstrap sample set.

3.3 Surrogates

In this study, genetic programming (GP) (Koza 1994) is used to construct surrogate models for predicting the aquifer responses to pumping. Recent GP applications in water resources management includes Citakoglu et al. (2014); Fallah-Mehdipour et al. (2012); Azamathulla and Ghani (2011) and Sreekanth and Datta (2011b). GP is used to develop surrogate models to predict pumping induced saltwater intrusion in coastal aquifers. GP learns by training and testing. Compared to the widely used neural network surrogate modeling approach genetic programming has the advantage that the genetic programming itself evolves the optimum model structure and parameters. A detailed comparison of genetic programming and neural network based surrogate modeling is reported in Sreekanth and Datta (2010).

Genetic programming initiates with a randomly chosen population of program structures. The programs are generated using the functional and terminal sets, where the functional set includes basic mathematical operators like addition, subtraction, multiplication, division, trigonometric functions etc. The terminal set is comprised of the constants and variables used in the model development. The programs generated using these components are then evaluated for their predictive ability by comparing the model predictions against the training and testing patterns input into the model development. They are tested against the criterion of minimizing an objective function which is usually the root mean square error. The programs in the population are ranked based on their objective function value and new programs are generated using the operators, mutation and cross-over. This series of operations are repeated over a number of generations to evolve the best fit programs.

In the present work an ensemble of surrogates are developed using genetic programming. Each surrogate in the ensemble is trained and tested using a bootstrap sample set generated from the original training and testing data set. When these bootstrap samples, which contain repeated samples of pumping-salinity patterns, are used in the training, different weighting of patterns occur in the objective function used in the GP to develop the surrogate. Since the pumping-salinity patterns in the data pool correspond to different combination of uncertain parameters, it results in the development of surrogates which are differently capable of making predictions in different regions of the decision - parameter space. Also, since the pumping patterns are also repeated in the training and testing data the resulting surrogates are different in their capability to make predictions in different regions of the pumping variable space. With sufficient representation of the entire parameter and decision space in the original data set and sufficient number of surrogates in the ensemble, the ensemble surrogate modeling approach can achieve sufficiently accurate approximation of the saltwater intrusion prediction at the selected monitoring locations. Sufficient accuracy of prediction is verified by validating the optimal solutions by checking the corresponding salinity levels at the monitoring locations using the numerical simulation model. If the prediction errors are low and the optimal solutions are still in the feasible domain, it may be considered that the representation of the parameter-decision space is sufficient. Else, an adaptive training as proposed by Yan and Minsker (2006) or Sreekanth and Datta (2010) may be required to improve the surrogate models. This may be required for more complex applications.

3.4 Ensemble Size and the Uncertainty in the Prediction of the Ensemble Surrogates

The number of surrogate models in the ensemble is determined by a criterion based on the uncertainty in the ensemble prediction. Root mean square errors of the individual surrogates in the ensemble were computed. Overall performance of the ensemble modeling approach was quantified by calculating the mean and standard deviation of the root mean square errors. An initial ensemble size with a few surrogates was chosen. The ensemble performance was determined using the coefficient of variation (CoV) of the RMSEs. CoV was calculated as standard deviation over the mean value. Then surrogates were added one by one and the CoV was recalculated. The ensemble size for which the CoV achieves a minimum value, when the difference between two consecutive CoV values are less than a limiting value, was selected as the actual ensemble size for the linked simulation optimization.

The predictive uncertainty of the ensemble surrogates may be attributed to two causes. The parameter uncertainty, represented by Latin-hypercube samples of parameters in the numerical model development, is reflected in the pumping-salinity patterns generated using the flow and transport model. This uncertainty propagates into the predictions by the approximations surrogates. The second cause of predictive uncertainty is the uncertainty inherent in the surrogate model structure and parameters (Sreekanth and Datta 2011a).

4 Coupled Simulation-Optimization

This study proposes multiple realization optimization (Wagner and Gorelick 1987, 1989; Morgan et al. 1993; Chan 1993; Feyen and Gorelick 2005; Bayer et al. 2008) together with ensemble surrogate modeling approach to solve the coastal aquifer pumping management problem considering uncertainty in the parameters. Here, the multiple realizations pertain to the salinity values obtained from different surrogate models in the ensemble. The surrogates developed using genetic programming are coupled to the multi-objective genetic algorithm NSGA-II (Deb 2001). The methodology is schematically represented in Fig. 1.

The multiple realizations of the concentration value are obtained from the ensemble of surrogates. The optimization algorithm searches to find the optimal pumping strategy which

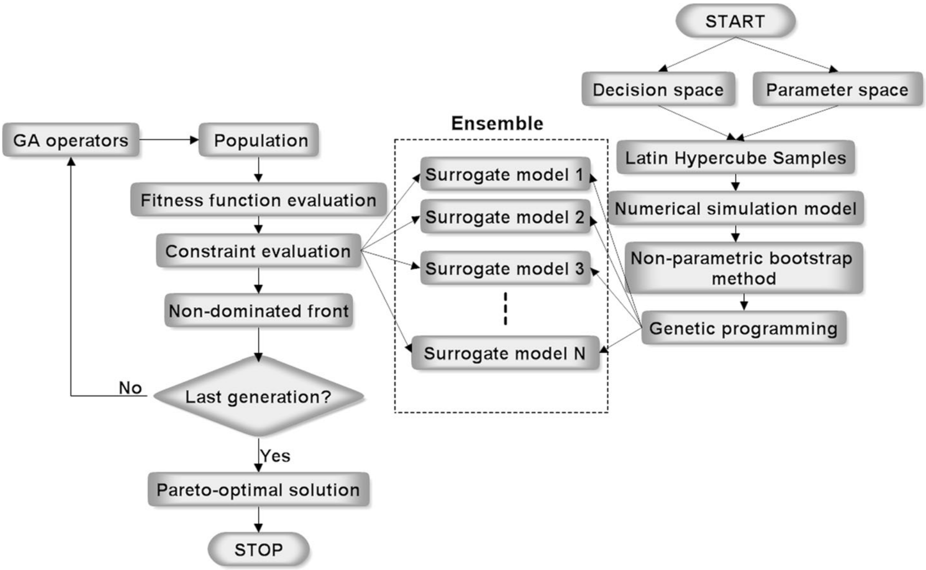

Fig. 1 Schematic representation of the ensemble based simulation-optimization

limits the concentration at the monitoring locations at prescribed values. In this multiple realization approach, reliability is implemented as the percentage of the surrogates in the entire ensemble whose concentration predictions do not violate the imposed constraints of maximum concentration levels (Sreekanth and Datta 2011a).

5 Case Study

The proposed methodology is applied to a near real groundwater model built with the aquifer geometry and parameters derived from a coastal aquifer in the Lower Burdekin area in Australia. The considered study area lies between the bifurcations of the Burdekin River near the sea. The total area is 60.2 km^2 out of which a major portion is irrigated for sugar cane cultivation. There is huge stress on the groundwater resources in this area due to the irrigation demand. The aquifer has an average depth of 60 m. The area is bounded on one side by the sea and on the other two sides by the Burdekin River. Constant head boundaries with the annual average water level are assigned for the river boundaries. The seaside boundary is assigned a constant head of 0 m and a constant concentration of 35 kg/m^3. A wide range of hydraulic conductivity estimates have been reported for the Lower Burdekin area (McMahon et al. 2000; Narayan et al. 2007). Narayan et al. (2007) tested three different homogeneous hydraulic conductivity values, 10, 50 and 100 m/d in their saltwater intrusion simulation study using two-dimensional SUTRA model. In this study we consider homogeneous but uncertain value of the hydraulic conductivity. For this, a log normal distribution of hydraulic conductivity with μ=log (32.67) and σ = 0.28 was used. Twenty five Latin hypercube samples were selected from this distribution.

A mean recharge value of 0.000484 m/d with a standard deviation of 0.000115. Latin hypercube samples were chosen from this normal distribution and paired randomly with the values of hydraulic conductivity to generate the random parameter space used in the simulation. Three dimensional coupled flow and transport simulation model FEMWATER was used to simulate the aquifer processes in response to pumping. FEMWATER uses a finite element method to solve the corresponding flow and transport equations.

For simplifying the model development for regional scale management, all the wells falling within a radial distance of 1 km were represented by a single pumping well at the central node. There is no barrier pumping well existing in this field. However, in this study we consider barrier wells pumping from the saltwater wedge as an additional measure for hydraulic control of saltwater intrusion. Altogether, 8 pumping well locations and 3 barrier well locations were considered within the study area.

The upper limit of pumping from each location in the study area is determined as 0.013 M m^3/d. For the transport simulation, longitudinal and lateral dispersivities of 80 m/d and 35 m/d respectively, molecular diffusion coefficient of 0.69 m2/d and soil porosity of 0.2 were used.

Although these data, as obtained from different sources, are used with the intent of developing a realistic simulation model, the primary objective and focus of this paper is to illustrate the application of the proposed new methodology of coastal aquifer management. FEMWATER model was run with the specified boundary conditions and average groundwater extraction rates at the pumping locations were run for a long period of 100 years to obtain the initial water table and saltwater wedge locations. These head and concentrations were used as the initial conditions for running the model for the actual management period of 3 years. Uniform extraction rates are assumed at each location for a time-step of 1 year.

The aquifer responses were monitored at three nodes, at the water table, in between the pumping and barrier wells. The simulated concentration values at these nodes are named C1, C2 and C3 respectively as indicated in Fig. 2. The pumping management model prescribes permissible maximum concentration levels at these locations as 0.5, 0.6 and 0.6 kg/m^3 respectively. Corresponding to each combination of the uncertain parameters different pumping patterns were used to simulate the aquifer responses. Multiple training and testing sets were generated by bootstrap sampling from the original data set of pumping-salinity patterns. For this, the original data set was split into two sets and bootstrap sampling was

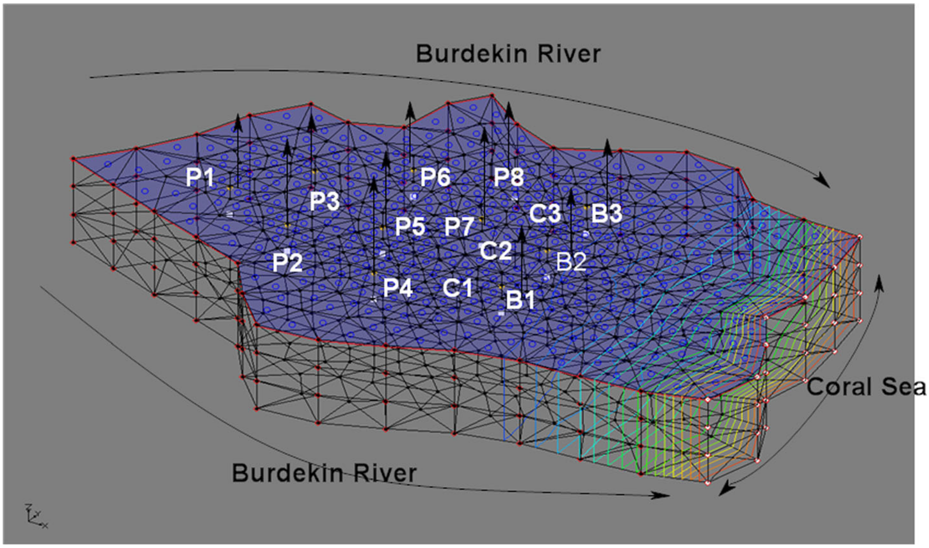

Fig. 2 Study area with the beneficial and barrier well locations

performed on each half to obtain separate training and testing sample sets. This ensures that training and testing of the surrogates are performed on mutually exclusive data sets.

Each bootstrap sample set has thrice the number of patterns contained in the original data sets. This ensures that different patterns are repeated multiple times in different bootstrap data set. However, increasing the bootstrap sample size largely may result in identical sample sets which are undesirable. A pair of training and testing sample sets is used to develop one surrogate model. Similarly, different pairs of training and testing sample sets are used with genetic programming to generate the ensemble of surrogates.

These data sets were input to genetic programming software Discipulus to generate the surrogate models. Forty models were required to reduce the uncertainty as described in Section 3.4. C codes of the developed models were generated and linked with the NSGA-II algorithm for optimization. For developing all the models, the parameters used in GP were as follows. The population size was fixed as 500, mutation frequency 90, and cross over frequency 60. Optimum values of these parameters were chosen by trial and error with different parameters tested against the criteria of minimizing the objective function of GP model training. Number of constants (the surrogate model parameters) used were limited to 30 in all the GP models These surrogate model parameters are comparable to the connection weights in a neural network surrogate model, in that way, the number of parameters used in the GP approach is very less compared to neural networks (Sreekanth and Datta 2010). It was ensured that training and testing errors were in the same range to avoid over-fitting. Bloating was prevented in GP trees by dynamically adjusting the maximum size of the programs.

These surrogate models were coupled individually to the multi-objective genetic algorithm, NSGA-II (Deb 2001) in such a way that in each iteration the new pumping solutions generated by the GA operators are tested using these surrogates for their constraint values of concentrations at the monitoring locations as described in the formulation.

Another bootstrap sample of training and testing sample set with a larger size was generated from the original data set to investigate the possibility of a single universal surrogate. Surrogates based on genetic programming were trained and tested using this data set. This surrogate was then coupled with NSGA-II to evolve optimal pumping strategies for the coastal aquifer.

6 Results and Discussion

6.1 Ensemble Modeling Approach

The inputs and outputs used in the surrogate model development are respectively the pumping rates and the resulting salinity levels. The uncertain parameters are not used as inputs into the GP surrogate models. Instead, input–output patterns obtained for different combinations of these parameters and these data sets are randomly (random sampling with replacement from the original data pool) used to train the surrogate models. Thus the parameter values are accounted for only implicitly. If the parameters are explicitly used as inputs for the surrogate model development the methodology may not be scalable for larger applications. As the parameter values are not used in the surrogate model development, the methodology can be extended for heterogeneous values of parameters, although a larger size of the ensemble may be required for the purpose. However, since linking the ensemble surrogate to optimization model does not increase the computational burden hugely, it is still not impossible to address heterogeneous parameter case with this approach.

6.2 Ensemble Surrogate Model Statistics

Forty surrogate models were developed for the prediction of salinities at each location C1, C2 and C3. The prediction uncertainty and other analyses were performed for these three locations. The prediction uncertainty reflects the uncertainties in the groundwater parameters used in the numerical simulation model and the uncertainties in the surrogate model structure and parameters. All the analyses showed similar results for locations C1 and C3. Hence, for brevity, results corresponding to C1 and C2 only are reported in the tables.

An initial ensemble size of 8 models was considered. The COV of RMSEs of the predictions by these models was computed. Then surrogate models were added one by one into the ensemble and the CoVs were computed. The CoVs of the RMSEs in the prediction of C1 for increasing sizes of the ensemble are plotted in Fig. 3.

From Fig. 3, for predicting the salinity C1, it is observed that there is a steady decrease in the value of CoV of the RMSE with the increase in the number of surrogate models in the ensemble. The CoV becomes the least when 37–40 surrogate models are present in the ensemble and it is observed that the slope of the CoV curve becomes close to zero indicating no further decrease. Therefore the optimum number of models in the ensemble for predicting C1 was fixed as 40. Similar results were obtained for C2 and C3.

6.3 Multi-Objective, Multiple Realization Optimization

The population size and number of generations used in the NSGA-II algorithm were respectively, 250 and 750. This means that at each stage of optimization 250 candidate solutions are evaluated in parallel for their objective function and constraint values. After a number of numerical experiments it was found that to obtain the full Pareto-optimal front, population size of at least 250 is required. When the population size was lesser, parts of the actual front were eliminated from the final solution. The cross-over and mutation probabilities were respectively 0.85 and 0.02. The candidate solutions are crossed over and mutated at these probabilities to generate a new population of solutions. NSGA-II algorithm uses a tournament selection and simulated binary cross-over (Deb 2001). This process is repeated 750 times to evolve the Pareto-optimal set of solutions.

In this study each surrogate model in the ensemble is individually called by the optimization routine to predict the concentration level at the monitoring node. Thus, 40 values of concentration are predicted each for C1, C2 and C3. The coastal aquifer management problem has 33 variables corresponding to pumping from 11 locations for three time periods. The multiple realization approach calls 120 different surrogate models, 40 each corresponding to the salinity concentrations C1, C2 and C3, during the evaluation of each candidate solution.

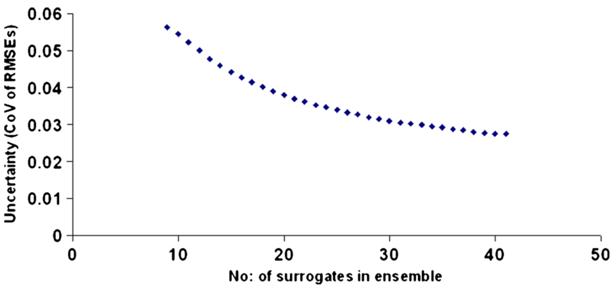

Fig. 3 Ensemble surrogate model uncertainty for salinity C1

6.4 Optimal Solutions with Different Reliabilities

Optimal solution to the pumping optimization problem considering two conflicting objectives is a Pareto-optimal front of solutions which defines a trade-off between the two objectives. The Pareto-optimal front which is obtained, when the constraints imposed by all the 40 surrogate models in the ensemble are satisfied in the optimization, is considered as the solution corresponding to a reliability level of 0.99. Similarly optimal solutions with reliabilities 0.8 and 0.6 satisfy 32 and 24 out of the total 40 models, respectively. The Pareto-optimal set of solutions corresponding to these different reliability levels are shown in Fig. 4. The figure also shows the Pareto-optimal front corresponding to the single surrogate model based optimization. This front appears to give better optimal solutions. However, when the corresponding pumping values are input in the numerical simulation model, it was observed that the all the solutions in the front violates the constraints. The predicted concentration values and corresponding constraint violations for five solutions from different regions of the front are shown in Table 1.

It was observed that this front of solutions is actually in the infeasible domain. This is primarily because of the wrong predictions by the single surrogate model. However, it was found that the RMSE values for the single surrogate models for C1, C2 and C3 were similar to that of the surrogate models in the ensemble. Thus the average prediction accuracy does not indicate accurate levels of prediction for the optimal solution. This is because in an attempt to search for the optimal values of the objective functions, the optimization algorithm chooses those candidate solutions which give the highest positive error (i.e., surrogate model prediction – numerical model observed) in the prediction of concentration. The probability distribution of the errors for C1 obtained from the single surrogate model are plotted in Fig. 5. From Table 1 and this figure it is evident that the errors in the concentration prediction for the optimal solutions belong to the positive tail end of the distribution and beyond.

From this we deduce that an original data set with 250 patterns is insufficient to train and validate a single surrogate model which satisfactorily predicts the concentrations in all regions of the parameter-decision space. It may not be impossible to develop a single surrogate model capable of doing this, but may require exponentially large number of training and testing patterns of pumping-salinity data. However, developing a surrogate model with such huge training data may defy the objective of obtaining computational efficiency using surrogate

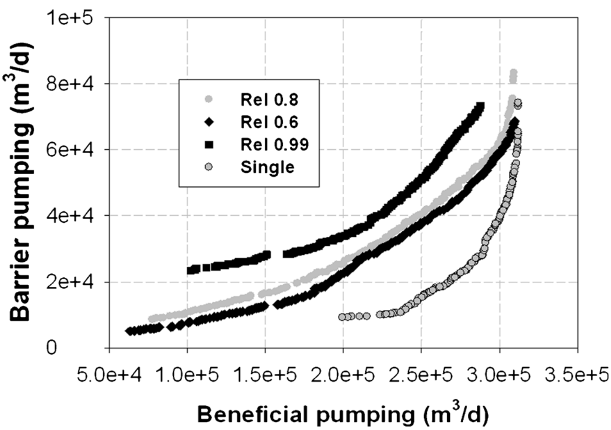

Fig. 4 Pareto-optimal fronts for different reliabilities and single surrogate modeling approach

Table 1 Optimal solutions and constraint violations using single surrogate model

Solution	Total pumping (× 10^3 m^3/d)		Constraint (× 10^{-3} kg/m^3)			
	Beneficial	Barrier	C1 (<500)	Violation	C2 (<600)	Violation
1.0	251.6	16.1	544.3	44.3	765.5	165.5
2.0	204.9	9.4	537.6	37.6	688.7	88.7
3.0	232.6	10.6	545.6	45.6	758.9	158.9
4.0	284.8	27.1	534.7	34.7	773.3	173.3
5.0	310.3	55.5	510.0	10.0	710.3	110.3

models. If uncertainty in more number of numerical model parameters is considered, a single surrogate may be infeasible as it may require large number of patterns to train the surrogate model which involves huge computational burden. This is because multiple uncertain parameters in the numerical model will be mapped in to a single set of surrogate model structure and parameters. Large number of surrogate model parameters may be required for this and may result in over-fitting of the model.

Multiple realization optimization with ensemble surrogate models is found to be an efficient methodology for evolving reliable optimal solutions in the Pareto-optimal front. The Pareto-optimal fronts for the reliability levels 0.99, 0.8 and 0.6 are shown in Fig. 4. The objective function values corresponding to reliability level of 0.99 appears to be the least optimal value amongst all the fronts. However, it will be closer to the actual pareto-optimal front because for the lesser reliability levels, at least some of the solutions in the front move into the infeasible region as they violate the constraints. Twenty five solutions from each front were cross checked for their constraint violation, using the numerical simulation model. The average value of constraint violation corresponding to three different reliability levels and three different combinations of parameter values are shown in Table 2. Five points from each front with their objective function values and corresponding constraint values for three different realizations of the uncertain parameters chosen from different regions of their respective distributions are shown in Table 3. The solutions with a reliability level 0.99 have virtually no constraint violation, where a violation within 1 % excess of the prescribed limit of concentration is considered acceptable. Also, it is observed that as the reliability level decreases the constraint violation increases.

In order to investigate the sensitivity of the optimal solutions to the optimal number of surrogate models in the ensemble numerical experiments were conducted using five different

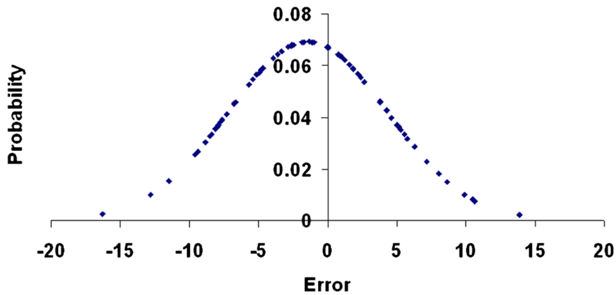

Fig. 5 Prediction error distribution for C1

Table 2 Average values of constraint violation by solutions of different reliabilities

Hydraulic conductivity, Recharge	32.67 m/d, 0.176 m/yr		24.44 m/d, 0.061 m/yr		45.59 m/d, 0.258 m/yr	
Constraint violation (% of the concentration limit C1=500 and C2=600)						
Reliability	C1 (<500)	C2 (<600)	C1 (<500)	C2 (<600)	C1 (<500)	C2 (<600)
0.99	−0.13	0.00	−0.35	0.00	−0.05	0.00
0.8	−1.35	−1.44	−1.63	−1.80	−0.49	0.00
0.6	−2.20	−3.56	−2.96	−3.90	−2.40	−3.45

Negative value indicates a constraint violation

optimization models with 38, 39, 40, 41, 42 and 46 models in the ensemble. All these models evolved the same Pareto-optimal front indicating that around 40 surrogate models are sufficient to constitute the ensemble.

Due to the random selection of patterns with repetition into the bootstrap samples, different bootstrap sample sets have different weighting of different regions of the decision space. Depending on the Latin hypercube samples of uncertain parameters used in the numerical model to simulate the concentration corresponding to these patterns, they have different weighting of different regions in the parameter space too. When a number of such models are used they adequately represent the total decision-parameter space. This is ensured using Latin hypercube samples of the pumping patterns, hydraulic conductivity and recharge values.

In the multiple realization approach optimal pumping strategy will not be dictated by one single "worst" realization (Feyen and Gorelick 2004). The most active constraint in different iterations of the optimization will be different.

6.5 Robustness of Optimal Solutions

The validation of the optimal solutions using FEMWATER for uncertain parameters chosen from different regions of the parameter space as shown in Table 3, indicate that the solutions obtained using the multiple realization optimization are also robust optimal solutions. The

Table 3 Concentrations corresponding to optimal solutions with reliability 0.99 obtained from FEMWATER with different values of uncertain parameters

Hydraulic conductivity, Recharge	Objectives		32.67 m/d, 0.176 m/yr		24.44 m/d, 0.061 m/yr		45.59 m/d, 0.258 m/yr	
Solution No:	Total pumping ($\times 10^3 m^3/d$)		Constraint ($\times 10^{-3} kg/m^3$)		Constraint ($\times 10^{-3} kg/m^3$)		Constraint ($\times 10^{-3} kg/m^3$)	
	Production	Barrier	C1 (<500)	C2 (<600)	C1 (<500)	C2 (<600)	C1 (<500)	C2 (<600)
1	286.7	69.3	485.2	564.1	502.95	584.92	481.10	550.18
2	228.9	43.3	502.9	577.9	501.53	590.42	499.21	555.25
3	175.5	30.1	503.0	563.7	501.22	582.87	499.24	551.43
4	105.9	23.7	485.1	565.6	488.09	575.92	478.96	550.15
5	134.3	26.4	498.4	555.6	501.11	562.58	492.11	546.86

concentration values obtained for the optimal solutions for different values of the parameters are very close to each other. It could be concluded that when multiple constraints are incorporated in optimization using different surrogate models, the algorithm searches for solutions which simultaneously satisfies the constraints imposed by all the surrogate models and thus result in robust optimal solutions.

7 Summary and Conclusion

An ensemble surrogate modeling approach together with multiple realization optimization is proposed for multi-objective pumping management of coastal aquifer. The proposed methodology is demonstrated with application to a realistic coastal aquifer system in Burdekin delta area in Australia.

Ensemble surrogate models coupled with multiple realization optimization has definite advantages over single surrogate modeling approach. It helps to better account for the uncertain groundwater parameters. Most often the errors in the surrogate model predictions for optimal solutions correspond to high values in the tail end regions of the error distribution, for objective functions like maximization of pumping. Hence, using single surrogate models to substitute numerical simulation models may result in infeasible or sub-optimal solutions. Ensemble surrogate models with multiple realization optimization helps to overcome this problem to a certain extent. The ensemble approach also reduces the computational requirement by reducing the number of patterns required to train and test the surrogate models. Thus the proposed ensemble surrogate modeling approach is a computationally efficient methodology that can be used to solve groundwater management problems considering uncertainty in groundwater parameters. The results also indicate that the solutions obtained are robust in nature.

It is noteworthy that methods like Monte-carlo simulations based on Bayesian statistics are required for comprehensive characterisation of uncertainty. When such methods are infeasible to be used together with optimization for management decision due to computational burden, the proposed approach could be beneficial.

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