Supplementary

1. Proof of eq. (7) and eq. (9)

In this section, we have suppressed the conditioning over $\boldsymbol{\rho}, \boldsymbol{Z}$ and $\boldsymbol{Z}^\star$ for brevity. Since $\boldsymbol{Y}|\boldsymbol{A} \sim N(\boldsymbol{\mu} + \boldsymbol{\Phi}\boldsymbol{A}, \sigma_\varepsilon^2 \mathbb{I})$ and $\boldsymbol{A} \sim N(\boldsymbol{0}, \boldsymbol{K}(\boldsymbol{Z}, \boldsymbol{Z}))$, we can show that the posterior distribution $\boldsymbol{A}|\boldsymbol{Y}$ also follows the multivariate Gaussian distribution:

$$\boldsymbol{A}|\boldsymbol{Y} \sim N(\boldsymbol{\mu}^{\star(2)}, \boldsymbol{\Sigma}^{\star(2)}),$$

where $\boldsymbol{\mu}^{\star(2)} = \boldsymbol{\Sigma}^{\star(2)} \left(\frac{1}{\sigma_\varepsilon^2} \boldsymbol{\Phi}^T (\boldsymbol{Y} - \boldsymbol{\mu}) \right)$ and $\boldsymbol{\Sigma}^{\star(2)} = \left(\frac{1}{\sigma_\varepsilon^2} \boldsymbol{\Phi}^T \boldsymbol{\Phi} + \boldsymbol{K}^{-1} \right)^{-1}$. Following the definition of GP, FPC scores of any finite number of subjects have a joint Gaussian distribution. Specifically, the FPC scores of the historical subjects $\boldsymbol{A}$ and those of a new subject $\boldsymbol{A}^\star$ have a joint Gaussian distribution:

$$\begin{pmatrix} \boldsymbol{A}^\star \\ \boldsymbol{A} \end{pmatrix} \sim N\left(\boldsymbol{0}, \begin{bmatrix} \boldsymbol{K}^{\star\star} & \boldsymbol{K}^\star \\ \boldsymbol{K}^{\star T} & \boldsymbol{K} \end{bmatrix} \right),$$

Since $p(\boldsymbol{A}^\star|\boldsymbol{A}) = p(\boldsymbol{A}^\star, \boldsymbol{A})/p(\boldsymbol{A})$, we can show that $\boldsymbol{A}^\star|\boldsymbol{A} \sim N(\boldsymbol{\mu}', \boldsymbol{\Sigma}')$, where $\boldsymbol{\mu}' = \boldsymbol{K}^\star \boldsymbol{K}^{-1} \boldsymbol{A}$ and $\boldsymbol{\Sigma}' = \boldsymbol{K}^{\star\star} - \boldsymbol{K}^\star \boldsymbol{K}^{-1} \boldsymbol{K}^{\star T}$. Marginalizing as $p(\boldsymbol{A}^\star|\boldsymbol{Y}) = \int p(\boldsymbol{A}^\star|\boldsymbol{A}) p(\boldsymbol{A}|\boldsymbol{Y}) d\boldsymbol{A}$, we can further prove that

$$\boldsymbol{A}^\star|\boldsymbol{Y} \sim N(\boldsymbol{\mu}^\star, \boldsymbol{\Sigma}^\star),$$

with parameters, $\boldsymbol{\mu}^\star = \boldsymbol{K}^\star \boldsymbol{K}^{-1} \boldsymbol{\mu}^{\star(2)}$ and $\boldsymbol{\Sigma}^\star = \boldsymbol{K}^\star \boldsymbol{K}^{-1} \boldsymbol{\Sigma}^{\star(2)} \boldsymbol{K}^{-1} \boldsymbol{K}^{\star T} + \boldsymbol{\Sigma}'$.

2. Sensitivity to Mis-specification of Inert Covariate

In this subsection, we consider the cases, where the distribution of the inert covariate is mis-specified due to the lack of prior knowledge or limited amount of historical dataset. In such scenarios, the proposed method may provide additional errors in terms of informative covariate identification. Here, we follow the detailed settings described in Section 3.2, except that the inert covariate is sampled from the symmetric beta distribution. The beta distribution is chosen as it has been widely used to model the behavior of random variables limited to a finite interval. Note that $Beta(1,1)$ is equivalent to $Uniform(0,1)$ and the distribution of existing covariates is $Uniform(0,1)$. Three distributions are used to sample inert covariates: $Beta(0.8, 0.8)$, $Beta(1,1)$ and $Beta(1.2, 1.2)$. Figure 1 shows the probability density functions of the corresponding beta distributions.

The simulation is repeated 50 times for each of the Beta distributions. The covariate selection results are in Table 1. The results show that the proposed method is quite robust with respect to the mis-specification of the inert covariate. In particular, the proposed method is able to correctly identify informative covariates despite a mis-specified inert covariate. Yet, when the distribution of the inert covariate is mis-specified (i.e., $Beta(0.8, 0.8)$ or $Beta(1.2, 1.2)$), there is a slightly higher

Figure 1 Probability density functions of the beta distributions of mis-specified inert covariates

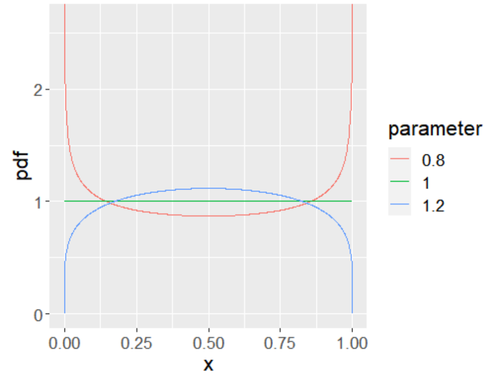

Table 1 Average proportion of simulations that a covariate is identified as informative/irrelevant when the inert covariate is mis-specified (correct distribution of the inert covariate is $Beta(1.0, 1.0)$)

Percentile	Inert covariate	Covariate	
		Informative	Irrelevant
90th	$Beta(0.8, 0.8)$	1	0.132
	$Beta(1.0, 1.0)$	1	0.123
	$Beta(1.2, 1.2)$	1	0.128
95th	$Beta(0.8, 0.8)$	1	0.083
	$Beta(1.0, 1.0)$	1	0.068
	$Beta(1.2, 1.2)$	1	0.075

chance of falsely identifying non-informative covariates as informative. Recall that the proposed method identifies informative covariates by measuring how rapidly the FPC score changes according to the covariate change. Roughly speaking, when the distribution of the inert distribution is mis-specified, the differences of the inert covariates between different subjects will be distorted, while the corresponding differences in the FPC score estimations between subjects remain the same. This may lead to "less" rapid changes in FPC scores, i.e., the significance of the inert covariate is underestimated, and increase the false positive rate (decrease the false negative rate).

3. Sensitivity to Correlated Covariates

This subsection investigates how the proposed method performs when there are multiple correlated covariates. We use the similar settings described in Section 3.2, except that $n_i = 5$ for all subjects, and only the first covariate is truly informative and the second covariate is correlated with the first covariate. In particular, the FPC scores of the i^{th} subject are calculated using $A_{i1} = 0.5 \times Z_{i1}^2$ and $A_{i2} = 0.5 \times \sin(2 \times Z_{i1})$, and the correlation coefficient between the first and second covariates is set to 0, 0.2 or 0.5. The simulation is repeated 50 times for each correlation coefficient value. Table 2 summarizes the results using the 95^{th} percentile of the reference distribution as a criterion. The table shows that as the correlation between the first and second covariates increases, the probability of incorrectly identifying the second covariate as informative increases as well. Recall that the

Table 2 Proportion of simulations that each covariate is identified as informative (Truly informative covariates are highlighted in bold)

	Covariate								
	1			2			Others		
Correlation	**0**	**0.2**	**0.5**	0	0.2	0.5	0	0.2	0.5
95^{th}	**1**	**1**	**1**	0.06	0.18	0.38	0.04	0.05	0.04

proposed method identifies a covariate as informative if the change of the covariate leads to the change of the response. Thus, the proposed method is more likely to identify the second covariate as informative when it has the stronger correlation with the first covariate, because we observe that the change of the second covariate value happens along with the change of the response. As a result, we recommend removing highly correlated covariates to avoid potential numerical instability and misleading covariate identification results.

4. Informative Covariate Identification Results on Void Swelling using Existing Methods

The point estimation of ρ_m using the MLE in the conventional GP is provided in Table 3. It is not straightforward to set an appropriate value of ξ to decide which covariates to screen out. More importantly, the conventional GP fails to identify well-known important covariates such as %wt. Cr and %wt. Fe, yet concludes other covariates as more informative, i.e., estimates smaller ρ_m, whose effects on void swelling are less clear.

Table 3 MLE results of ρ_m of conventional ARD

Covariate	Value	Covariate	Value
Total Damage	0.094	Irradiation Temperature	0.086
B	$>10^3$	Mn	$>10^3$
C	0.562	Fe	$>10^3$
N	$>10^3$	Cu	0.120
Al	0.022	Ni	4.067
Si	0.642	Mo	34.10
P	0.152	Ni6+	$>10^3$
S	558.1	Fe2+	0.015
Ti	7.155	Neutron	121.3
V	0.042	Proton	0.153
Cr	$>10^3$	Electron	0.126

Next, the linear mixed-effects model is fitted on the void swelling dataset. In this model, the swelling value is a response variable and total damage and other covariates (i.e., irradiation temperature, irradiation type, and alloy compositions) are predictors. The significance testing results are summarized in Table 4. In particular, the Satterthwaite's method for approximating degrees of freedom is used to conduct F test and obtain the p-values (Hrong-Tai Fai and Cornelius 1996).

The method also fails to identify the important covariates such as irradiation temperature and first-order major elements (%wt. Cr and %wt. Fe). Note that the design matrix is not full rank, and 3 covariates are dropped.

Table 4 **Significance testing results of the linear mixed-effects model**

Covariate	p-value	Covariate	p-value
Total Damage	≈ 0	Irradiation Temperature	0.106
B	0.847	Mn	0.239
C	0.415	Fe	0.170
N	0.039	Cu	≈ 0
Al	0.020	Ni	0.173
Si	0.725	Mo	0.206
P	0.481	Ni6+	0.013
S	0.965	Fe2+	0.011
Ti	0.796	Neutron	0.123
Cr	0.153		

Lastly, we apply the well-known lasso method to the void swelling dataset. The lasso uses the L_1-norm of the coefficient as a penalty for predictor (covariate) selection (Tibshirani 1996). In particular, three benchmark methods based on the lasso are implemented as summarized in Table 5. In the table, covariates that are known to be informative are highlighted in bold. "Gamma_LASSO" is the results using a generalized linear model with log link and gamma distribution, "Quadratic_LASSO" is the results when the quadratic transformation of continuous covariates are added as predictors, and "Adaptive LASSO" is the results using the adaptive lasso proposed in Zou (2006). The adaptive lasso is similar to the conventional lasso method, except that it imposes different penalty weights for different predictors. In each model, 10-fold cross validation is employed to find the optimal tuning parameters. Table 5 shows that these methods fail to select some informative covariates such as irradiation temperature or %wt. Cr. One of the main reason is because in void swelling, it has been shown that different covariates do not have *additive* effects.

5. Computer codes

R codes which generate the simulation dataset and implement the developed methodology are attached.

References

Hrong-Tai Fai A, Cornelius PL (1996) Approximate f-tests of multiple degree of freedom hypotheses in generalized least squares analyses of unbalanced split-plot experiments. *Journal of statistical computation and simulation* 54(4):363–378.

Table 5 Estimated coefficient results of the LASSO-based methods

Covariate	Gamma_LASSO	Quadratic_LASSO	Adaptive LASSO
Total Damage	**-41.46**	**0**	**0.20**
Irradiation Temperature	**0**	**0**	**0**
B	0	0	0
C	0	0	0
N	0.59	0	0
Al	0	0	0
Si	18.67	0	-0.11
P	0	0	0
S	0	0	0
Ti	0	0	0
V	0	0	0
Cr	**0**	**0**	**0**
Mn	0	0	0
Fe	**-7.99**	**0.10**	**0.12**
Cu	-13.17	0	0.50
Ni	0	0	0
Mo	9.56	0	0
Ni6+	0	0	0
Neutron	0	0	0
Proton	0	-0.01	0
Fe2+	6.89	0	0.01
Electron	0	0	0
Total Damage^2	-	**0.25**	-
Irradiation Temperature^2	-	**0**	-
B^2	-	0	-
C^2	-	0	-
N^2	-	-0.02	-
Al^2	-	0	-
Si^2	-	-0.11	-
P^2	-	0	-
S^2	-	0	-
Ti^2	-	0	-
V^2	-	0	-
Cr^2	-	**0**	-
Mn^2	-	0	-
Fe^2	-	**0**	-
Cu^2	-	0.54	-
Ni^2	-	0	-
Mo^2	-	-0.02	-

Tibshirani R (1996) Regression Shrinkage and Selection Via the Lasso. *Journal of the Royal Statistical Society: Series B (Methodological)* 58(1):267–288, URL `http://dx.doi.org/10.1111/j.2517-6161.1996.tb02080.x`.

Zou H (2006) The Adaptive Lasso and Its Oracle Properties. *Journal of the American Statistical Association* 101(476):1418–1429, ISSN 0162-1459, URL `http://dx.doi.org/10.1198/016214506000000735`.