# B Supplementary Online Material

### Additional simulations and examples

For the $d = 2$ setting, we considered overall four models (see Table 3) and six designs (see Figure 6). The six designs are based on the work of Li et al. [3], but the four models go beyond the simulations of Li et al. [3]. Note that the domain for the model with a logarithmic term is different than the others. This is because the function $\boldsymbol{x}(\boldsymbol{z})$ is not a continuous function on the domain $\mathcal{D} = [0, 1]^2$. For reference, contour plots of the four models are shown in Figure 7.

We first show examples of $\mathrm{CR}_{\mathrm{S},0.95}$ and $\mathrm{CR}_{0.95}$, for all four models in Figure 8. The confidence intervals are based on one sample from each model with $\kappa = 36, m = 10$ (i.e. $n = 360$) and under the first design, under the asymptotic distribution. The results for the linear and quadratic models appear also in the main paper, and are repeated here only for ease of comparison. The confidence regions are given in Figure 8 (top and middle rows) and the sizes of the regions are reported in Table 4 as the proportion of the domain covered by the confidence superset. We see that $\mathrm{CR}_{0.95}$ and $\mathrm{CR}_{\mathrm{S},0.95}$ are relatively similar in size (with $\mathrm{CR}_{0.95}$ being slightly bigger), except for the quadratic model. The fact that $\mathrm{CR}_{0.95}$ is smaller than $\mathrm{CR}_{\mathrm{S},0.95}$ for the quadratic model is probably caused by the fact that Scheffé's bounds are conservative, and this is particularly emphasized with an increase in the difference between $k + 1$ (the number of parameters in the model) and $d$ (the dimension of the covariates).

Figure 8 (bottom row) also shows the confidence region $\mathrm{CR}_{0.95}$, along with 25 bootstrap samples $\widehat{\mathrm{ED}}_{50}^*$, again from the asymptotic model. This shows how the confidence region describes visually the variability of $\widehat{\mathrm{ED}}_{50}$. In particular, we see how in the quadratic model, $\widehat{\mathrm{ED}}_{50}$ can "dip down" in the upper right hand corner, a property not revealed by looking solely at the observed $\widehat{\mathrm{ED}}_{50}$.

Further to that presented in the main paper, we performed simulations in the $d = 2$ case for all four models of Table 3 and the six designs given in Fig 6. We consider design one for all four models in Tables 5 and 6. A less complete version of Table 6 appears in the main paper. Here, we studied empirical coverage of the three confidence regions when the true variance $\Sigma$ is estimated from the data. In Table 5, we assume that $\Sigma$ is known.

Table 3: True model parameters for $\boldsymbol{z} = (z_1, z_2) \in \mathbb{R}^2$

| | true model | domain |
|---|---|---|
| linear | $-6 + 6z_1 + 6z_2$ | $[0, 1]^2$ |
| interaction | $-6 + 6z_1 + 6z_2 - 3z_1z_2$ | $[0, 1]^2$ |
| quadratic | $-6 + 6z_1 + 6z_2 + 10z_1^2 + 3z_1z_2 + z_2^2$ | $[0, 1]^2$ |
| log term | $-10 + 6\log z_1 + 6z_2$ | $[1, 2]^2$ |

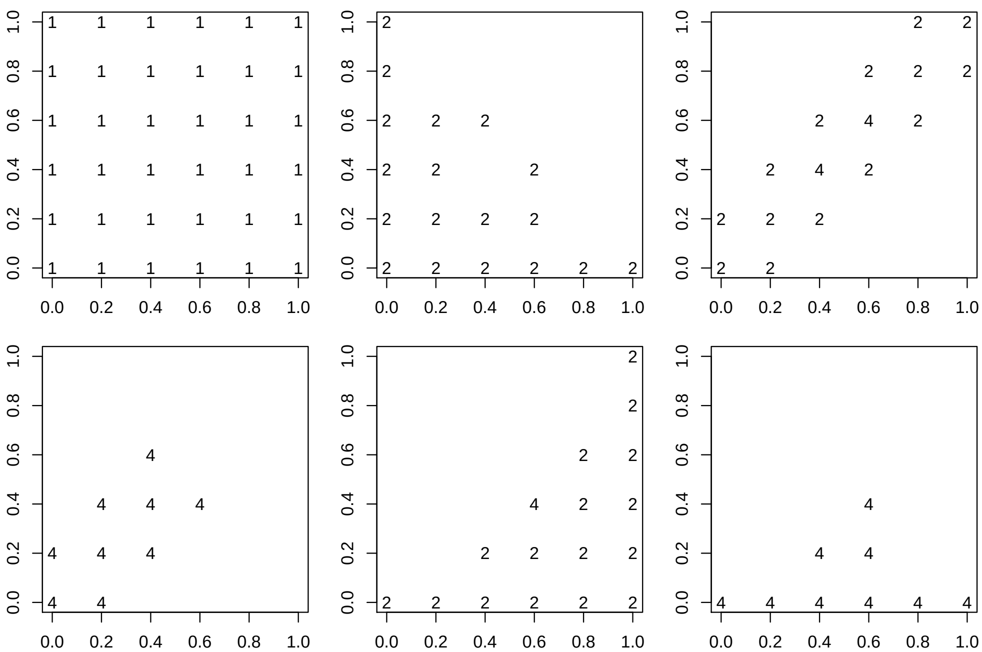

Figure 6: Different design matrices considered for the parametric model. The designs are shown from left to right: 1–3 in the top row and 4–6 in the bottow row.

We first look at the behaviour of the confidence regions when sampling from the asymptotic distribution (i.e. $\Sigma$ is known) given in Table 5. For the linear, interaction and log term models, the coverage of $\mathrm{CR}_{0.95}$ is either better or similar to that of $\mathrm{CR}_{\mathrm{S},0.95}$, while the sizes of the confidence regions are similar. For the quadratic model, the coverage of $\mathrm{CR}_{0.95}$ is smaller than that of $\mathrm{CR}_{\mathrm{S},0.95}$, as is the mean size of the region. $\mathrm{CR}_{0.95}$ is the only region which achieves its nominal coverage, if only in a few instances. Since we are sampling from the asymptotic distribution, the behaviour of the confidence regions is relatively similar as the sample size varies. The mean sizes of the regions do decrease with the sample size, which is again expected.

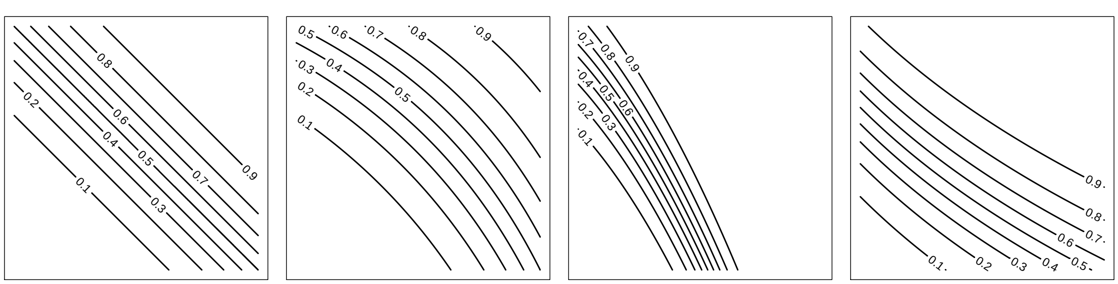

Figure 7: Contour plots for the true function $f$ in the parametric setting. From left the right the models from Table 3 are linear, interaction, quadratic, and log-term.

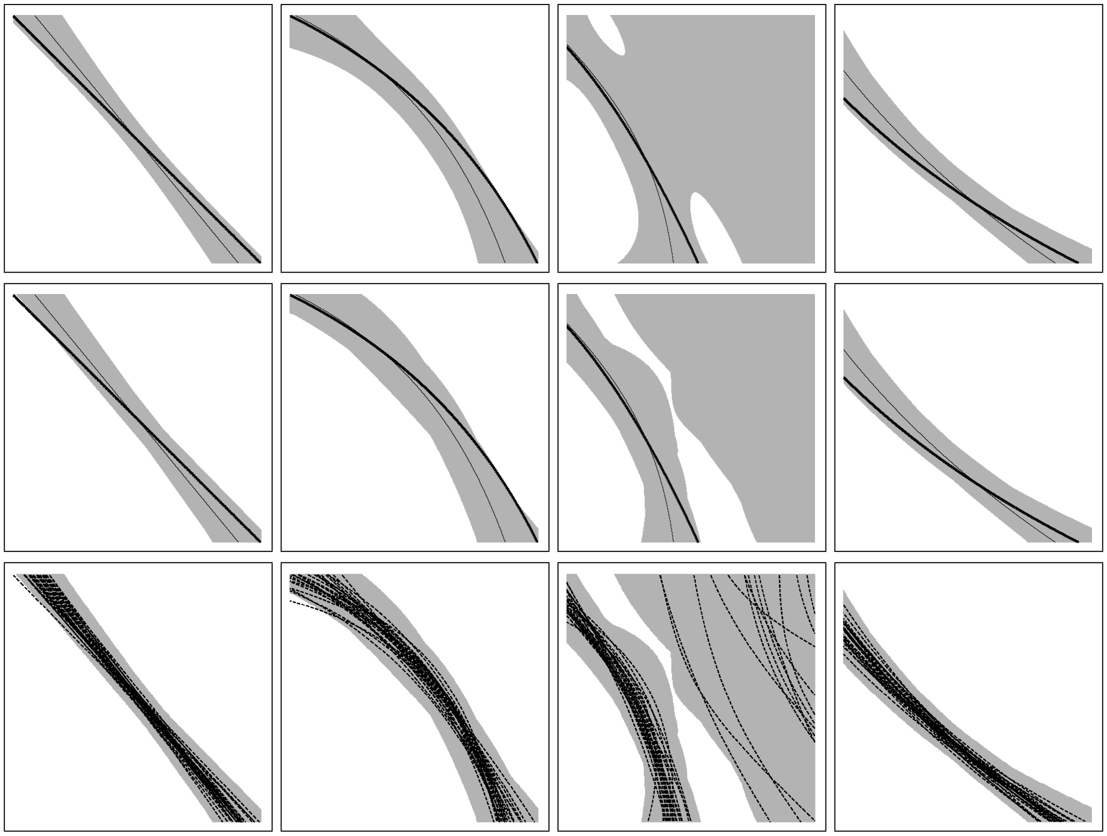

Figure 8: Confidence regions (gray) for $\mathrm{ED}_{50}$ (bold); $\widehat{\mathrm{ED}}_{50}$ is shown as the thin line in the first two rows. The regions are $\mathrm{CR}_{\mathrm{S},0.95}$ (top row) and $\mathrm{CR}_{0.95}$ (middle row). The bottom row shows the regions $\mathrm{CR}_{0.95}$ along with 25 bootstrap samples of $\widehat{\mathrm{ED}}_{50}^{*}$ (dashed lines). From left to right, the models are linear, interaction, quadratic, and log term with a sample size of $n = 360$ under the asymptotic model.

We next assume that the true $\Sigma$ is unknown. The results are shown in Table 6. Note that we did not report the results for the quadratic model when $n = 36$. This is because there was too large a proportion of observations in “complete separation” [10] in this case. When the sample size is $n = 360$ and $n = 3600$, the results in Table 6 and Table 5 are similar. When $n = 36$, however, $\mathrm{CR}_{\mathrm{S},0.95}$ and $\mathrm{CR}_{0.95}$ behave comparably. In the parametric bootstrap the results are similar to those in Table 6, while for the nonparametric bootstrap the results again undercover in a manner similar to that in Table 5.

Table 4: Proportion of the domain covered by the confidence regions shown in Figure 8.

| | linear | interaction | quadratic | log-term |
|---|---|---|---|---|
| $\mathrm{CR}_{\mathrm{S},0.95}$ | 0.161 | 0.230 | 0.803 | 0.159 |
| $\mathrm{CR}_{0.95}$ | 0.168 | 0.245 | 0.718 | 0.172 |

Following Li et al. [3], we also consider several different experimental designs in our simulations. The various designs are given in Figure 6, and recall that contours of the true models are given in Figure 7. In these simulations we consider only the case where $\Sigma$ must be estimated from the data. The results for $n = 36$ are given in Table 7 and those for $n = 360$ in Table 8. We note that for $n = 36$ and the linear and interaction models, under designs 1,3, and 5 one expects at least 10 failures and 10 successes, but not so for designs 2,4, and 6. This is also holds for $n = 36$ and $n = 360$ for all designs in the log term model. As before, we do not report the simulations which had a large proportion (more than $\sim 20\%$) of data in complete separation.

Table 5: Empirical coverage probabilities of $95\%$ confidence regions for $\mathrm{ED}_{100p}$ for the parametric models in Table 3 for design 1 (see Figure 6) for simulations from the asymptotic normal distribution. Results *not* statistically different from 0.95 are shown in bold. The corresponding sizes of the confidence regions, measured as the mean proportion of the domain covered by the region, are given in brackets. SCH denotes Scheffé's method, while CR denotes the new bootstrap approach.

| | | linear | | interaction | | quadratic | | log term | |
|---|---|---|---|---|---|---|---|---|---|
| $n$ | $p$ | SCH | CR | SCH | CR | SCH | CR | SCH | CR |
| 36 | .1 | .993 | .976 | .995 | .972 | 1.00 | .985 | .994 | .983 |
| | | (.46) | (.50) | (.59) | (.60) | (.95) | (.91) | (.26) | (.32) |
| | .5 | .984 | .969 | .995 | .980 | .997 | .980 | .985 | .974 |
| | | (.75) | (.80) | (.90) | (.90) | (.99) | (.98) | (.72) | (.79) |
| | .9 | .990 | .996 | 1.00 | 1.00 | .998 | .987 | .982 | .992 |
| | | (.47) | (.51) | (.42) | (.45) | (.96) | (.93) | (.64) | .(70) |
| 360 | .1 | .993 | .973 | .995 | .968 | 1.00 | .989 | .994 | .981 |
| | | (.18) | ( .17) | (.26) | (.21) | (.37) | (.32) | (.10) | (.10) |
| | .5 | .984 | **.947** | .995 | **.942** | .998 | .982 | .985 | **.963** |
| | | (.19) | (.20) | (.27) | (.27) | (.57) | (.47) | (.18) | (.19) |
| | .9 | .991 | .990 | 1.00 | .997 | .998 | .972 | .982 | **.962** |
| | | (.18) | (.19) | (.12) | (.10) | (.64) | (.59) | (.26) | (.28) |
| 3600 | .1 | .993 | .975 | .995 | .968 | 1.00 | .987 | .994 | .981 |
| | | (.06) | ( .05) | (.08) | (.07) | (.06) | (.05) | (.03) | (.03) |
| | .5 | .984 | **.948** | .996 | **.942** | .998 | .970 | .985 | .970 |
| | | (.06) | (.06) | (.09) | (.09) | (.06) | (.05) | (.06) | (.06) |
| | .9 | .993 | .985 | 1.00 | .976 | .998 | **.959** | .982 | .967 |
| | | (.06) | (.06) | (.05) | (.05) | (.09) | (.08) | (.08) | (.09) |

Table 6: Empirical coverage probabilities of $95\%$ confidence regions for $\mathrm{ED}_{100p}$ for the parametric models in Table 3 for design one (see Figure 6) using the maximum likelihood estimate of $\Sigma$. Results *not* statistically different from 0.95 are shown in bold. The corresponding sizes of the confidence regions, measured as the mean proportion of the domain covered by the region, are given in brackets. SCH denotes Scheffé's method, while CR denotes the new bootstrap approach.

| | | linear | | interaction | | quadratic | | log term | |
|---|---|---|---|---|---|---|---|---|---|
| $n$ | $p$ | SCH | CR | SCH | CR | SCH | CR | SCH | CR |
| 36 | .1 | .989 | .995 | .995 | .992 | * | * | .990 | .997 |
| | | (.47) | (.54) | (.61) | (.64) | * | * | (.28) | (.36) |
| | .5 | 1.00 | .998 | 1.00 | 1.00 | * | * | 1.00 | .993 |
| | | (.93) | (.95) | (1.0) | (1.0) | * | * | (.85) | (.96) |
| | .9 | .991 | .993 | .997 | .997 | * | * | .994 | .996 |
| | | (.47) | (.53) | (.43) | (.49) | * | * | (.67) | .(72) |
| 360 | .1 | .988 | .977 | .992 | .966 | 1.00 | .994 | .988 | .980 |
| | | (.18) | (.17) | (.26) | (.21) | (.34) | (.29) | (.10) | (.10) |
| | .5 | .988 | **.946** | .994 | **.945** | 1.00 | .995 | .983 | .965 |
| | | (.19) | (.20) | (.27) | (.27) | (.51) | (.40) | (.18) | (.19) |
| | .9 | .990 | .985 | .997 | .989 | .996 | .973 | .980 | .971 |
| | | (.18) | (.19) | (.12) | (.11) | (.69) | (.66) | (.26) | (.28) |
| 3600 | .1 | .995 | .980 | .999 | .980 | 1.00 | .971 | .988 | .970 |
| | | (.06) | (.05) | (.08) | (.07) | (.06) | (.05) | (.03) | (.03) |
| | .5 | .986 | **.944** | .989 | **.937** | .999 | .982 | .991 | .968 |
| | | (.06) | (.07) | (.09) | (.09) | (.06) | (.05) | (.06) | (.06) |
| | .9 | .991 | .973 | .996 | .969 | .999 | .975 | .989 | .973 |
| | | (.06) | (.06) | (.05) | (.05) | (.08) | (.07) | (.08) | (.09) |

Table 7: Empirical coverage probabilities of $95\%$ confidence regions for $\mathrm{ED}_{100p}$ for the parametric models give in Table 3 using $\widehat{\Sigma}_n$ throughout. The designs are shown in Figure 6. Results not statistically different from 0.95 are shown in bold. The mean proportion of the domain covered by the region is given in brackets. SCH denotes Scheffé's method, while CR denotes the new bootstrap approach.

| | | | linear | | interaction | | log term | |
|---|---|---|---|---|---|---|---|---|
| $n$ | design | $p$ | SCH | CR | SCH | CR | SCH | CR |
| 36 | 2 | .1 | .989 | .993 | .992 | .992 | .984 | .993 |
| | | | (.70) | (.83) | (.98) | (.98) | (.23) | (.32) |
| | | .5 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | .997 |
| | | | (.93) | (.98) | (.99) | (.98) | (.92) | (.97) |
| | | .9 | 1.00 | 1.00 | 1.00 | 1.00 | .993 | .997 |
| | | | (.51) | (.57) | (.59) | (.62) | (.65) | (.68) |
| | 3 | .1 | .989 | .993 | .996 | .995 | .992 | .998 |
| | | | (.74) | (.81) | (.85) | (.87) | (.59) | (.68) |
| | | .5 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | .999 |
| | | | (.98) | (1.0) | (1.0) | (1.0) | (.95) | (.98) |
| | | .9 | .979 | .986 | .995 | .992 | .981 | .989 |
| | | | (.74) | (.81) | (.80) | (.82) | (.84) | (.88) |
| | 4 | .1 | .985 | .932 | * | * | .989 | .993 |
| | | | (.85) | (.93) | * | * | (.49) | (.61) |
| | | .5 | 1.00 | 1.00 | * | * | .998 | .997 |
| | | | (.97) | (.99) | * | * | (.93) | (.98) |
| | | .9 | 1.00 | 1.00 | * | * | .994 | .997 |
| | | | (.71) | (.77) | * | * | (.78) | (.81) |
| | 5 | .1 | .993 | .995 | .999 | .997 | .989 | .994 |
| | | | (.65) | (.74) | (.81) | (.83) | (.51) | (.62) |
| | | .5 | 1.00 | .998 | 1.00 | 1.00 | 1.00 | .999 |
| | | | (.99) | (1.0) | (1.0) | (1.0) | (.98) | (.99) |
| | | .9 | .987 | .989 | .994 | .994 | .986 | .992 |
| | | | (.65) | (.74) | (.73) | (.76) | (.78) | (.84) |
| | 6 | .1 | .989 | .996 | .993 | .993 | .990 | .996 |
| | | | (.85) | (.93) | (1.0) | (.1.0) | (.59) | (.75) |
| | | .5 | 1.00 | 1.00 | 1.00 | 1.00 | .998 | .998 |
| | | | (.97) | (.99) | (1.0) | (1.0) | (1.0) | (1.0) |
| | | .9 | .999 | 1.00 | 1.00 | 1.00 | .993 | .997 |
| | | | (.65) | (.72) | (.96) | (.97) | (.74) | (.78) |

Table 8: Empirical coverage probabilities of $95\%$ confidence regions for $\mathrm{ED}_{100p}$ for the parametric models give in Table 3 using $\widehat{\Sigma}_n$ throughout. The designs are shown in Figure 6. Results not statistically different from 0.95 are shown in bold. The mean proportion of the domain covered by the region is given in brackets. SCH denotes Scheffé's method, while CR denotes the new bootstrap approach.

| | | | linear | | interaction | | quadratic | | log term | |
|---|---|---|---|---|---|---|---|---|---|---|
| $n$ | design | $p$ | SCH | CR | SCH | CR | SCH | CR | SCH | CR |
| 360 | 2 | .1 | .983 | .972 | .987 | .970 | .998 | .995 | .991 | .980 |
| | | | (.16) | ( .15) | (.30) | (.29) | (.33) | (.29) | (.08) | (.08) |
| | | .5 | .983 | **.947** | .993 | .979 | 1.00 | .987 | .986 | .965 |
| | | | (.23) | (.26) | (.53) | (.54) | (.46) | (.38) | (.16) | (.17) |
| | | .9 | .994 | .983 | 1.00 | .999 | .997 | .968 | .990 | .971 |
| | | | (.27) | (.28) | (.27) | (.24) | (.63) | (.57) | (.30) | (.32) |
| | 3 | .1 | .985 | .969 | .992 | .986 | * | * | .987 | .984 |
| | | | (.34) | (.36) | (.49) | (.45) | * | * | (.18) | (.21) |
| | | .5 | .986 | **.944** | .992 | **.947** | * | * | .985 | .970 |
| | | | (.39) | (.40) | (.47) | (.46) | * | * | (.37) | (.40) |
| | | .9 | .987 | .991 | .995 | .993 | * | * | .982 | .968 |
| | | | (.34) | (.33) | (.30) | (.31) | * | * | (.42) | (.43) |
| | 4 | .1 | .985 | **.961** | .986 | .988 | .996 | .981 | .993 | .978 |
| | | | (.29) | (.31) | (.77) | (.78) | (.69) | (.64) | (.12) | (.14) |
| | | .5 | .987 | **.956** | .992 | **.963** | 1.00 | .985 | .973 | **.960** |
| | | | (.37) | (.40) | (.71) | (.72) | (.74) | (.69) | (.30) | (.32) |
| | | .9 | .991 | .995 | .995 | .992 | .998 | .982 | .988 | .970 |
| | | | (.36) | (.37) | (.51) | (.52) | (.78) | (.74) | (.38) | (.40) |
| | 5 | .1 | .985 | .970 | .991 | .989 | * | * | .993 | .975 |
| | | | (.27) | (.27) | (.48) | (.48) | * | * | (.14) | (.16) |
| | | .5 | .987 | .971 | .992 | **.963** | * | * | .977 | .968 |
| | | | (.31) | (.31) | (.49) | (.46) | * | * | (.30) | (.31) |
| | | .9 | .990 | .972 | .995 | .992 | * | * | .983 | **.963** |
| | | | (.27) | (.26) | (.35) | (.35) | * | * | (.37) | (.38) |
| | 6 | .1 | .994 | .977 | .991 | .992 | .999 | .997 | .991 | .976 |
| | | | (.16) | (.26) | (.85) | (.85) | (.91) | (.90) | (.11) | (.12) |
| | | .5 | .994 | .976 | .994 | .983 | 1.00 | .996 | .982 | **.966** |
| | | | (.36) | (.38) | (.83) | (.84) | (.94) | (.92) | (.28) | (.31) |
| | | .9 | .996 | .994 | .998 | .998 | .997 | .990 | .988 | **.967** |
| | | | (.35) | (.34) | (.69) | (.70) | (.96) | (.95) | (.43) | (.44) |