Design of DOE-Based Automatic Process Controller With Consideration of Model and Observation Uncertainties

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***Abstract*—Robust parameter design (RPD) has been widely used as a cost-effective tool in quality control to reduce variability, in which the controllable factors are set to minimize the variability of response variables due to noise factors, assuming their distributions are known. It is essentially an offline tool without considering that some noise factors can be measured online. Recently, the concept of design of experiment (DOE)-based automatic process control (APC) has been proposed for online process control based on regression models obtained from DOE and with consideration of the online measurement of noise factors. The existing literature investigates the DOE-based APC with assumption that both regression models and the online noise measurement are precisely known, which limits the applicability of the technique. This paper develops the DOE-based APC scheme that considers both the observation and the modeling uncertainties. The controller is implemented under two APC strategies, i.e., cautious control strategy and certainty equivalence control strategy. The comparison among online APC and robust design approaches demonstrates that automatic controller with consideration of both uncertainties can achieve better process performance than conventional design, and is more stable than normal DOE-based APC controllers. The proposed approach is illustrated using an industrial process.**

***Note to Practitioners*—Manufacturing processes usually involve complicated interactions among process variables, and traditional robust design explores these interactions to eliminate the impact of noise as much as possible. Nowadays the in-process sensing technology provides real-time estimations of the process variables, and using this additional information, automatic process control should be able to further improve the quality of process. However, overtrusting these observations in reality will be reacting to noise, and may lead to an even worse control performance. This paper develops a new automatic process control strategy that will setup and adjust the controllable variables according to the online observations. It also considers the uncertainties during observation and estimation, which further improves the control performance and robustness to sensor noises.**

***Index Terms*—Automatic process control (APC), design of experiment (DOE), cautious control, robust parameter design (RPD), variation reduction.**

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I. Introduction

In complex manufacturing processes, there are many process variables that interact in a complicated manner. In general, these variables can be classified into control (or controllable) factors, $\mathbf{x}$ (variables that can be easily manipulated), and noise (or uncontrollable) factors, $\mathbf{n}$ (variables that vary randomly and are difficult to manipulate in real time). Let y denote a quality response of interest, then the relationship between $\mathbf{x}, \mathbf{n}$ and y can be generally expressed as

$$y = f(\mathbf{x}, \mathbf{n}). \tag{1}$$

Taguchi's robust parameter design (RPD) is considered a cost-effective tool for reducing process variability, which aims to set the values of controllable factors to eliminate the effect of noise factors on response [1]. This is done by exploiting the control-by-noise interactions and setting the controllable factors to "optimal" levels so that the response is insensitive to the variations in noise factors within certain ranges. Experimental design is then employed to obtain the relationship of $f(\cdot)$ in (1).

RPD is essentially a technique for determining the control factors' settings at design stage to maximize the robustness of process performance to the disturbances of noise. In this effort, only the distributions of noise factors are assumed to be known. While with the advancement of sensing technology, some noise factors can be measured or estimated through in-process sensing during production. Examples of such factors include temperature, humidity, etc. It is reasonable to anticipate the process performance to be further improved if the process control factors are adjusted according to the online sensing information of noise factors, rather than based only on the assumptions of their distributions.

Some research efforts have been made to utilize online observations of noise factors for process variation reduction. One approach is explicitly introducing online measurable noise factors into a designed experiment, as described in [2]. It shows that the additional information gained from online observations can enhance the choice of values for the controllable factors. A robust parameter design methodology in the presence of feed-forward or feedback control systems and measurable noise factors is proposed by [3], [4]. However, they do not implement the control variables under automatic control scheme.

The study of automatic control strategy based on regression models obtained from DOE is initiated by [5], where noise factors are classified into "measurable noise factors" and "immeasurable noise factors." They investigate two types of control strategies: cautious control and certainty equivalence control, and compare them with robust parameter design. Their approach assumes all controllable factors are online adjustable, which limits the applicability of the methodology in the case where some control factors cannot be changed in real-time. Shi *et al.* in [6] further classifies controllable factors into online controllable and controllable ones, with the latter denoting factors that are difficult to be adjusted online but can be set at the design stage. A corresponding control strategy is proposed in their paper.

The aforementioned DOE-based APC approaches are developed based on the precise regression models with no assumptions or considerations of modeling error. However, in practice, the model parameters are often estimated from experimental data, and these estimates will be affected by the design and unknown random effects in experiments. Thus, it is unavoidable that all regression models used in the APC design have inherent modeling errors. Other than modeling uncertainties, the precision of online sensing of noise factors is constrained by the sensing capabilities. Therefore, it is important to investigate the impacts of those modeling and sensing errors on the performance of the DOE-based APC control strategy, as well as further develop effective ways to improve the robustness of the control strategy to both uncertainties.

This paper develops a generic APC method based on experimental design and modeling, which considers modeling and sensing errors simultaneously. The paper is organized as follows. In Section II, a new process modeling and an online control strategy is proposed with consideration of model uncertainties. Section III illustrates the proposed strategies using an injection molding process and carries out comparisons to existing approaches. Finally, the paper is summarized in Section IV.

II. Online Control Algorithm

A. General Model and Assumptions

A generic response model with single response y can be expressed in terms of $\mathbf{X}, \mathbf{U}, \mathbf{e}$, and $\mathbf{n}$ as

$$y = f(\mathbf{X}, \mathbf{U}, \mathbf{e}, \mathbf{n}) + \varepsilon \quad (2)$$

where the controllable factors are classified into setting factors $\mathbf{X}$ and online controllable factors $\mathbf{U}$, while noise factors are classified into measurable noise $\mathbf{e}$ and immeasurable noise $\mathbf{n}$, and ε is the regression residual error.

Regression model $f(\mathbf{X}, \mathbf{U}, \mathbf{e}, \mathbf{n})$ is generally nonlinear for inputs but still linear for model parameters. A model of interest should include main effects of all factors together with control-by-noise interactions. Thus, model (2) becomes

$$\begin{aligned} y = \beta_0 &+ \boldsymbol{\beta}_1^T\mathbf{X} + \boldsymbol{\beta}_2^T\mathbf{U} + \boldsymbol{\beta}_3^T\mathbf{e} + \boldsymbol{\beta}_4^T\mathbf{n} \\ &+ \mathbf{X}^T\mathbf{B}_1\mathbf{e} + \mathbf{U}^T\mathbf{B}_2\mathbf{e} \\ &+ \mathbf{X}^T\mathbf{B}_3\mathbf{n} + \mathbf{U}^T\mathbf{B}_4\mathbf{n} + \varepsilon \end{aligned} \quad (3)$$

where $\mathbf{X} \in \mathrm{R}^{m\times 1}, \mathbf{U} \in \mathrm{R}^{n\times 1}, \mathbf{e} \in \mathrm{R}^{p\times 1}, \mathbf{n} \in \mathrm{R}^{q\times 1}$, and other vectors and matrices are of appropriate dimensions. This model has the typical form of regression models obtained from a designed experiment. The details of modeling strategy and procedures can be found in [7]. The higher order interactions among controllable variables and noise variables are not included in (3), since the consideration of these interactions will only add to the complexity of solving the problem, but not on the optimization procedure.

Define $\boldsymbol{\beta}$ as $\boldsymbol{\beta} \equiv [\beta_0, \boldsymbol{\beta}_1^T, \ldots, \boldsymbol{\beta}_4^T, \mathrm{vec}(\mathbf{B}_1)^T, \ldots, \mathrm{vec}(\mathbf{B}_4)^T]^T$, representing the set of all model parameters. Here $\mathrm{vec}(\mathbf{B})$ is the stack up of column vectors of a matrix $\mathbf{B}$.

To develop the process control methodology, the following assumptions have been made.

A1. The manufacturing process is time-invariant for the period of time when the same control law is applied. This would be appropriate for many real-life manufacturing processes with stable and in-control productions. The model and control law can be adjusted in case the process setting has changed. The parameters are estimated from designed experiments, denoted by $\hat{\boldsymbol{\beta}} = \boldsymbol{\beta} + \tilde{\boldsymbol{\beta}}$, where $\boldsymbol{\beta}$ is the underlying true model parameter, $\hat{\boldsymbol{\beta}}$ is its estimate from experiments, and $\tilde{\boldsymbol{\beta}}$ is the estimation error. The estimation uncertainty is represented by $\mathrm{Cov}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}) = \Sigma_{\tilde{\boldsymbol{\beta}}}$. This modeling uncertainty is of the same definition as the parameter estimation error. The estimation error is assumed to be normally distributed.

A2. The noise terms $\mathbf{e}$, $\mathbf{n}$ and ε are independent of each other, with $E(\mathbf{e}) = \mathbf{0}, \mathrm{Cov}(\mathbf{e}) = \sum_{\mathbf{e}}, E(\mathbf{n}) = \mathbf{0}, \mathrm{Cov}(\mathbf{n}) = \Sigma_{\mathbf{n}}$, and $E(\varepsilon) = 0, \mathrm{Var}(\varepsilon) = \sigma_\varepsilon^2$. The model residual errors, represented as ε's, are independently and identically distributed.

A3. The online noise observer can provide an unbiased estimation of measurable noise factor $\mathbf{e}$, denoted by $\hat{\mathbf{e}} = \mathbf{e} + \tilde{\mathbf{e}}$, where $\mathbf{e}$ is the true value of the observable noises, $\hat{\mathbf{e}}$ is its observation, and $\tilde{\mathbf{e}}$ is the observation error. The observation of noise variable is unbiased, i.e., $E[\hat{\mathbf{e}} - \mathbf{e}|\hat{\mathbf{e}}] = 0$, and $\mathrm{Cov}(\hat{\mathbf{e}} - \mathbf{e}|\hat{\mathbf{e}}) = \sum_{\tilde{\mathbf{e}}}$ represents the observation uncertainty.

The modeling uncertainty $\sum_{\tilde{\boldsymbol{\beta}}}$ in assumption A1 can be obtained from experimental design together with the model coefficients [7]. The observation uncertainty $\sum_{\tilde{\mathbf{e}}}$ in assumption A3 can be estimated from the specifications of observer, or gauge repeatability and reproducibility study.

B. Optimal Control Strategy

The objective process control is usually to keep the deviation of response y from the target value as small as possible, which is called a "nominal-the-best problem." A quadratic loss function $L(y,t) = k(y-t)^2$ should be chosen as the performance measure, where t is the target value and k is a monetary coefficient. Since there is only one quality response characteristic y considered in this paper, k can be assumed to be 1 without loss of generality. The optimal control algorithm is developed to minimize $L(y,t)$.

Thus, when the process parameter $\hat{\boldsymbol{\beta}}$ is estimated and measurement $\hat{\mathbf{e}}$ is obtained, the conditional control objective function can be expressed as

$$\begin{aligned} &J_{\mathrm{APC}}(\mathbf{X}, \mathbf{U}|\hat{\mathbf{e}}, \hat{\boldsymbol{\beta}}) \\ &= E_{\mathbf{e},\mathbf{n},\tilde{\boldsymbol{\beta}},\varepsilon}[L(y,t)|\hat{\mathbf{e}}, \hat{\boldsymbol{\beta}}] \\ &= E_{\mathbf{e},\mathbf{n},\tilde{\boldsymbol{\beta}},\varepsilon}[(y|\hat{\mathbf{e}}, \hat{\boldsymbol{\beta}}) - t]^2 \\ &= (E_{\mathbf{e},\mathbf{n},\tilde{\boldsymbol{\beta}},\varepsilon}[y|\hat{\mathbf{e}}, \hat{\boldsymbol{\beta}}] - t)^2 + \mathrm{Var}_{\mathbf{e},\mathbf{n},\tilde{\boldsymbol{\beta}},\varepsilon}(y|\hat{\mathbf{e}}, \hat{\boldsymbol{\beta}}). \end{aligned} \quad (4)$$

In this equation, if $\mathbf{a}$ is a random vector and b is a random variable as a function of $\mathbf{a}$, $E_{\mathbf{a}}[b]$ represents the expectation of b taken over the distribution of $\mathbf{a}$. Similarly, $\mathrm{Var}_{\mathbf{a}}(b)$ represents the variance of b taken over the distribution of $\mathbf{a}$. For regression model (3), it can be shown that (see Appendix A for details)

$$\begin{aligned} &J_{\mathrm{APC}}(\mathbf{X},\mathbf{U}|\hat{\mathrm{e}},\hat{\boldsymbol{\beta}}) \\ &= \Big(\hat{\beta}_0 - t + \hat{\boldsymbol{\beta}}_1^T\mathbf{X} + \hat{\boldsymbol{\beta}}_2^T\mathbf{U} \\ &\quad + \hat{\boldsymbol{\beta}}_3^T\hat{\mathrm{e}} + \mathbf{X}^T\hat{\mathbf{B}}_1\hat{\mathrm{e}} + \mathbf{U}^T\hat{\mathbf{B}}_2\hat{\mathrm{e}}\Big)^2 \\ &\quad + \Big(\hat{\boldsymbol{\beta}}_3 + \hat{\mathbf{B}}_1^T\mathbf{X} + \hat{\mathbf{B}}_2^T\mathbf{U}\Big)^T \sum_{\tilde{\mathbf{e}}} \Big(\hat{\boldsymbol{\beta}}_3 + \hat{\mathbf{B}}_1^T\mathbf{X} + \hat{\mathbf{B}}_2^T\mathbf{U}\Big) \\ &\quad + \Big(\hat{\boldsymbol{\beta}}_4 + \hat{\mathbf{B}}_3^T\mathbf{X} + \hat{\mathbf{B}}_4^T\mathbf{U}\Big)^T \sum_{\mathbf{n}} \Big(\hat{\boldsymbol{\beta}}_4 + \hat{\mathbf{B}}_3^T\mathbf{X} + \hat{\mathbf{B}}_4^T\mathbf{U}\Big) \\ &\quad + \sigma^2_{\tilde{\beta}_0} + \mathbf{X}^T\sum_{\tilde{\boldsymbol{\beta}}_1}\mathbf{X} + \mathbf{U}^T\sum_{\tilde{\boldsymbol{\beta}}_2}\mathbf{U} + \hat{\mathrm{e}}^{\mathbf{T}}\sum_{\tilde{\boldsymbol{\beta}}_3}\hat{\mathrm{e}} \\ &\quad + E_{\mathbf{n}}\left[\mathbf{n}^T\sum_{\tilde{\boldsymbol{\beta}}_4} n\right] + \mathrm{Var}_{\tilde{\boldsymbol{\beta}}}(\mathbf{X}^T\mathbf{B}_1\mathbf{e}) + \mathrm{Var}_{\tilde{\boldsymbol{\beta}}}(\mathbf{U}^T\mathbf{B}_2\mathbf{e}) \\ &\quad + E_{\mathbf{n}}[\mathrm{Var}_{\tilde{\boldsymbol{\beta}}}(\mathbf{X}^T\mathbf{B}_3\mathbf{n})] + E_{\mathbf{n}}[\mathrm{Var}_{\tilde{\boldsymbol{\beta}}}(\mathbf{U}^T\mathbf{B}_4\mathbf{n})] + \sigma^2_{\varepsilon}. \end{aligned} \tag{5}$$

The optimal controller should minimize $J_{\mathrm{APC}}(\mathbf{X},\mathbf{U}|\hat{\boldsymbol{\beta}}) = E_{\hat{\mathrm{e}}}[J_{\mathrm{APC}}(\mathbf{X},\mathbf{U}|\hat{\mathrm{e}},\hat{\boldsymbol{\beta}})]$, i.e., taking into account of all possible observations of noise factors. If constraints on the controllable factors are considered, this optimization problem can be written as

$$(\mathbf{X}^*,\mathbf{U}^*) = \arg\min_{\|\mathbf{X}\|_\infty \le \mathbf{1}, \|\mathbf{U}\|_\infty \le \mathbf{1}} J_{\mathrm{APC}}(\mathbf{X},\mathbf{U}|\hat{\boldsymbol{\beta}}) \tag{6}$$

where $\|\cdot\|_\infty$ is the maximum absolute row sum norm of the corresponding matrix, and $\mathbf{1}$ indicates the experimental region and constraints for the controllable variables.

Since $\mathbf{X}$ is the setting factor that cannot be adjusted during production, the following **two-step approach** is proposed to obtain an optimal solution to the optimization problem.

1) Solve the optimal control law of $\mathbf{U}^*$. The restricted solution is given as

$$\mathbf{U}^* = \arg\min_{\|\mathbf{U}\|_\infty \le \mathbf{1}} J_{\mathrm{APC}}(\mathbf{X},\mathbf{U}|\mathbf{X},\hat{\mathrm{e}},\hat{\boldsymbol{\beta}}). \tag{7}$$

A closed-form solution of $\mathbf{U}^* = h(\mathbf{X},\hat{\mathrm{e}},\hat{\boldsymbol{\beta}},\sum_{\tilde{\mathrm{e}}},\sum_{\mathbf{n}}\sum_{\tilde{\boldsymbol{\beta}}})$ can be obtained from (5) and (7) by solving the equation of $(\partial J_{\mathrm{APC}}(\mathbf{X},\mathbf{U}|\mathbf{X},\hat{\mathrm{e}},\hat{\boldsymbol{\beta}}))/(\partial\mathbf{U}) = 0$. However, this closed-form solution is a function of $\mathbf{X}$, and is not guaranteed to be within the constrained region. A numerical search for optimum should be employed under this situation using optimization methods such as DIRECT [11], [12], which will be illustrated in details in case study.

2) Minimize the quadratic loss at $\mathbf{U} = \mathbf{U}^*$ over the distribution of $\hat{\mathrm{e}}$. Thus, the constrained optimal setting of $\mathbf{X}^*$ can be obtained as

$$\mathbf{X}^* = \arg\min_{\|\mathbf{X}\|_\infty \le \mathbf{1}} E_{\hat{\mathrm{e}}}\{J_{\mathrm{APC}}(\mathbf{X},\mathbf{U}^*|\hat{\mathrm{e}},\hat{\boldsymbol{\beta}})\}. \tag{8}$$

TABLE I
FACTORS IN THE INJECTION MOLDING EXPERIMENT

Controllable Factors	
Off-Line (**X**)	*On-Line* (**U**)
x_1: Mold temperature x_2: Cavity thickness x_3: Gate size	U_1: Cycle time U_2: Holding pressure U_3: Injection speed u_4: Holding time
Noise Factors	
Measurable (**e**)	*Immeasurable* (**n**)
e_1: Moisture content e_2: Ambient temperature	n_1: Percentage reground

It should be noted that, the second step requires a direct plug-in of the closed-form solution of $\mathbf{U}^*$ obtained in the first step. Since it cannot be foreseen whether this solution falls into the constrain region or not before numerically solving it, this step might not lead to a globally optimal $\mathbf{X}^*$; however, the suboptimal performance is guaranteed as comparing to robust design. This is because the suboptimal is still the best solution in the feasible region, which includes the solution from robust design. The efficiency will be shown in the case study.

Then the control strategy can be implemented as

1) Offline set $\mathbf{X} = \mathbf{X}^*$ at the process setup stage.
2) Online adjust $\mathbf{U}$ to $\mathbf{U}^*$ according to observations during production.

If there are no measurement errors, i.e., $\sum_{\tilde{\mathrm{e}}}$ is zero, the corresponding control law becomes certainty equivalence control, which will be discussed in the following case study.

III. Injection Molding Process

A. Injection Process Description

Injection molding is widely used in the manufacturing of fabricated plastic products. The process is very complex due to the high degree of interaction of material, machine, and process variables [8].

In this experiment, percentage of shrinkage of the molded parts is determined as the quality response. The problem is considered as a nominal-the-best as discussed in Section II-B.

A designed experiment on this injection molding process was reported in [9]. The experiment consists of seven controllable factors and three noise factors as listed in Table I. The lowercase letters are used to denote the process variables in each set of factors.

For classification of the noise factors, percentage reground is considered immeasurable, since it is very costly to be measured during the process run. Ambient temperature can be easily measured; moisture content can be estimated through the measurements of ambient humidity and the amount of time the material is exposed to the air [2]. Thus, these two variables are considered measurable noise factors. The experiment design response values are shown in Table II, as presented in [10].

By fitting a straight line in the half-normal probability plot of all main effects and two-factor interactions (shown in Fig. 1), any effect or interaction whose corresponding point falls off the line is considered significant.

The estimated effects of all significant terms and some nonsignificant main effects (x_1, x_2, e_1 and n_1) are listed in Table III [6].

TABLE II
DESIGN AND RESPONSES FOR THE INJECTION MOLDING EXPERIMENT

Controllable Factors								Percent Shrinkage for Noise Factors n_1, e_1, e_2			
Cell	u_1	x_1	x_2	u_2	u_3	u_4	x_3	(-1,-1,-1)	(-1,+1,+1)	(+1,-1,+1)	(+1,+1,-1)
1	-1	-1	-1	-1	-1	-1	-1	2.2	2.1	2.3	2.3
2	-1	-1	-1	+1	+1	+1	+1	2.5	0.3	2.7	0.3
3	-1	+1	+1	-1	-1	+1	+1	0.5	3.1	0.4	2.8
4	-1	+1	+1	+1	+1	-1	-1	2.0	1.9	1.8	2.0
5	+1	-1	+1	-1	+1	-1	+1	3.0	3.1	3.0	3.0
6	+1	-1	+1	+1	-1	+1	-1	2.1	4.2	1.0	3.1
7	+1	+1	-1	-1	+1	+1	-1	4.0	1.9	4.6	2.2
8	+1	+1	-1	+1	-1	-1	+1	2.0	1.9	1.9	1.8

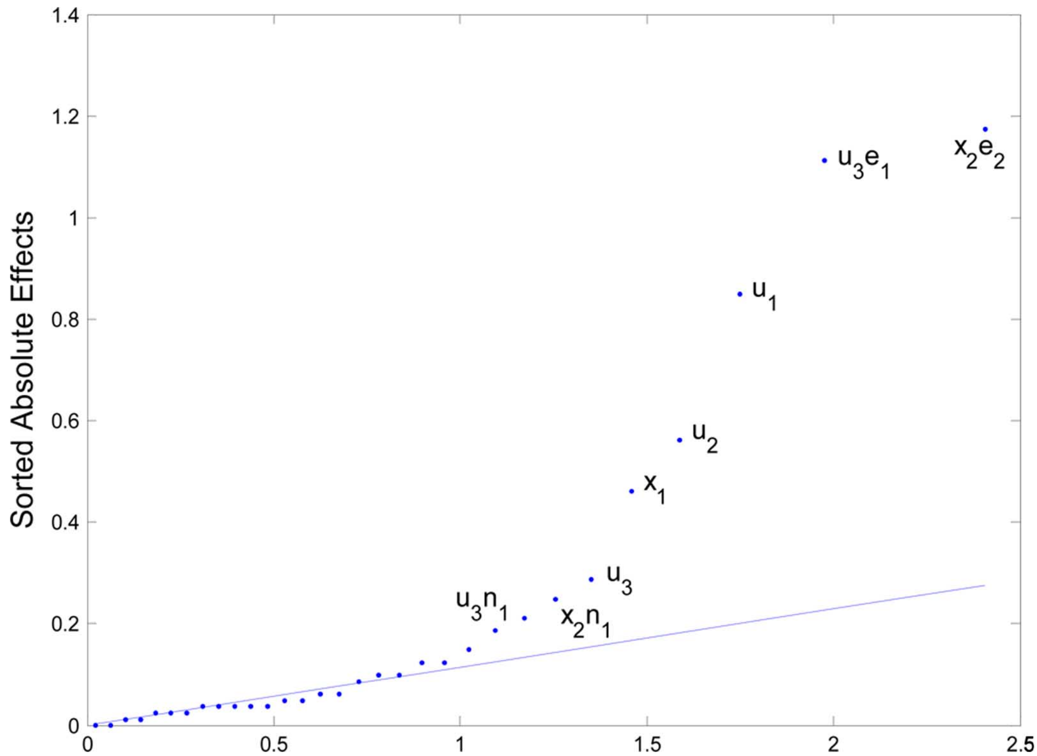

Fig. 1. Half-normal probability plot of main effects and interactions.

TABLE III
EFFECT ESTIMATES

Main Effects			
Effect	Estimate	Effect	Estimate
x_1	-0.150	u_2	-0.563
x_2	0.125	u_3	0.288
x_3	-0.463	e_1	0
u_1	0.850	n_1	-0.100
2-way Interactions			
Effect	Estimate	Effect	Estimate
$x_2\, e_1$	1.175	$x_2\, n_1$	-0.250
$u_3\, e_1$	-1.113	$u_2\, n_1$	-0.188
$x_1\, n_1$	0.125	$u_3\, n_1$	0.213

From the above results, the following model can be obtained:

$$\begin{aligned} y = \beta_0 + \boldsymbol{\beta}_1^T \mathbf{X} + \boldsymbol{\beta}_2^T \mathbf{U} + \beta_3 e_1 + \beta_4 n_1 \\ + \mathbf{X}^T \mathbf{B}_1 e_1 + \mathbf{U}^T \mathbf{B}_2 e_1 \\ + \mathbf{X}^T \mathbf{B}_3 n_1 + \mathbf{U}^T \mathbf{B}_4 n_1 + \varepsilon \end{aligned} \tag{9}$$

where $\mathbf{X} = [x_1, x_2, x_3]^T$ and $\mathbf{U} = [u_1, u_2, u_3, u_4]^T$. Estimated model parameters are $\beta_0 = 2.25, \boldsymbol{\beta}_1^T = [-0.075\ 0.063\ -0.232], \boldsymbol{\beta}_2^T = [0.425\ -0.282\ 0.144], \beta_3 = 0, \beta_4 = -0.05, \mathbf{B}_1^T = [0\ 0.588\ 0]$, $\mathbf{B}_2^T = [0\ 0\ -0.557], \mathbf{B}_3^T = [0.063\ -0.125\ 0]$, and $\mathbf{B}_4^T = [0\ -0.094\ 0.106]$. Other controllable factors not appearing in the model can be set according to economic advantages during the production. The uncertainty of estimated model parameters $\Sigma_{\tilde{\boldsymbol{\beta}}}$ is $4.084 \cdot 10^{-4} \times \mathbf{I}^{21\times 21}$, as can be obtained as a standard output of statistical regression process.

B. Implemented Process Control Strategies

This section first develops the robust parameter design and the optimal control scheme for the injection molding. They will be implemented under both the cautious control strategy and certainty equivalence control strategy in the next section.

1) Robust Parameter Design: According to the transmitted variance model approach in [7], the variance of $\hat{y}$ is

$$\begin{aligned} \mathrm{Var}(\hat{y}) = (-0.05 + 0.0625x_1 - 0.125x_2 - 0.0938u_2 \\ + 0.1063u_3)^2\sigma_{n_1}^2 + (0.5875x_2 - 0.5563u_3)^2\sigma_{e_1}^2. \end{aligned} \tag{10}$$

To minimize the transmitted variance $\mathrm{Var}(\hat{y})$ over the experimental region, the robust settings can be obtained

TABLE IV
SETTINGS OF FACTOR u_1 AND x_3 IN TERMS OF PERCENT SHRINKAGE

Percent shrinkage t	Factor u_1^*	Factor x_3^*
≤1.85	-1	1
(1.85, 2.25]	-1	-1
(2.25, 2.70]	1	1
>2.70	1	-1

as $(x_1, x_2, u_2, u_3) = (0.4664, 0, -0.2222, 0)$ by solving a quadratic problem for continuous x_i's and u_i's. Factors u_1 and x_3 are significant effects in the response model but not in the transmitted variance model, so they are set to values between -1 and $+1$ to bring the expected response close to target value, which means

$$\mathbf{X}^* = [0.4664 \quad 0 \quad x_3^*]^T$$
$$\mathbf{U}^* = [u_1^* \quad -0.2222 \quad 0]^T \tag{11}$$

where u_1 and x_3 are given in Table IV, based on different target value (percent shrinkage) t [6].

2) Optimal Control: The model (9) has one measurable noise factor e_1 and one immeasurable noise factor n_1. Assuming the variance of the immeasurable noise factor n_1 is $\sigma_{n_1}^2$ and the measurement uncertainty of the measurable noise factor e_1 is $\sigma_{\tilde{e}_1}^2$, the objective loss function for this application example becomes

$$\begin{aligned} J_{\mathrm{APC}}&(\mathbf{X}, \mathbf{U}|\hat{e}_1, \hat{\boldsymbol{\beta}}) \\ &= \Big(\hat{\beta}_0 - t + \hat{\boldsymbol{\beta}}_1^T\mathbf{X} + \hat{\boldsymbol{\beta}}_2^T\mathbf{U} \\ &\quad + \hat{\beta}_3^T\hat{e}_1 + \mathbf{X}^T\hat{\mathbf{B}}_1\hat{e}_1 + \mathbf{U}^T\hat{\mathbf{B}}_2\hat{e}_1\Big)^2 \\ &\quad + \left(\hat{\beta}_3 + \hat{\mathbf{B}}_1^T\mathbf{X} + \hat{\mathbf{B}}_2^T\mathbf{U}\right)^T \sum_{\tilde{e}_1}\left(\hat{\beta}_3 + \hat{\mathbf{B}}_1^T\mathbf{X} + \hat{\mathbf{B}}_2^T\mathbf{U}\right) \\ &\quad + \left(\hat{\beta}_4 + \hat{\mathbf{B}}_3^T\mathbf{X} + \hat{\mathbf{B}}_4^T\mathbf{U}\right)^T \sum_{n_1}\left(\hat{\beta}_4 + \hat{\mathbf{B}}_3^T\mathbf{X} + \hat{\mathbf{B}}_4^T\mathbf{U}\right) \\ &\quad + \sigma_{\tilde{\beta}_0}^2 + \mathbf{X}^T\sum_{\tilde{\boldsymbol{\beta}}_1}\mathbf{X} + \mathbf{U}^T\sum_{\tilde{\boldsymbol{\beta}}_2}\mathbf{U} + \hat{e}_1^2\sigma_{\tilde{\beta}_3}^2 + \sigma_{n_1}^2\sigma_{\tilde{\beta}_4}^2 \\ &\quad + \hat{e}_1^2\mathbf{X}^T\sum_{\tilde{\mathbf{B}}_1}\mathbf{X} + \hat{e}_1^2\mathbf{U}^T\sum_{\tilde{\mathbf{B}}_2}\mathbf{U} + \sigma_{n_1}^2\mathbf{X}^T\sum_{\tilde{\mathbf{B}}_3}\mathbf{X} \\ &\quad + \sigma_{n_1}^2\mathbf{U}^T\sum_{\tilde{\mathbf{B}}_4}\mathbf{U} + \sigma_\varepsilon^2. \end{aligned} \tag{12}$$

Thus, the closed-form control law of $\mathbf{U}^*$ can be obtained as a function of $\mathbf{X}$ (see Appendix B for details)

$$\begin{aligned} \mathbf{U}^* = -&\left\{(\hat{\boldsymbol{\beta}}_2 + \hat{\mathbf{B}}_2\hat{e}_1)(\hat{\boldsymbol{\beta}}_2 + \hat{\mathbf{B}}_2\hat{e}_1)^T + \hat{\mathbf{B}}_2\sigma_{\tilde{e}_1}^2\hat{\mathbf{B}}_2^T \right. \\ &\left. + \hat{\mathbf{B}}_4\sigma_{n_1}^2\hat{\mathbf{B}}_4^T + \sum_{\tilde{\boldsymbol{\beta}}_2}^2 + \hat{e}_1^2\sum_{\tilde{\mathbf{B}}_2} + \sigma_{n_1}^2\sum_{\tilde{\mathbf{B}}_4}\right\}^{-1} \\ &\cdot\left\{\left(\hat{\beta}_0 - t + \hat{\boldsymbol{\beta}}_1^T\mathbf{X} + \hat{\beta}_3^T\hat{e}_1 + \mathbf{X}^T\hat{\mathbf{B}}_1\hat{e}_1\right)(\hat{\boldsymbol{\beta}}_2 + \hat{\mathbf{B}}_2\hat{e}_1) \right. \\ &\left. + \hat{\mathbf{B}}_2\sigma_{\tilde{e}_1}^2\left(\hat{\boldsymbol{\beta}}_3 + \hat{\mathbf{B}}_1^T\mathbf{X}\right) + \hat{\mathbf{B}}_4\sigma_{n_1}^2\left(\hat{\boldsymbol{\beta}}_4 + \hat{\mathbf{B}}_3^T\mathbf{X}\right)\right\}. \end{aligned} \tag{13}$$

As aforementioned, the optimal setting $\mathbf{X}^*$ can be obtained by first substituting the optimal $\mathbf{U}^* = [u_1^* \quad u_2^* \quad u_3^*]^T$ as (13) into the quadratic loss function (12), and then minimizing (12) by integrating over the distribution of e_1.

C. Case Study

A simulated case study is conducted here to evaluate and compare the performance of 1) robust parameter design, 2) control law proposed by [6], and 3) online cautious process control developed in this paper.

The residual term ε in model (9) represents the model accuracy, which is determined by the DOE model structure, factor test levels, effect de-aliasing, sensitivity analysis, and parameter estimation methods. Therefore, reduction of the model residual can only be obtained by improved designed experiments and/or modeling algorithms. A control strategy alone cannot reduce the variation contributed by the residual noise in the model. Thus, the following performance evaluation will compare only the response value of the predicted model without considering the regression residual ε, nor the residual variance σ_ε^2.

The optimization problems were solved by using DIRECT, an algorithm that is able to search the global minimum of a multivariate function subject to simple bounds on the variables [11], [12]. The optimization was carried out by using Matlab.

If the measurement uncertainty $\sum_{\tilde{\mathbf{e}}}$ is considered, the optimal control law is known as "cautious control (CC) law" [6]. The basic idea is that magnitudes of the controllable factors adjustments consider both the estimated noise factor levels and the covariance of the estimator errors. When the measurement errors $\tilde{\mathbf{e}}$ is not considered, i.e., $\sum_{\tilde{\mathbf{e}}} = \mathbf{0}$, the designed controller is known as "certainty equivalence (CE) control." Furthermore, if a controller does not consider the model parameter estimation error, nor the measurement error, it is a traditional APC controller.

The process performances of robust parameter design and online process control are compared, and APC is carried out under cautious control, certainty equivalence control and traditional control.

In this simulation study, both n_1 and e_1 are assumed to follow zero-mean normal distributions with variance of 0.25, i.e., $n_1 \sim \mathrm{N}(0, 0.25), e_1 \sim \mathrm{N}(0, 0.25)$. Thus, 95% of the random noises will fall in the region of $[-1, 1]$. $\hat{e}_1$ is the measurement of e_1 with certain observation errors, and the performance of the control laws are compared under different levels of noise estimation uncertainties. The model parameter uncertainties are set to $4.084 \cdot 10^{-4}$, which is obtained from the deigned experiment data.

Fig. 2 shows the comparison of the performances of different controllers. The horizontal axis of the figure is the ratio of uncertainty of sensor noise $(\sigma_{\tilde{e}_1})$ to that of measurable noise factor (σ_{e_1}). The vertical axis is the ratio between controller performances and robust design performance $(J_{\mathrm{APC}}/J_{\mathrm{RPD}})$, and thus a value smaller than 1 indicates a preference of employing the corresponding APC strategy at that noise level. The figure shows that robust design is outperformed by both control strategies at a lower noise level, since it ignores the uncertainties of model parameter estimation and observation. However, CE control works well only if there is no (or small) estimation errors. As the uncertainties get larger, $(\sigma_{\tilde{e}_1}/\sigma_{e_1} > 0.24$ in this study), the CE

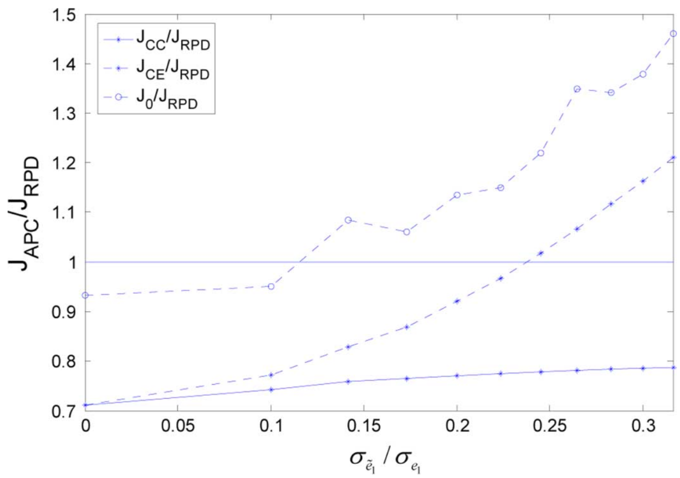

Fig. 2. Comparison of variability of $\hat{y}$ under RPD and APC Strategies.

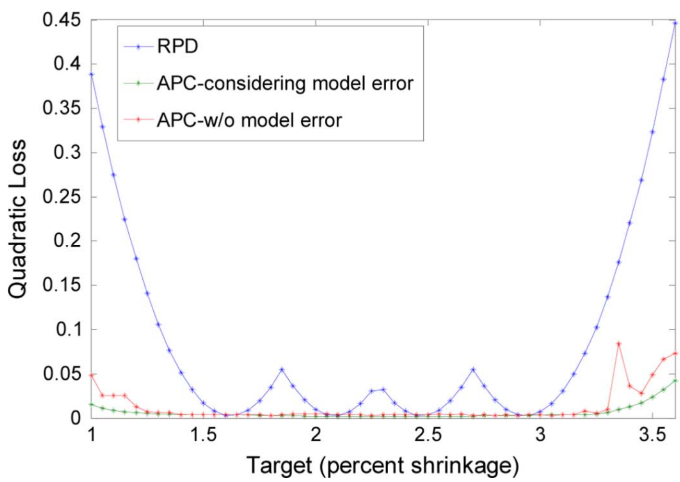

Fig. 3. Comparison of quadratic losses of the three approaches.

controller deteriorates and performs worse than the RPD. While a CC further considers the observation uncertainty and is "cautious" about each control action it takes; thus, its performance is better than the RPD until a large noise level.

The control performances for different target values are also compared, as shown in Fig. 3. The horizontal axis indicates that the comparison of the performances is carried out under shrinkage percentages ranging from 1% to 3.6%. This range contains the designed experimental range, within which the correctness of the DOE regression model can be ensured. The vertical axis in Fig. 3 represents the performances (or quadratic loss) under different control strategies. The peaks of the RPD are resulted from the adjustment of u_1 and x_3 according to different target regions.

A closer look of Fig. 3 indicates that 1) the control performance is improved by considering modeling error; and 2) the control performance is still acceptable when other strategies are not functioning properly. It is also observed that the controller performance gets worse closer to the edge of target range. This performance deterioration is because the optimal controlled solution is close to being out of the experimental region and needs to be set to the boundary, which greatly decreases the control efficiency.

Fig. 4 provides a zoom-in comparison from Fig. 3. This figure focuses on the two APC control strategies, ranging from 2.0%

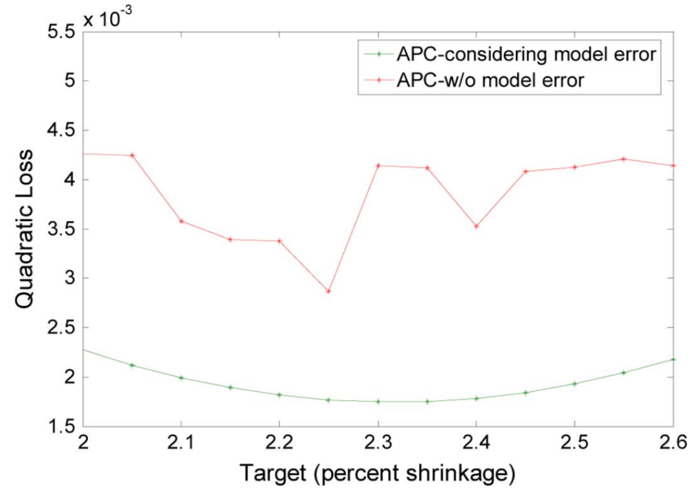

Fig. 4. Comparison of quadratic losses of two APC.

to 2.6%, which is in the center of the previously mentioned working range of controllers. This closer look clearly shows that APC with consideration of modeling errors is consistently better than that without considering them.

IV. Conclusion

An automatic process control strategy is developed based on regression models obtained from design of experiments. The control strategy takes into account modeling and observation uncertainties and demonstrated superior performance when the uncertainties are large. The performances of the proposed control strategy and existing control approaches have been compared via a case study on an injection molding process. Generally, the proposed strategy can significantly improve the control performance by considering in-process observation of noise factors and errors in parameter estimation. The comparison study also indicates that the certainty equivalence control provides better performance than robust design when online sensing uncertainties are small.

There are some open issues to be addressed in the future research. Some examples of those topics include 1) increasing the model (3) complexity by including high interaction terms among control variables and noise variables, 2) considering model uncertainties due to model structure errors, and 3) investigating the sensitivity of the control performance to the model assumptions. More efforts are needed to consider the integrated system modeling and control to achieve better control performance.

Appendix A

Proof of (5): Consider the quadratic loss function $L(y,t) = [y-t]^2$. The objective function is

$$\begin{aligned} &J_{\rm APC}(\mathbf{X},\mathbf{U}|\hat{\mathbf{e}},\hat{\boldsymbol{\beta}}) \\ &\quad = E_{\mathbf{e},\mathbf{n},\tilde{\boldsymbol{\beta}},\varepsilon}[L(y,t)|\hat{\mathbf{e}},\hat{\boldsymbol{\beta}}] \\ &\quad = E_{\mathbf{e},\mathbf{n},\tilde{\boldsymbol{\beta}},\varepsilon}[(y|\hat{\mathbf{e}},\hat{\boldsymbol{\beta}}) - t]^2 \\ &\quad = (E_{\mathbf{e},\mathbf{n},\tilde{\boldsymbol{\beta}},\varepsilon}[y|\hat{\mathbf{e}},\hat{\boldsymbol{\beta}}] - t)^2 + {\rm Var}_{\mathbf{e},\mathbf{n},\tilde{\boldsymbol{\beta}},\varepsilon}(y|\hat{\mathbf{e}},\hat{\boldsymbol{\beta}}). \end{aligned} \quad (14)$$

Plugging in the response model (3), the two items in (14) become

$$\begin{aligned}
&E_{\mathbf{e},\mathbf{n},\tilde{\boldsymbol{\beta}},\varepsilon}[y|\hat{\mathbf{e}},\hat{\boldsymbol{\beta}}]\\
&\quad= E_{\mathbf{e},\mathbf{n},\tilde{\boldsymbol{\beta}},\varepsilon}\Big[\beta_0+\boldsymbol{\beta}_1^T\mathbf{X}+\boldsymbol{\beta}_2^T\mathbf{U}+\boldsymbol{\beta}_3^T\mathbf{e}+\boldsymbol{\beta}_4^T\mathbf{n}\\
&\qquad+\mathbf{X}^T\mathbf{B}_1\mathbf{e}+\mathbf{U}^T\mathbf{B}_2\mathbf{e}+\mathbf{X}^T\mathbf{B}_3\mathbf{n}\\
&\qquad+\mathbf{U}^T\mathbf{B}_4\mathbf{n}+\varepsilon|\hat{\mathbf{e}},\hat{\boldsymbol{\beta}}\Big]\\
&\quad=\hat{\beta}_0+\hat{\boldsymbol{\beta}}_1^T\mathbf{X}+\hat{\boldsymbol{\beta}}_2^T\mathbf{U}\\
&\qquad+E_{\mathbf{e}}\Big[\boldsymbol{\beta}_3^T\mathbf{e}|\hat{\mathbf{e}},\hat{\boldsymbol{\beta}}\Big]+E_{\mathbf{e}}[\mathbf{X}^T\mathbf{B}_1\mathbf{e}|\hat{\mathbf{e}},\hat{\boldsymbol{\beta}}]\\
&\qquad+E_{\mathbf{e}}[\mathbf{U}^T\mathbf{B}_2\mathbf{e}|\hat{\mathbf{e}},\hat{\boldsymbol{\beta}}]\\
&\quad=\hat{\beta}_0+\hat{\boldsymbol{\beta}}_1^T\mathbf{X}+\hat{\boldsymbol{\beta}}_2^T\mathbf{U}+\hat{\boldsymbol{\beta}}_3^T\hat{\mathbf{e}}\\
&\qquad+\mathbf{X}^T\hat{\mathbf{B}}_1\hat{\mathbf{e}}+\mathbf{U}^T\hat{\mathbf{B}}_2\hat{\mathbf{e}},\\
&\mathrm{Var}_{\mathbf{e},\mathbf{n},\tilde{\boldsymbol{\beta}},\varepsilon}(y|\hat{\mathbf{e}},\hat{\boldsymbol{\beta}})\\
&\quad=E_{\mathbf{n}}(\mathrm{Var}_{\mathbf{e},\tilde{\boldsymbol{\beta}},\varepsilon}[y|\hat{\mathbf{e}},\hat{\boldsymbol{\beta}},\mathbf{n}])\\
&\qquad+\mathrm{Var}_{\mathbf{n}}(E_{\mathbf{e},\tilde{\boldsymbol{\beta}},\varepsilon}[y|\hat{\mathbf{e}},\hat{\boldsymbol{\beta}},\mathbf{n}]).
\end{aligned}\tag{15}$$

For (15)

$$\begin{aligned}
&\mathrm{Var}_{\mathbf{n}}\{E_{\mathbf{e},\tilde{\boldsymbol{\beta}},\varepsilon}[y|\hat{\mathbf{e}},\hat{\boldsymbol{\beta}},\mathbf{n}]\}\\
&\quad=\mathrm{Var}_{\mathbf{n}}\Big\{\hat{\beta}_0+\hat{\boldsymbol{\beta}}_1^T\mathbf{X}+\hat{\boldsymbol{\beta}}_2^T\mathbf{U}+\hat{\boldsymbol{\beta}}_3^T\hat{\mathbf{e}}+\hat{\boldsymbol{\beta}}_4^T\mathbf{n}\\
&\qquad+\mathbf{X}^T\hat{\mathbf{B}}_1\hat{\mathbf{e}}+\mathbf{U}^T\hat{\mathbf{B}}_2\hat{\mathbf{e}}+\mathbf{X}^T\hat{\mathbf{B}}_3\mathbf{n}+\mathbf{U}^T\hat{\mathbf{B}}_4\mathbf{n}\Big\}\\
&\quad=\Big(\hat{\boldsymbol{\beta}}_4+\hat{\mathbf{B}}_3^T\mathbf{X}+\hat{\mathbf{B}}_4^T\mathbf{U}\Big)^T\sum_{\mathbf{n}}\Big(\hat{\boldsymbol{\beta}}_4+\hat{\mathbf{B}}_3^T\mathbf{X}+\hat{\mathbf{B}}_4^T\mathbf{U}\Big),\\
&E_{\mathbf{n}}\{\mathrm{Var}_{\mathbf{e},\tilde{\boldsymbol{\beta}},\varepsilon}(y|\hat{\mathbf{e}},\hat{\boldsymbol{\beta}},\mathbf{n})\}\\
&\quad=E_{\mathbf{n}}\{E_{\mathbf{e}}[\mathrm{Var}_{\tilde{\boldsymbol{\beta}},\varepsilon}(y|\hat{\mathbf{e}},\hat{\boldsymbol{\beta}},\mathbf{n},\tilde{\mathbf{e}})]\\
&\qquad+\mathrm{Var}_{\mathbf{e}}[E_{\tilde{\boldsymbol{\beta}},\varepsilon}(y|\hat{\mathbf{e}},\hat{\boldsymbol{\beta}},\mathbf{n},\tilde{\mathbf{e}})]\}\\
&\quad=E_{\mathbf{n}}\Bigg\{E_{\mathbf{e}}\Bigg[\sigma_\varepsilon^2+\sum_{\tilde{\beta}_0}+\mathbf{X}^T\sum_{\tilde{\boldsymbol{\beta}}_1}\mathbf{X}+\mathbf{U}^T\sum_{\tilde{\boldsymbol{\beta}}_2}\mathbf{U}\\
&\qquad+\mathbf{e}^T\sum_{\tilde{\boldsymbol{\beta}}_3}\mathbf{e}+\mathbf{n}^T\sum_{\tilde{\boldsymbol{\beta}}_4}\mathbf{n}\\
&\qquad+\mathrm{Var}_{\tilde{\boldsymbol{\beta}}}(\mathbf{X}^T\mathbf{B}_1\mathbf{e})+\mathrm{Var}_{\tilde{\boldsymbol{\beta}}}(\mathbf{U}^T\mathbf{B}_2\mathbf{e})\\
&\qquad+\mathrm{Var}_{\tilde{\boldsymbol{\beta}}}(\mathbf{X}^T\mathbf{B}_3\mathbf{n})+\mathrm{Var}_{\tilde{\boldsymbol{\beta}}}(\mathbf{U}^T\mathbf{B}_4\mathbf{n})\Bigg]\\
&\qquad+\mathrm{Var}_{\mathbf{e}}\Big[\hat{\beta}_0+\hat{\boldsymbol{\beta}}_1^T\mathbf{X}+\hat{\boldsymbol{\beta}}_2^T\mathbf{U}\\
&\qquad+\hat{\boldsymbol{\beta}}_3^T\hat{\mathbf{e}}+\hat{\boldsymbol{\beta}}_4^T\mathbf{n}+\mathbf{X}^T\hat{\mathbf{B}}_1\hat{\mathbf{e}}\\
&\qquad+\mathbf{U}^T\hat{\mathbf{B}}_2\hat{\mathbf{e}}+\mathbf{X}^T\hat{\mathbf{B}}_3\mathbf{n}+\mathbf{U}^T\hat{\mathbf{B}}_4\mathbf{n}\Big]\Bigg\}\\
&\quad=\sigma_\varepsilon^2+\sum_{\tilde{\beta}_0}+X^T\sum_{\tilde{\boldsymbol{\beta}}_1}X+\mathbf{U}^T\sum_{\tilde{\boldsymbol{\beta}}_2}\mathbf{U}\\
&\qquad+\hat{\mathbf{e}}^T\sum_{\tilde{\boldsymbol{\beta}}_3}\hat{\mathbf{e}}+E_{\mathbf{n}}\Bigg[\mathbf{n}^T\sum_{\tilde{\boldsymbol{\beta}}_4}\mathbf{n}\Bigg]\\
&\qquad+\mathrm{Var}_{\tilde{\boldsymbol{\beta}}}(\mathbf{X}^T\mathbf{B}_1\mathbf{e})+\mathrm{Var}_{\tilde{\boldsymbol{\beta}}}(\mathbf{U}^T\mathbf{B}_2\mathbf{e})\\
&\qquad+E_{\mathbf{n}}[\mathrm{Var}_{\tilde{\boldsymbol{\beta}}}(\mathbf{X}^T\mathbf{B}_3\mathbf{n})]\\
&\qquad+E_{\mathbf{n}}[\mathrm{Var}_{\tilde{\boldsymbol{\beta}}}(\mathbf{U}^T\mathbf{B}_4\mathbf{n})]\\
&\qquad+\Big(\hat{\boldsymbol{\beta}}_3+\hat{\mathbf{B}}_1^T\mathbf{X}+\hat{\mathbf{B}}_2^T\mathbf{U}\Big)^T\sum_{\tilde{\mathbf{e}}}\Big(\hat{\boldsymbol{\beta}}_3+\hat{\mathbf{B}}_1^T\mathbf{X}+\hat{\mathbf{B}}_2^T\mathbf{U}\Big).
\end{aligned}\tag{16}$$

(16) holds since $\mathrm{Cov}(\mathbf{e}|\hat{\mathbf{e}})=\mathrm{Cov}(\tilde{\mathbf{e}}|\hat{\mathbf{e}})+\mathrm{Cov}(\hat{\mathbf{e}}|\hat{\mathbf{e}})=\sum_{\tilde{\mathbf{e}}}$.

Thus, the expected quadratic loss function is given by

$$\begin{aligned}
&J_{\mathrm{APC}}(\mathbf{X},\mathbf{U}|\hat{\mathbf{e}},\hat{\boldsymbol{\beta}})\\
&\quad=\sigma_\varepsilon^2+\Big(\hat{\beta}_0-t+\hat{\boldsymbol{\beta}}_1^T\mathbf{X}+\hat{\boldsymbol{\beta}}_2^T\mathbf{U}\\
&\qquad+\Big(\hat{\boldsymbol{\beta}}_3^T+\mathbf{X}^T\hat{\mathbf{B}}_1+\mathbf{U}^T\hat{\mathbf{B}}_2\Big)\hat{\mathbf{e}}\Big)^2\\
&\qquad+\Big(\hat{\boldsymbol{\beta}}_3+\hat{\mathbf{B}}_1^T\mathbf{X}+\hat{\mathbf{B}}_2^T\mathbf{U}\Big)^T\Sigma_{\tilde{\mathbf{e}}}\Big(\hat{\boldsymbol{\beta}}_3+\hat{\mathbf{B}}_1^T\mathbf{X}+\hat{\mathbf{B}}_2^T\mathbf{U}\Big)\\
&\qquad+\Big(\hat{\boldsymbol{\beta}}_4+\hat{\mathbf{B}}_3^T\mathbf{X}+\hat{\mathbf{B}}_4^T\mathbf{U}\Big)^T\Sigma_{\mathbf{n}}\Big(\hat{\boldsymbol{\beta}}_4+\hat{\mathbf{B}}_3^T\mathbf{X}+\hat{\mathbf{B}}_4^T\mathbf{U}\Big)\\
&\qquad+\sigma_{\tilde{\beta}_0}^2+\mathbf{X}^T\Sigma_{\tilde{\boldsymbol{\beta}}_1}\mathbf{X}+\mathbf{U}^T\Sigma_{\tilde{\boldsymbol{\beta}}_2}\mathbf{U}\\
&\qquad+\hat{\mathbf{e}}^T\Sigma_{\tilde{\boldsymbol{\beta}}_3}\hat{\mathbf{e}}+E_{\mathbf{n}}\Big[\mathbf{n}^T\Sigma_{\tilde{\boldsymbol{\beta}}_4}\mathbf{n}\Big]\\
&\qquad+\mathrm{Var}_{\tilde{\boldsymbol{\beta}}}(\mathbf{X}^T\mathbf{B}_1\mathbf{e})+\mathrm{Var}_{\tilde{\boldsymbol{\beta}}}(\mathbf{U}^T\mathbf{B}_2\mathbf{e})\\
&\qquad+E_{\mathbf{n}}[\mathrm{Var}_{\tilde{\boldsymbol{\beta}}}(\mathbf{X}^T\mathbf{B}_3\mathbf{n})]\\
&\qquad+E_{\mathbf{n}}[\mathrm{Var}_{\tilde{\boldsymbol{\beta}}}(\mathbf{U}^T\mathbf{B}_4\mathbf{n})].
\end{aligned}$$

This proves (5).

Appendix B

Proof of (13): From (12), take the first-order partial derivative of $J_{\mathrm{APC}}(\mathbf{X},\mathbf{U}|\mathbf{X},\hat{e}_1,\hat{\boldsymbol{\beta}})$ on $\mathbf{U}$ and set it zero

$$\begin{aligned}
&\frac{\partial J_{\mathrm{APC}}(\mathbf{X},\mathbf{U}|\mathbf{X},\hat{e}_1,\hat{\boldsymbol{\beta}})}{\partial\mathbf{U}}\\
&\quad=2\Big(\beta_0-t+\hat{\boldsymbol{\beta}}_1^T\mathbf{X}+\hat{\beta}_3^T\hat{e}_1+\mathbf{X}^T\hat{\mathbf{B}}_1\hat{e}_1\Big)(\hat{\boldsymbol{\beta}}_2+\hat{\mathbf{B}}_2\hat{e}_1)\\
&\qquad+2(\hat{\boldsymbol{\beta}}_2+\hat{\mathbf{B}}_2\hat{e}_1)(\hat{\boldsymbol{\beta}}_2+\hat{\mathbf{B}}_2\hat{e}_1)^T\mathbf{U}\\
&\qquad+2\sigma_{n_1}^2\hat{\mathbf{B}}_4\Big(\hat{\beta}_4+\hat{\mathbf{B}}_3^T\mathbf{X}\Big)+2\Big(\hat{\mathbf{B}}_4\sigma_{n_1}^2\hat{\mathbf{B}}_4^T\Big)\mathbf{U}\\
&\qquad+2\sigma_{\tilde{e}_1}^2\hat{\mathbf{B}}_2\Big(\hat{\beta}_3+\hat{\mathbf{B}}_1^T\mathbf{X}\Big)+2\Big(\hat{\mathbf{B}}_2\sigma_{\tilde{e}_1}^2\hat{\mathbf{B}}_2^T\Big)\mathbf{U}\\
&\qquad+2\mathrm{Var}\Big(\hat{\boldsymbol{\beta}}_2^T\mathbf{U}\Big)+2\hat{e}_1^2\mathrm{Var}\Big(\hat{\mathbf{B}}_2^T\mathbf{U}\Big)\\
&\qquad+2\sigma_{n_1}^2\mathrm{Var}\Big(\hat{\mathbf{B}}_4^T\mathbf{U}\Big)\\
&\quad=0.
\end{aligned}$$

It follows that if $(\hat{\boldsymbol{\beta}}_2 + \hat{\mathbf{B}}_2\hat{\mathbf{e}})(\hat{\boldsymbol{\beta}}_2 + \hat{\mathbf{B}}_2\hat{\mathbf{e}})^T + \hat{\mathbf{B}}_2\sigma^2_{\tilde{e}_1}\hat{\mathbf{B}}_2^T + \hat{\mathbf{B}}_4\sigma^2_{n_1}\hat{\mathbf{B}}_4^T + \sum_{\tilde{\boldsymbol{\beta}}_2}^2 + \hat{e}_1^2\sum_{\tilde{\mathbf{B}}_2} + \sigma^2_{n_1}\sum_{\widehat{\mathbf{B}}_4}$ is invertible

$$\mathbf{U}^* = -\left\{(\hat{\boldsymbol{\beta}}_2 + \hat{\mathbf{B}}_2\hat{e}_1)(\hat{\boldsymbol{\beta}}_2 + \hat{\mathbf{B}}_2\hat{e}_1)^T + \hat{\mathbf{B}}_2\sigma^2_{\tilde{e}_1}\hat{\mathbf{B}}_2^T + \hat{\mathbf{B}}_4\sigma^2_{n_1}\hat{\mathbf{B}}_4^T + \sum_{\tilde{\boldsymbol{\beta}}_2}^{2} + \hat{e}_1^2\sum_{\tilde{\mathbf{B}}_2} + \sigma^2_{n_1}\sum_{\tilde{\mathbf{B}}_4}\right\}^{-1} \cdot \left\{\left(\hat{\beta}_0 - t + \hat{\boldsymbol{\beta}}_1^T\mathbf{X} + \hat{\beta}_3^T\hat{e}_1 + \mathbf{X}^T\hat{\mathbf{B}}_1\hat{e}_1\right) \times (\hat{\boldsymbol{\beta}}_2 + \hat{\mathbf{B}}_2\hat{e}_1) + \hat{\mathbf{B}}_2\sigma^2_{\tilde{e}_1}(\hat{\beta}_3 + \hat{\mathbf{B}}_1^T\mathbf{X}) + \hat{\mathbf{B}}_4\sigma^2_{n_1}(\hat{\beta}_4 + \hat{\mathbf{B}}_3^T\mathbf{X})\right\}.$$

This proves (13).

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