Data Mining for State Space Orthogonalization in Adaptive Dynamic Programming

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Abstract

Dynamic programming (DP) is a mathematical programming approach for optimizing a system which changes over time, and is applied to solve multi-stage optimization problems in environmental engineering, manufacturing systems and many other areas. However, exact solutions are only possible for problems with low dimensions or under very limiting circumstances. Given recent advances in computational power, approximate DP (ADP) methods are developed; however, they are still subject to the "curse of dimensionality", which render DP problem computationally intractable in high-dimensions, with few exceptions. In addition, an approximate solution through discretization of the state space is required for most continuous-state problems. By incorporating a design and analysis of computer experiments (DACE) approach, computationally-tractable ADP methods for continuous-state problems are possible. However, ideal experimental designs need to be orthogonal, and ideal experimental designs will not appropriately represent the state space when the state variables are correlated. Data mining methods are applied in this study for two purposes: (1) to reduce the dimensionality of a DP problem and (2) to orthogonalize a DP state space and enable the use of ideal experimental designs. Results are presented by employing the proposed approach into an Atlanta ozone pollution problem.

Keywords

Data Mining, Design and Analysis of Computer Experiments, Approximate Dynamic Programming, Ozone Pollution.

1. Introduction

Dynamic programming (DP) problems with a high dimension are known to be difficult to solve. Exact solutions are only possible for small DP problems or under very limiting circumstances (linear dynamics, Gaussian random variables, quadratic cost). Consequently, many approximate DP (ADP) methods are developed to address this issue (Barto et al. (2004). In this research, ADP methods for solving stochastic DP (SDP) problems, with continuous (or near-continuous) state variables, are studied. The objective of this SDP is to minimize expected cost (E[c_t(.)]) over T discrete stages and subject to certain restrictions (Γ_t), where the expected value is taken over a random vector (ε_t), with a known probability distribution that forms the stochasticity in the system. For a given current stage (t), the initial state of the system is represented by $\boldsymbol{x}_1$ and the state variables (x_t) specify the state of the system at the beginning of stage t. The transition of the state variables from the current stage (x_t) to the next stage (x_{t+1}) is defined by the state transition function (f_t(.)). For an ozone pollution problem, the state variables consist of concentrations of ozone and its precursor gases, such as nitrogen oxide. The decision (or control) variables (u_t) in each stage are chosen in order to achieve the minimum expected cost. For ozone pollution, the decisions are the reductions in precursor gas emissions at specific times and locations. In each stage, there is a cost function $c_t(\cdot)$, and the decision variables will be chosen to minimize current plus future expected costs. Finally, the optimal value function ($V_t(x_t)$) is defined for stage t as the minimum expected cost, so as to operate the system from stage t forward to the end of the time horizon. Given the state x_t of the system at any stage t, optimal value function can be resolved recursively using equation (1), and the optimal policy obtained from solving (1) will be employed to control the system at stage t.

$$\begin{aligned} &\mathbf{V}_t(x_t) = \min_{\mathbf{u}_t} E\left\{c_t(\boldsymbol{x}_t, \mathbf{u}_t, \boldsymbol{\varepsilon}_t) + \mathbf{V}_{t+1}(x_{t+1})\right\} \\ &\text{s.t.} \quad \boldsymbol{x}_{t+1} = f_t(\boldsymbol{x}_t, \mathbf{u}_t, \boldsymbol{\varepsilon}_t), \text{for } t = 1,..., T \\ &\qquad \mathbf{u}_t \in \Gamma_t, \text{ for } t = 1,..., T \\ &\text{where } \mathbf{V}_T(\boldsymbol{x}_T) = \min_{\mathbf{u}_T} E\left\{c_T(\boldsymbol{x}_T, \mathbf{u}_T, \boldsymbol{\varepsilon}_T)\right\} \end{aligned} \tag{1}$$

All possible values for $V_t(x_t)$ can be acquired if there are a finite number of states. However, when the state space is continuous, as it is for ozone pollution, it is impossible to get all the possible values. Most continuous-state problems require an estimation of the optimal value function and a discretization of the state space. Typically, an approach for approximating the solution in a continuous-state ADP is to firstly form a finite grid of discretization points and then approximate the optimal value function among grid points. However, in high-dimensional problems, a grid of points will grow exponentially when the number of state variables increases. This is one form of the "curse of dimensionality", which makes DP problems computationally intractable. Chen et al. (1999) recognized that state space discretization can profit from design of experiments (DOE), and then an orthogonal array experimental design is used in place of the full factorial design to create a computationally tractable solution method. This is an approach named as design and analysis of computer experiments (DACE), where the computer experiment is the optimization that occurs in each stage of the DP. To approximate the continuous optimal value function, Chen et al. (1999) made use of a regression splines method.

1. For each stage t: Use DOE to sample N points from the state space $\{\boldsymbol{x}_{jt}\}_{t=1}^{N}$.
2. In each stage $t = T-1, \ldots, 1$:
   (a) For each sampled state point $\boldsymbol{x}_{jt}$, $j = 1, \ldots, N$, solve the minimization problem (1), where $t < T-1$, the future value function $\mathbf{V}_{t+1}(\cdot)$ is estimated by $\hat{\mathbf{V}}_{t+1}(\cdot)$.
   (b) Construct the estimated $\hat{\mathbf{V}}_t(\cdot)$ via a statistical model using the data from step 2(a).

Algorithm 1: DACE-ADP algorithm for optimizing a multi-dimensional, T-stage, continuous-state problem (Chen et al. 1999)

The DACE-based ADP solution method from Chen et al. (1999) is introduced in Algorithm 1. In each DP stage t, an experimental design is applied to specify values of the state variables. The computer experiment is resolved for these design state values to achieve the optimized objective, which is the response variable. Then a statistical model is used to fit this data in order to approximate the future value function.

Due to the fact that for ideal experimental designs, orthogonality in the experimental design space is a required assumption (Chen et al. 2006), DOE will not be able to properly represent the state space when the state variables are correlated. Another issue due to the multicollinearity in a state space, is that the collinear variables contain the related or almost the same information corresponding to the dependent variable, which means they are redundant. A principal danger of this data redundancy is that it will result in an overfitting of the regressed model. In statistics, even though the multicollinearity issue does not decrease the predictive power of the model within the sample data set, at least the small changes in the data or the model may change the coefficient estimates of the regression model erratically, which indicates that the created regression model is not robust. Therefore, considering these conditions, this paper presents a preliminary study that uses data mining (DM) to address multicollinearity in a DP state space. DM methods are applied in this study for two reasons: (1) to reduce the dimensionality of a DP problem, (2) to orthogonalize a DP state space, so as to enable the use of ideal experimental designs to build a robust metamodel. The next section will introduce how data mining techniques can be used to reduce the dimension of a DP problem and deal with multicollinearity issues. In section 3, an Atlanta ozone pollution case study is conducted with a comparison of different DM modeling scenarios. Finally, the conclusion is given in the last section.

2. Data mining techniques used in this research

In extremely high-dimensional problems with over 100 state variables, directly conducting DACE-based ADP would require a particularly large experimental design, under the assumption that all these state variables are important. However, not all of them are vital in practice, and it is not known in advance which ones should be deleted and which ones should be maintained. Hence, DM feature selection methods with small exploratory experimental designs are able to provide important dimension reductions to decrease computations. Figure 1 is an example from the Atlanta ozone pollution problem. It very clearly identifies that the state variable "ykm3p1" has strong correlation with the state variable "ykm3p2" and the state variable "ykm3p2" also has strong correlation with

"ykm3p3". However, when transforming these four state variables from the current state space to the Z space, the relationship between these four variables is orthogonalized as shown in Figure 2.
Therefore, for the state variables in Figure 1, it is difficult to conduct an appropriate experimental design to represent them, since DOE only renders ideal designs that are “square” (or circular), as shown in Figure 2. To handle this multicollinearity issue, the state space should be orthogonalized by using DM tools before implementing DACE. The DM techniques used in this study can be divided into two types, feature selection and feature extraction. Both tools are combined to generate an efficient and orthogonal DP state space.

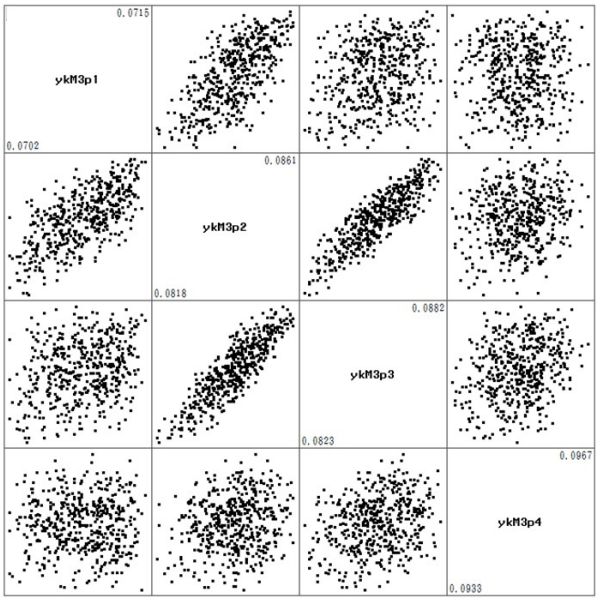

Figure 1. The relationship between state variables in X-state space

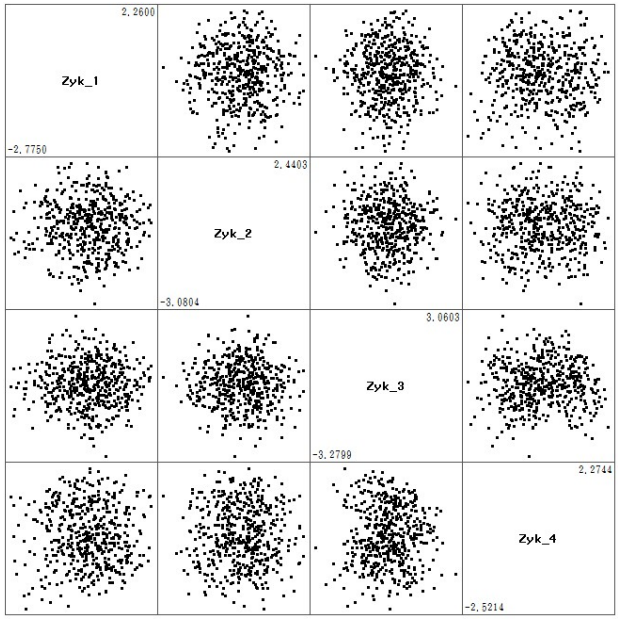

Figure 2. The relationship of state variables in Z-state space

2.1 Feature selection

Feature (variable) selection DM techniques are used to shrink the size of a DP problem by identifying the vital subset of the original features. The feature selection techniques used in this study are comprised of stepwise regression, classification and regression trees (Breiman et al. 1984), and a multiple testing procedure based on the false discovery rate (FDR) (Benjamini and Hochberg, 1995). These techniques have already been studied by Shih et al. (2006), who found out that FDR performed well for the Atlanta ozone pollution problem from Yang et al. (2009).

2.1.1 Stepwise regression

Stepwise regression is an automatic variable selection procedure that uses forward selection and backward elimination processes. In the forward selection process, variables are added one by one to the model if they are statistically significant. Where as in the backward selection process, all of the variables already included in the model are evaluated, and insignificant variables will be deleted. These two processes, forward selection and backward elimination, are repeated until none of the variables outside of the model are significant. In this study, the significance level threshold for a variable to enter or to remain in the model was specified at 0.05.

2.1.2 Classification and regression trees

Classification and regression trees (CART) developed by Breiman et al. (1984) have become a very popular data mining tool for supervised learning. The CART forward algorithm uses binary recursive partitioning to separate the variable space into rectangular regions based on the similarity of the response values. In this research, regression trees are conducted using CART software from Salford Systems (www.salfordsystems.com). For variable selection, this software provides "variable importance scores." The variable that receives a 100 score indicates the most influential variable for prediction, followed by other variables based on their relative importance to the most important variable. However, there are some different options for calculating the scores, and selecting the threshold of the scores to identify important variables may be subjective.

2.1.3 Multiple testing procedure based on the false discovery rate (FDR)

Variable selection using FDR usually divides a dataset into c groups based on a categorical response variable. For each predictor variable ($\boldsymbol{x}_i$), we test the differences in the c samples, using a t-test or F-test. For an n-dimensional problem, a collection of hypothesis tests, that uses the corresponding p-values $\{p_i\}_{i=1}^{n}$, where p_i is the p-value of testing the null hypothesis for variable $\boldsymbol{x}_i$ (where a rejected null hypothesis corresponds to a significant variable), are conducted. In the literature, it is standard to choose a p-value threshold (α) and declare the variable $\boldsymbol{x}_i$ is significant if and only if the corresponding p-value $p_i \leq \alpha$. The FDR is defined as the "expected proportion of false positives among all the hypotheses rejected" (Benjamini and Hochberg, 1995). The general FDR-procedure to identify significant variables is shown as follows:

1. Choose a fixed α, where $0 \leq \alpha \leq 1$.
2. Find $\hat{t} = \max\left[t: p_i \leq \frac{i}{m} \cdot \frac{\alpha}{\pi_0}\right]$, where $\pi_0 (= \frac{m_0}{m})$ denotes the proportion of true H_i.
3. If $\hat{t} \geq 1$, $\Omega =$ {All rejected H_i with $p_i < p_{(i)}$} with FDR(Ω) $\leq \alpha$.

   If $\hat{t} = 0$, do not reject any hypothesis since $\Omega = \varnothing$.

In this study, $\alpha = 0.05$ and $\pi_0 = 1$ are pre-specified.

2.2 Feature extraction

Feature extraction DM techniques try to create new orthogonal features based on transformations of the original features that can supply useful information for modeling [8]. The new orthogonal features are linear combinations of the originals. Feature extraction can be used for both orthogonalization and dimension reduction. Principal component analysis (PCA) and partial least squares (PLS) are the feature extraction tools used in this study. Brief descriptions of PCA and PLS are presented in the following section.

2.2.1 Principal Component Analysis

PCA can be regarded as a method to compute a new coordinate system formed by principal components (PCs), the latent variables or scores, which are orthogonal. Only a small number of the most informative PCs are used. In PCA, correlated original variables ($\boldsymbol{X}$) with p columns (variables) and n rows (samples or observations) are transformed to uncorrelated PCs ($\boldsymbol{Z}$) which are linear combinations of X and are defined in (2). Each consecutive PC is orthogonally selected in descending order of the proportion of explained variation in X.

$$\boldsymbol{Z} = XE \quad (2)$$
$$\text{where } \boldsymbol{E} = [\boldsymbol{E}_1, \boldsymbol{E}_2, \ldots, \boldsymbol{E}_p],\ \boldsymbol{Z} = [\boldsymbol{Z}_1, \boldsymbol{Z}_2, \ldots, \boldsymbol{Z}_p].$$

The eigenvectors of the covariance matrix of X are $\boldsymbol{E} = [\boldsymbol{E}_1, \boldsymbol{E}_2, \ldots, \boldsymbol{E}_p]$, with corresponding ordered eigenvalues ($\boldsymbol{\lambda}_1 > \boldsymbol{\lambda}_2 > \ldots > \boldsymbol{\lambda}_p$), where $\boldsymbol{\lambda}_i$ indicates the variance of $\boldsymbol{Z}_i$. Thus, the first PC ($\boldsymbol{Z}_1$) clarifies the most variation in the original data $\boldsymbol{X}$. The second PC ($\boldsymbol{Z}_2$) is orthogonal to the first one, and explains the next largest variation in the data, and so forth. PCA will produce p PCs, if the original data $\boldsymbol{X}$ has p dimensions.. The PCs illustrate the latent structure of $\boldsymbol{X}$ and can be employed as regressors to predict a response in the regression model.

2.2.2 Partial Least Squares

The model structures of PLS and PCA are very similar. The only difference between them is that the new orthogonal variables (PLS components, $\boldsymbol{Z}$) are chosen to maximize the covariance between $\boldsymbol{X}$ (predictors) and $\boldsymbol{Y}$ (responses). The PLS can be regarded as a compromised approach between PCA and ordinary least squares. The covariance of $\boldsymbol{X}$ and $\boldsymbol{Y}$ merges high variance of $\boldsymbol{X}$ and high correlation with $\boldsymbol{Y}$. The PLS components of $\boldsymbol{Z}$ are achieved by exploring a weight vector $\boldsymbol{w}$ which maximizes the covariance between the scores of $\boldsymbol{X}$ and $\boldsymbol{Y}$ as shown in (3), then regressing $\boldsymbol{Z}$ on $\boldsymbol{X}$ and $\boldsymbol{Y}$, through (4)-(5), and finally the prediction model $\boldsymbol{Y}$ from original $\boldsymbol{X}$ can be obtained by (6). $\boldsymbol{E}$ and $\boldsymbol{F}$ are residual matrices, and $\boldsymbol{P}$ and $\boldsymbol{Q}$ are loading matrices. PLS components of $\boldsymbol{Z}$ can be acquired from many algorithms, but in this study, Wold's PLS (Wold et al. 2001) is applied, where each PLS component $\boldsymbol{Z}$ and weight $\boldsymbol{w}$, are orthogonal ($\boldsymbol{Z}_i^T \boldsymbol{Z}_j = 0$, $\boldsymbol{w}_i^T \boldsymbol{w}_j = 0$; $\boldsymbol{i} \neq \boldsymbol{j}$).

$$\boldsymbol{Z} = \boldsymbol{X}\boldsymbol{w} \quad (3)$$
$$\boldsymbol{X} = \boldsymbol{Z}\boldsymbol{P}^T + \boldsymbol{E} \quad (4)$$
$$\boldsymbol{Y} = \boldsymbol{Z}\boldsymbol{Q}^T + \boldsymbol{F} \quad (5)$$
$$\boldsymbol{Y}_{hat} = \boldsymbol{Z}\boldsymbol{Q}^T = \boldsymbol{X}\boldsymbol{w}\,\boldsymbol{Q}^T = \boldsymbol{X}\,\boldsymbol{B}_{hat} \quad (6)$$
$$\text{where } \boldsymbol{B}_{hat} = \boldsymbol{w}\,\boldsymbol{Q}^T$$

In general, PLS performs better for prediction than PCA since the new orthogonal predictors $\boldsymbol{Z}$ are chosen by incorporating information in $\boldsymbol{Y}$. In the following section, combinations of DM scenarios are employed to the Atlanta ozone pollution problem from Yang et al. [7].

3. Atlanta Ozone Pollution Problem Case Study

One of the main reasons for this research is to enable the use of ideal experimental designs for a DACE based SDP solution method when the state variables are highly correlated. The Atlanta ground-level ozone pollution problem from Yang et al. (2009) is selected as our case study because ozone state variables at different monitoring stations and at different time-periods are highly correlated. In addition, the air quality computer model used in the Atlanta ozone problem, called the Atlanta Urban Airshed Model (UAM), is computationally impractical to use directly in the SDP implementation. Therefore, more efficient approaches are studied.

Natural ozone that stays in the upper atmosphere is good for our earth. This ozone protects the earth from harmful ultraviolet (UV) rays. However, ozone is a harmful pollutant when it is generated at ground-level because ground-level ozone irritates the human nose and eyes and also damages vegetation. Ground-level ozone is not emitted directly but is formed by the chemical reactions of nitrogen oxides (NO_x) and volatile organic compounds (VOCs) in sunlight. Hence, ozone falls at night but rises during the day. Therefore, in order to control ground-level ozone, it is required to control emissions of NO_x and VOC. However, Atlanta is "NO_x-limited," which denotes that targeting VOC emissions is not effective. Thus, for this case study, we only focus on NO_x emissions. To control NO_x, we

should have power over the sources of NO_x, which are point sources and non-point sources. Power plants and other heavy industries are categorized as point sources of NO_x emission, while other sources, such as automobiles and small industries, are treated as non-point sources.

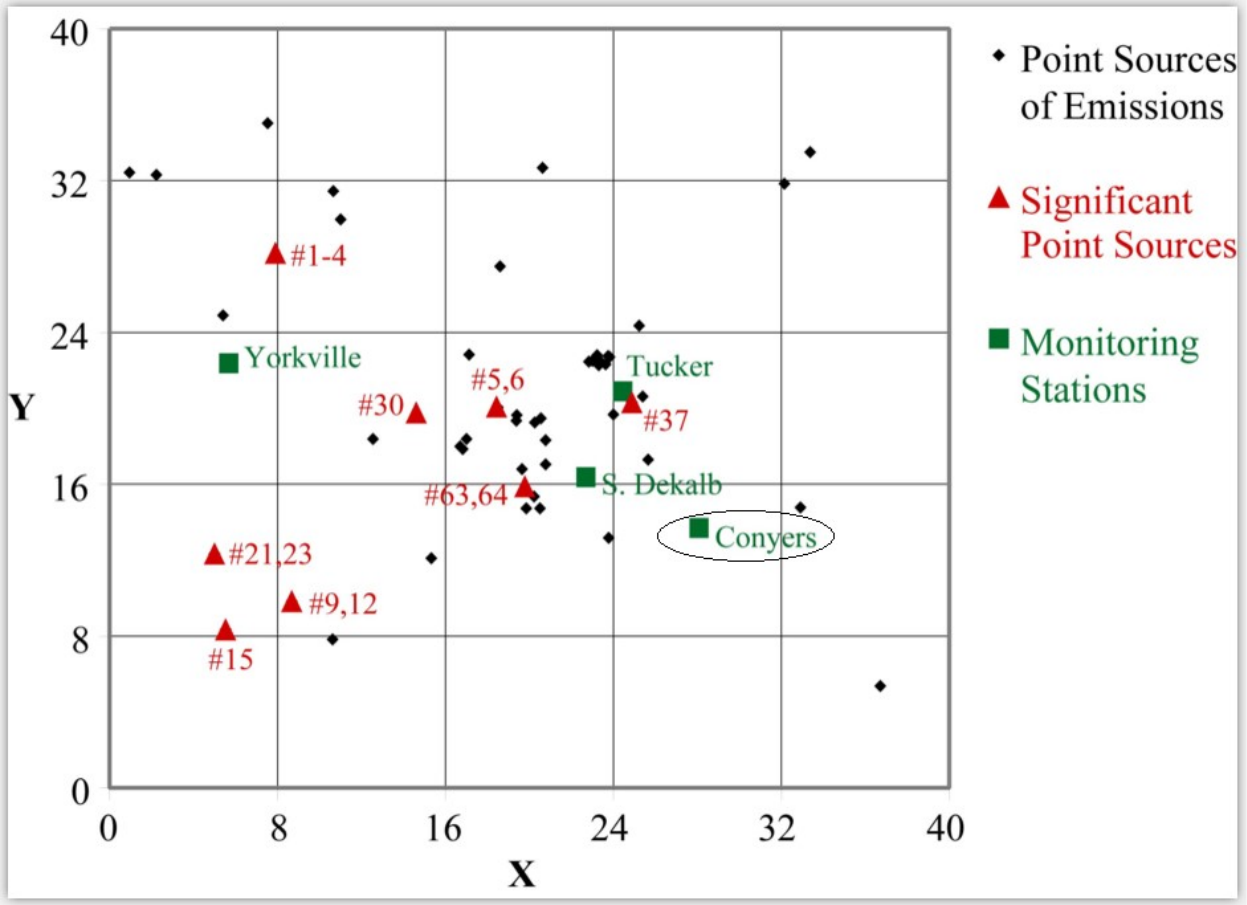

Figure 3. Illustration of the emission sources of the Atlanta ozone problem (Yang et al. 2009)

Figure 3 shows a spatial representation of the Atlanta area using the UAM's 40 x 40 grid covering a 160 x 160 kilometer square region of the metropolitan area. Yang et al. (2009) aggregated the 40 x 40 grid into a 5 x 5 grid to represent the non-point source emissions for the Atlanta metropolitan area. In this region, there are a total of 102 point sources. The Ozone level is monitored by four Photochemical Assessment Monitoring Stations (PAMS) located at Conyers, S. Dekalb, Tucker, and Yorkville, because only these four stations are monitored. The case they studied happened on the dates July 29 – August 1, 1987.

As to the application of ADP to solve this ozone problem, at time stage t, the known state variables describe the status of all the factors at the beginning of SDP stage t that may have an impact on ozone concentrations. A sequence of decisions must be made in the four time stages to minimize the total cost to achieve the ozone attainment goals. According to the SDP formulation in Eq. (1), state variables (x_t) at time t include all historical information on ozone concentrations and NO_x emissions at various spatial locations across the metropolitan Atlanta area. In other words, the initial set of potential state variables for SDP stage t includes information related to ozone air chemistry occurring from time periods 0 though t - 1. Decision variables (u_t) are the actions to be chosen in SDP stage t to control the amount of emissions at various locations and times over the course of the day in order to minimize the reduction of emissions needed to prevent an ozone exceedance.

The objective of the Atlanta ozone pollution problem is to minimize the cost of preventing ozone from exceeding the US EPA standard limit, which was 0.12 parts per million in this research (and more recently has been decreased,

see http://www.epa.gov/air/criteria.html). To reduce ozone concentrations, emission controls are applied to specific areas and times. Since ozone rises during the daytime when the sun is present, only time periods from 4 a.m. to 7 p.m. are considered as potential time periods for reducing emissions. For the ozone pollution SDP approach, five 3-hour time periods are defined: time period 0 is from 4 a.m. to just before 7 a.m, time period 1 is from 7 am to just before 10 am, time period 2 is from 10 am to just before 1 pm, time period 3 is from 1 pm to just before 4 pm and time period 4 is from 4 p.m. to just before 7 p.m. Time period 0 is an initialization period. The SDP stages are based on time periods 1 through 4.

In Yang et al. (2009), the Atlanta UAM model was used as a computer model for generating data on the relevant air chemistry. They studied one of the worst cases in ozone history in urban Atlanta, which occurred between July 29th and August 1st, 1987, where the episode began on July 31st and peaked on August 1st. They focused on July 31st with the logic that if the first day of the episode could be controlled, then there might be hope for controlling the second day. The UAM includes meteorological conditions and nominal emissions as input for this ozone episode. A 500-point Latin Hypercube experimental design was used to scale emissions in different grid regions, different point sources, and different times, from zero up to the nominal (maximum) level. These runs were input into the UAM, and the resulting ozone concentrations across the 40 x 40 UAM's model grid were collected and then aggregated into the 5 x 5 grid. Figure 4 shows the metamodeling process that uses the input emissions from experimental design and the ozone output from the UAM to construct statistical models as metamodel surrogates of the UAM. In adaptive DP (ADP), the metamodels are then used to represent the ozone state transition from stage to stage in a DACE based SDP implementation.

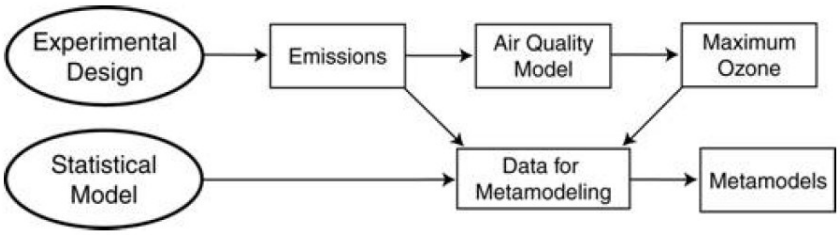

Figure 4. Process of developing metamodel (Yang et al. 2009)

Because the development of the state transition function is an integral part of the ADP process, its accuracy of the transition function has a direct impact on the achievement of optimal decision making. Therefore, it is important to conduct dimension reduction for high-dimensional problems, so as to eliminate the redundancy of states and enable better computational efficiency and accuracy. In this study, the statistical metamodeling approach is studied in the presence of a highly correlated state space. In this section, the proposed data mining techniques in section 2, feature selection to reduce dimension and feature extraction to handle the multicollinearity, are applied.

3.1 Proposed Data Mining Modeling Approaches

In an evaluation study, 19 modeling approaches are proposed which are shown in Table 1. Most of these approaches start with a feature selection procedure to reduce the dimension of the original problem, such as using stepwise regression, FDR, or regression trees. Then orthogonalization and dimension reduction are performed using PCA or PLS. For example, approach A-3 first uses stepwise regression on the original dataset to select a significant subset of state variables, then utilizes PCA on the selected subset to make them orthogonal, and finally conducted stepwise regression again, with the respect to the original response on the orthogonal predictors (PCs), to select a final subset of significant PCs. However, in Table 1, it is noted that there are two versions of using FDR to conduct the pre-feature selection: one is FDR with (2) categorized response and the other is FDR with continuous response. For the FDR with (2) categorized response, we first employ the median of the response to split the response into two groups and then apply the original FDR procedure from Benjamini and Hochberg (1995). In addition, for FDR with continuous response, we first apply the ordinary least square to obtain the estimates for all variables, second, the t-statistics for the estimates are calculated, third, the *p*-values of all the estimates from t-statistics are obtained, and finally, the original FDR procedure from Benjamini and Hochberg (1995) is utilized to select important variables by taking advantage of a set of *p*-values.

Table 1. Proposed Data Mining Modeling Approaches

Approach	Pre-Feature Selection	Feature Extraction	Post-Feature Selection
A-1	Stepwise Regression		
A-2	Stepwise Regression	PCA	
A-3	Stepwise Regression	PCA	Stepwise Regression
A-4	Stepwise Regression	PLS	
B-1	FDR w / (2)Categorized Response		
B-2	FDR w / (2)Categorized Response	PCA	
B-3	FDR w / (2)Categorized Response	PCA	Stepwise Regression
B-4	FDR w / (2)Categorized Response	PLS	
C-1	FDR w / Continuous Response		
C-2	FDR w / Continuous Response	PCA	
C-3	FDR w / Continuous Response	PCA	Stepwise Regression
C-4	FDR w / Continuous Response	PLS	
D-1	Regression Tree		
D-2	Regression Tree	PCA	
D-3	Regression Tree	PCA	Stepwise Regression
D-4	Regression Tree	PLS	
E-1	-	PAM Sites – PCA	Stepwise Regression
E-2	-	PCA	Stepwise Regression
F	-	PLS	

3.2. Evaluating the metamodel

Each proposed approach is evaluated on the Atlanta ozone data described above (500-Latin Hypercube design points with ozone concentrations from the UAM) to predict ozone levels for time stage 1 to time stage 4. Table 2 shows the numbers of variables involved in the Atlanta ozone SDP problem after the mining phase in Yang et al. (2009). In each stage, the metamodel uses both state and decision variables as initial predictors. It should be noted that the original dimension of the SDP state space, prior to the mining phase, is over 500.

For the Atlanta ozone problem, non-point sources of emissions are controlled separately in the 5 x 5 grid areas. These comprise of 25 non-point source decision variables. Initially, there are a total of 102 point sources, but after the mining phase in Yang et al. (2009), only 15 were statistically significant; thus, the number of point source decision variables maintained in this study is 15. In each time stage, there are 40 potential decision variables that the decision-maker must control. These decision variables are kept and considered as state variables in the next time stage. Past monitored ozone level information from the four PAMS sites, are additional state variables, so the number of potential state variables occurring in each time period is 44. For example, in time stage 4, the state variables entering this stage include all previous ozone levels at all stations and all previous NO_x emissions, i.e., ozone levels and emissions from time periods 0, 1, 2, and 3 yield 176 state variables. The 40 decision variables are the reductions in NO_x emissions for each grid region (5 x 5 = 25) and 15 point sources in time period 4.

Table 2. Number of Predictors for the Atlanta Ozone Problem.

	State Space (x_t) (Past Ozone & NOx)	**Decision Space (u_t)** (NOx emission)	**Total # Predictors**
Stage-1	44 (40 + 4)	40 (5 x 5 + 15)	84
Stage-2	88 (44 x 2)	40	128
Stage-3	132 (44 x 3)	40	172
Stage-4	176 (44 x 4)	40	216

In the evaluation study, all of the proposed metamodels, using the initial dataset shown in Table 2, were constructed separately by time stage to predict only the ozone level at the Conyers monitoring station, which is circled in Fig. 3, Each modeling approach was evaluated using the following performance measures;

(1) Model R^2 measures how well the model fits to the data.
(2) Number of variables left in the model represents ability to reduce dimension.
(3) Variance Inflation Factor (VIF) indicates degree of multicollinearity.
(4) Percent of prediction error (%Error) measures model prediction accuracy.

All evaluation results of the proposed metamodeling approach are presented in the following.

3.2.1. Results of various modeling scenarios for the metamodel of Conyers stage 1

The results of 19 modeling scenarios for the metamodel of Conyers at stage 1 are shown in Table 3. From it, it is easy to determine that no matter what approaches are used, the metamodel of Conyers at stage 1 has very low R^2, which denotes that the number of state variables at stage 0 is not enough to represent the whole state space, but more state variables are needed. However, feature selection reduces the dimension of variables successfully, and feature extraction also helps each approach obtain a very low VIF (the VIF of most approaches is 1), which denotes the state variables are orthogonalized to each other.

Table 3. Results of Various Modeling Scenarios for the metamodel of Conyers stage 1

Approaches		R^2	Vars. left in model	VIF	% Error
A-1	Stepwise	0.2646	7	(1.0006 - 1.0137)	1.08925
A-2	Stepwise-PCA	0.2646	7	1	1.08925
A-3	Stepwise-PCA-Stepwise	0.2597	4	1	1.09229
A-4	**Stepwise-PLS**	**0.2636**	**1**	**1**	**1.08741**
B-1	FDR	0.2219	3	(1.003 - 1.008)	1.10580
B-2	FDR_PCA	0.2219	3	1	1.10580
B-3	FDR_PCA_StepwiseReg	0.2208	2	1	1.10352
B-4	FDR_PLS	0.2205	1	1	1.10384
C-1	conFDR	0.1894	1	1	1.13779
C-2	conFDR_PCA	0.1894	1	1	1.13779
C-3	conFDR_PCA_Stepwise	0.1894	1	1	1.13779
C-4	conFDR_PLS	0.1894	1	1	1.13779
D-1	Tree	0.1937	2	1.00061	1.13840
D-2	Tree_PCA	0.1937	2	1	1.13840
D-3	Tree_PCA_Stepwise	0.1937	2	1	1.13840
D-4	Tree_PLS	0.1936	1	1	1.13890
E-1	PCA-Stepwise	0.2476	20	1	1.15553
E-2	PAMsSites-PCA-Stepwise	0.2646	7	(1.002 - 1.014)	1.08925
F	PLS	0.3048	1	1	1.18912

3.2.2. Results of various modeling scenarios for the metamodel of Conyers stage 2

To build up the metamodel of Conyers at stage 2, the state variables from stage 1 are also included in the state space. With the help of the metamodel, it is easy to identify that R^2 is very high and close to 1 for all approaches and percentage of error is low. From Table 4, we can also observe that the variables left in each model are different when using different approaches. In Table 5, the results of each criteria are ranked, after removing the approaches with VIF >1. From it, it is observed that approach FDR_PLS is able to reduce the dimension the most, Stepwise_PCA_stepwise can make the metamodel have lowest error, and PLS is likely to achieve a high R^2. However, these three methods only perform well under these three criteria. If the four criteria (R^2, Vars. left in model, VIF, %Error) are considered simultaneously, the general approach would start with stepwise regression to conduct the feature selection procedure, followed by PLS. This approach performs better than the other methods since, in combination, its R^2 is very high (but not the highest), 3 variables are left in the model, VIF is equal to 1 and

the percentage of prediction error is very low (but not the lowest). Moreover, compared to Table 3, the R^2 values in Table 4 are all more than 0.99, which connotes that the number of state variables at stage 0 and stage 1 are able to represent the whole state space.

Table 4. Results of Various Modeling Scenarios for the metamodel of Conyers stage 2

Approaches		R^2	Vars. left in model	VIF	% Error
A-1	Stepwise	0.9937	10	(1.009 - 1.260)	0.33001
A-2	Stepwise-PCA	0.9937	10	1	0.33001
A-3	Stepwise-PCA-Stepwise	0.9937	10	1	0.33001
A-4	**Stepwise-PLS**	**0.9934**	**3**	**1**	**0.34289**
B-1	FDR	0.9894	3	(1.01 - 1.23)	0.45582
B-2	FDR_PCA	0.9894	3	1	0.45582
B-3	FDR_PCA_Stepwise	0.9894	3	1	0.45582
B-4	FDR_PLS	0.9894	1	1	0.45582
C-1	conFDR	0.9900	6	(1.01302 - 1.24359)	0.45066
C-2	conFDR_PCA	0.9900	6	1	0.45066
C-3	conFDR_PCA_Stepwise	0.9900	6	1	0.45066
C-4	conFDR_PLS	0.9897	3	1	0.45497
D-1	Tree	0.9894	4	(1.00064 - 1.23411)	0.45593
D-2	Tree_PCA	0.9894	4	1	0.45593
D-3	Tree_PCA_Stepwise	0.9894	4	1	0.45593
D-4	Tree_PLS	0.9894	3	1	0.45652
E-1	PCA-Stepwise	0.9946	110	1	0.42443
E-2	PAMsSites-PCA-Stepwise	0.9935	14	(1.02 - 2.11)	0.34485
F	PLS	0.9947	10	1	0.43429

Table 5. Ranking Results of the Scenarios for the metamodel of Conyers stage 2

Approaches*	Vars. left in model
FDR_PLS	1
Stepwise-PLS	**3**
FDR_PCA	3
FDR_PCA_Stepwise	3
conFDR_PLS	3
Tree_PLS	3
Tree_PCA	4
Tree_PCA_Stepwise	4
conFDR_PCA	6
conFDR_PCA_Stepwise	6
Stepwise-PCA	10
Stepwise-PCA-Stepwise	10
PLS	10
PCA-Stepwise	110

Approaches*	% Error
Stepwise-PCA-Stepwise	0.33001
Stepwise-PCA	0.33001
Stepwise-PLS	**0.34289**
PCA-Stepwise	0.42443
PLS	0.43429
conFDR_PCA	0.45066
conFDR_PCA_Stepwise	0.45066
conFDR_PLS	0.45497
FDR_PCA_Stepwise	0.45582
FDR_PLS	0.45582
FDR_PCA	0.45582
Tree_PCA_Stepwise	0.45593
Tree_PCA	0.45593
Tree_PLS	0.45652

Approaches*	R^2
PLS	0.9947
PCA-Stepwise	0.9946
Stepwise-PCA	0.9937
Stepwise-PCA-Stepwise	0.9937
Stepwise-PLS	**0.9934**
conFDR_PCA	0.9900
conFDR_PCA_Stepwise	0.9900
conFDR_PLS	0.9897
FDR_PLS	0.9894
Tree_PLS	0.9894
FDR_PCA	0.9894
FDR_PCA_Stepwise	0.9894
Tree_PCA	0.9894
Tree_PCA_Stepwise	0.9894

*** VIF > 1 are removed.**

*** Ordered by better to worse**

3.2.3. Results of various modeling scenarios for the metamodel of Conyers stage 3

In Conyers stage 3, the state variables used in stage 0, 1 and 2 are also included in the state space. By applying the same procedure used in stage 2, after removing the approaches with VIF>1, the results are ordered from better to worse for each criteria, except VIF, and shown in Table 6. It is interesting to find out that the FDR_PLS method also performs well in the reduction of dimension; Stepwise-PCA can generate the lowest percentage of prediction error; and PLS can generate the highest R^2. As the same in stage 2, the approach Stepwise_PLS performs better in general than the other methods.

Table 6. Ranking Results of the Scenarios for the metamodel of Conyers stage 3

Approaches*	Vars. left in model
FDR_PLS	1
conFDR_PLS	2
Tree_PLS	2
Stepwise-PLS	**3**
FDR_PCA	3
FDR_PCA_Stepwise	3
Tree_PCA_Stepwise	3
Tree_PCA	4
conFDR_PCA	7
conFDR_PCA_Stepwise	7
PLS	11
Stepwise-PCA-Stepwise	20
Stepwise-PCA	21
PCA-Stepwise	135

Approaches*	% Error
Stepwise-PCA	0.51086
Stepwise-PCA-Stepwise	0.51669
Stepwise-PLS	**0.52170**
PCA-Stepwise	0.71002
PLS	0.71337
conFDR_PLS	0.72316
conFDR_PCA	0.72409
conFDR_PCA_Stepwise	0.72409
Tree_PCA_Stepwise	0.74759
FDR_PCA	0.75258
FDR_PCA_Stepwise	0.75258
Tree_PCA	0.75327
Tree_PLS	0.75677
FDR_PLS	0.75727

Approaches*	R^2
PLS	0.9879
PCA-Stepwise	0.9871
Stepwise-PCA	0.9847
Stepwise-PLS	**0.9846**
Stepwise-PCA-Stepwise	0.9846
conFDR_PCA	0.9727
conFDR_PCA_Stepwise	0.9727
conFDR_PLS	0.9727
FDR_PCA	0.9659
FDR_PCA_Stepwise	0.9659
Tree_PCA	0.9659
Tree_PCA_Stepwise	0.9659
Tree_PLS	0.9659
FDR_PLS	0.9652

*** VIF > 1 are removed.**

*** Ordered by better to worse**

3.2.4. Results of various modeling scenarios for the metamodel of Conyers stage 4

During stage 4, there are 176 state variables including all previous ozone levels at all stations and all previous NO_x emissions with 40 decision variables. Therefore, there are 216 predictor variables in total. By making use of the above methods, after eliminating the approaches with VIF>1 and ranking the rest, it is determined from Table 7 that conFDR_PLS performs best in reducing the dimensions with 4 variables left. In this case, FDR_PLS also can be ranked as the second best because it can decrease dimensions to 7. As same as in section 3.2.2 and 3.2.3, Stepwise_PCA approach has the lowest percentage of prediction error and PLS method has the highest R^2. In general, Stepwise_PLS approach performs better than the other methods.

Table 7. Ranking Results of the Scenarios for the metamodel of Conyers stage 4 (Ariyajunya et al. 2010)

Approaches*	Vars. left in model
conFDR_PLS	4
FDR_PLS	7
PLS	7
FDR_PCA_Stepwise	8
Stepwise-PLS	**9**
FDR_PCA	9
conFDR_PCA	9
conFDR_PCA_Stepwise	9
Tree_PLS	9
Tree_PCA_Stepwise	11
Tree_PCA	12
Stepwise-PCA-Stepwise	25
Stepwise-PCA	**26**
PCA-Stepwise	167

Approaches*	% Error
Stepwise-PCA	**0.76287**
Stepwise-PLS	**0.76289**
Stepwise-PCA-Stepwise	0.76405
Tree_PCA	1.03436
Tree_PLS	1.03437
PCA-Stepwise	1.03480
Tree_PCA_Stepwise	1.03789
FDR_PCA_Stepwise	1.08940
FDR_PLS	1.09064
FDR_PCA	1.09164
PLS	1.09891
conFDR_PCA	1.25593
conFDR_PCA_Stepwise	1.25593
conFDR_PLS	1.25641

Approaches*	R^2
PLS	0.9877
PCA-Stepwise	0.9864
Stepwise-PCA	**0.9841**
Stepwise-PCA-Stepwise	0.9841
Stepwise-PLS	**0.9841**
Tree_PCA	0.9676
Tree_PLS	0.9676
Tree_PCA_Stepwise	0.9675
FDR_PCA	0.9628
FDR_PLS	0.9627
FDR_PCA_Stepwise	0.9627
conFDR_PCA	0.9548
conFDR_PCA_Stepwise	0.9548
conFDR_PLS	0.9548

*** VIF > 1 are removed.**

*** Ordered by better to worse**

After conducting these experiments, we can conclude that the number of state variables is very important. If the quantity of state variables is not sufficient, R^2 will be very low, as shown in Table 3. When the state variables are able to represent the whole state space accurately, as the results shown in 3.2.2, 3.2.3 and 3.2.4, R^2 is very high. In addition, based on the four criteria, FDR_PLS only performs well in the dimension reduction, Stepwise_PCA only performs well in achieving the lowest percentage of prediction error and PLS can only reach the highest R^2. However, in practice, an approach that can satisfy every criterion is expected, which is identified in the Stepwise_PLS approach. Thus, in order to acquire the metamodel of Conyers at stage 2, 3 and 4, Stepwise_PLS approach is recommended.

4. Conclusions

In conclusion, this paper addresses the multicollinearity issue in DP state space using DM techniques (PCA and PLS). Moreover, these DM techniques also achieve significant reduction in dimensions, as shown from Table 3 to Table 8. Furthermore, by applying different combinations of DM techniques, it is identified that not all approaches behave well and some combinations only perform well under certain criteria. The results demonstrate that approaches starting with stepwise regression have higher R^2 and lower prediction error, but they are not the best in term of dimension reduction and VIF value. The combination of FDR and regression trees is very good for dimension reduction, but they are less accurate. The approaches that incorporate feature extraction methods, including PCA and PLS, are able to handle multicollinearity indicated by VIFs equal to 1, which denotes that the method provides an uncorrelated state space. Therefore, before employing DM tools into DP problems, it is necessary to select the best one among all approaches. In this study, the Stepwise_PLS method can achieve all our goals to enable a more computationally-efficient DP solution. Based on this preliminary experiment, it is necessary to apply DM techniques to DP metamodel building procedures, including the metamodel of unknown transition function, in future research.

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