

Optimal Robust Bounded Bias and Bounded Variance Designs

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Abstract

Designs which are minimax in the presence of model misspecifications have been constructed so as to minimize the maximum, over classes of alternate response models, of the integrated mean squared error of the predicted values. This mean squared error decomposes into a term arising solely from variation, and a bias term arising from the model errors. Here we consider two associated problems: (i) design so as to minimize the variance, subject to a bound on the bias, and (ii) design so as to minimize the bias, subject to a bound on the variance. We show that solutions to both problems are given by the minimax designs, with appropriately chosen values of their tuning constant. Conversely, any minimax design solves both problems for appropriate choices of the bounds on the bias or variance.

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1. Introduction and summary

The theory of robustness of design was largely initiated by Box and Draper (1959), who investigated the robustness of some classical experimental designs in the presence of certain model inadequacies, e.g. designs optimal for a low order polynomial response when the true response was a polynomial of higher order. Huber (1975) derived designs for straight line regression, robust in the presence of alternate response functions. Wiens (1990, 1992) extended these results to multiple regression responses and in a variety of other directions – see Wiens (2015) for a summary of these and other approaches to robustness of design.

Designs which are *minimax* in the presence of model misspecifications aim to minimize the maximum, over classes of alternate response models, of the integrated mean squared error (IMSE) of the predicted values. In this note we first briefly review the theory of such designs, and discuss a decomposition of the IMSE into a convex combination of

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two terms – one arising solely from variation, and the other arising from the bias due to the model errors. Then in §3 we propose two associated problems: (i) design so as to minimize the variance, subject to a bound on the bias, and (ii) design so as to minimize the bias, subject to a bound on the variance. We show that solutions to both problems are given by the minimax designs, with appropriately chosen values of the mixing parameter. Conversely, any minimax design solves both problems for appropriate choices of the bounds on the bias or variance. Examples and methods of implementation are studied in §4. The MATLAB code used to prepare these examples is available on the author’s personal website.

2. Minimax robustness of design

The general minimax design problem is phrased in terms of an approximate regression response

$$E[Y(\mathbf{x})] \approx f'(\mathbf{x})\boldsymbol{\theta}, \quad (1)$$

for p regressors f , each functions of q independent variables \mathbf{x} , and a parameter $\boldsymbol{\theta}$. Since (1) is an approximation the interpretation of $\boldsymbol{\theta}$ is unclear; we *define* this target parameter by

$$\boldsymbol{\theta} = \arg \min_{\boldsymbol{\eta}} \int_{\mathcal{X}} (E[Y(\mathbf{x})] - f'(\mathbf{x})\boldsymbol{\eta})^2 \mu(d\mathbf{x}), \quad (2)$$

where $\mu(d\mathbf{x})$ represents either Lebesgue measure or counting measure, depending upon the nature of the *design space* \mathcal{X} with $\int_{\mathcal{X}} \mu(d\mathbf{x}) < \infty$. We then define $\psi(\mathbf{x}) = E[Y(\mathbf{x})] - f'(\mathbf{x})\boldsymbol{\theta}$. This results in the class of responses $E[Y(\mathbf{x})] = f'(\mathbf{x})\boldsymbol{\theta} + \psi(\mathbf{x})$, with – by virtue of (2) – ψ satisfying the orthogonality requirement

$$\int_{\mathcal{X}} f(\mathbf{x})\psi(\mathbf{x})\mu(d\mathbf{x}) = \mathbf{0}. \quad (3)$$

Assuming that \mathcal{X} is rich enough that the matrix $\mathbf{A} = \int_{\mathcal{X}} f(\mathbf{x})f'(\mathbf{x})\mu(d\mathbf{x})$ is invertible, the parameter defined by (2) and (3) is unique.

We identify a design with its design measure – a probability measure $\xi(d\mathbf{x})$ on \mathcal{X} . Define

$$\mathbf{M}_{\xi} = \int_{\mathcal{X}} f(\mathbf{x})f'(\mathbf{x})\xi(d\mathbf{x}), \quad \mathbf{b}_{\psi,\xi} = \int_{\mathcal{X}} f(\mathbf{x})\psi(\mathbf{x})\xi(d\mathbf{x}),$$

and assume ξ is such that \mathbf{M}_{ξ} is invertible. For an anticipated design of n , not necessarily distinct, points the covariance matrix of the least squares estimator $\hat{\boldsymbol{\theta}}$, assuming homoscedastic errors with variance σ_{ε}^2 , is $(\sigma_{\varepsilon}^2/n)\mathbf{M}_{\xi}^{-1}$, and the bias is $E[\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}] = \mathbf{M}_{\xi}^{-1}\mathbf{b}_{\psi,\xi}$; together these yield the mean squared error (*mse*) matrix

$$\text{MSE}[\hat{\boldsymbol{\theta}}] = \frac{\sigma_{\varepsilon}^2}{n}\mathbf{M}_{\xi}^{-1} + \mathbf{M}_{\xi}^{-1}\mathbf{b}_{\psi,\xi}\mathbf{b}'_{\psi,\xi}\mathbf{M}_{\xi}^{-1}$$

of the parameter estimates, whence the *mse* of the fitted values $\hat{Y}(\mathbf{x}) = f'(\mathbf{x})\hat{\boldsymbol{\theta}}$ is

$$\text{MSE}[\hat{Y}(\mathbf{x})] = \frac{\sigma_{\varepsilon}^2}{n}f'(\mathbf{x})\mathbf{M}_{\xi}^{-1}f(\mathbf{x}) + (f'(\mathbf{x})\mathbf{M}_{\xi}^{-1}\mathbf{b}_{\psi,\xi})^2 + \psi^2(\mathbf{x}).$$

A loss function that is commonly employed is the *integrated mse* of the *predictions*:

$$\begin{aligned}\text{IMSE}(\xi|\psi) &= \int_X \text{MSE}[\hat{Y}(\mathbf{x})] \mu(d\mathbf{x}) \\ &= \frac{\sigma_\varepsilon^2}{n} \text{tr}(A M_\xi^{-1}) + \mathbf{b}'_{\psi,\xi} M_\xi^{-1} A M_\xi^{-1} \mathbf{b}_{\psi,\xi} + \int_X \psi^2(\mathbf{x}) \mu(d\mathbf{x}).\end{aligned}\quad (4)$$

The dependence on ψ is eliminated by adopting a *minimax* approach, according to which one first maximizes (4) over a neighbourhood of the assumed response. This neighbourhood is constrained by (3) and by a bound $\int_X \psi^2(\mathbf{x}) \mu(d\mathbf{x}) \leq \tau^2/n$, required so that errors due to bias and to variation remain of the same order, asymptotically. Define $\psi_0(\mathbf{x}) = \sqrt{n}\psi(\mathbf{x})/\tau$ and $\nu = \tau^2/(\sigma_\varepsilon^2 + \tau^2)$. Then $\max_\psi \text{IMSE}(\xi|\psi)$ is $(\sigma_\varepsilon^2 + \tau^2)/n$ times

$$I_\nu(\xi) = (1 - \nu) \text{VAR}(\xi) + \nu \text{BIAS}(\xi),$$

where $\text{VAR}(\xi) = \text{tr} A M_\xi^{-1}$ is the integrated variance of the predictors and $\text{BIAS}(\xi) = \max_{\psi_0} \text{BIAS}(\xi|\psi_0)$, where

$$\text{BIAS}(\xi|\psi_0) = \mathbf{b}'_{\psi_0,\xi} M_\xi^{-1} A M_\xi^{-1} \mathbf{b}_{\psi_0,\xi} + 1 \quad (5)$$

is the integrated (squared) bias, with ψ_0 constrained by (3) and $\int_X \psi_0^2(\mathbf{x}) \mu(d\mathbf{x}) = 1$.

3. Optimal Bounded Bias and Bounded Variance designs

Let Ξ be a class of designs on χ , for instance all probability measures on $[-1, 1]$ – requiring appropriate approximations to make them implementable – or all exact designs, i.e. with integer allocations, on a finite design space. For

$$\min_{\xi \in \Xi} \text{BIAS}(\xi) \leq b^2 \leq \max_{\xi \in \Xi} \text{BIAS}(\xi), \quad (6)$$

consider the problem

(B): Minimize $\text{VAR}(\xi)$ in the class $\Xi_b \subset \Xi$ of designs for which $\text{BIAS}(\xi) \leq b^2$.

We call a solution to (B) an *Optimal Bounded Bias* design with bias bound b^2 , denoted $\text{OBB}(b^2)$. For

$$\min_{\xi \in \Xi} \text{VAR}(\xi) \leq s^2 \leq \max_{\xi \in \Xi} \text{VAR}(\xi), \quad (7)$$

consider the problem

(S): Minimize $\text{BIAS}(\xi)$ in the class $\Xi_s \subset \Xi$ of designs for which $\text{VAR}(\xi) \leq s^2$.

We call a solution to (S) an *Optimal Bounded Variance* design with variance bound s^2 , denoted $\text{OBV}(s^2)$.

For $\nu \in [0, 1]$ define $\xi_\nu = \arg \min_\xi I_\nu(\xi)$. Set $b^2(\nu) = \text{BIAS}(\xi_\nu)$ and $s^2(\nu) = \text{VAR}(\xi_\nu)$. Note that then

$$\xi_\nu \in \Xi_{b(\nu)} \cap \Xi_{s(\nu)}.$$

In §3.1 we prove and discuss Theorem 1. This asserts that solutions to (B) and (S) are given by ξ_ν , for some $\nu \in [0, 1]$, for any b^2 and any s^2 . Conversely, any ξ_ν is a solution to (B) and (S) for appropriate values of b^2 and s^2 .

Theorem 1. (a) Optimal Bounded Bias designs with bias bound b^2 satisfying (6) are given by

$$\xi = \begin{cases} \xi_\nu, & \text{if } b^2 = b^2(\nu), \text{ for } 0 \leq \nu \leq 1; \\ \xi_0, & \text{if } b^2 \geq b^2(0). \end{cases}$$

(b) Optimal Bounded Variance designs with variance bound s^2 satisfying (7) are given by

$$\xi = \begin{cases} \xi_\nu, & \text{if } s^2 = s^2(\nu), \text{ for } 0 \leq \nu \leq 1; \\ \xi_1, & \text{if } s^2 \geq s^2(1). \end{cases}$$

3.1. Proof of Theorem 1

By the *I-optimal* design Studden (1977) we mean the minimizer of $I_0(\xi)$, i.e. of the Integrated Variance of the Predicted Values. By the *uniform* design we mean the design $\xi(dx) \propto \mu(dx)$. These designs play special roles – they turn out to be ξ_0 and ξ_1 , respectively.

Lemma 1. The design ξ_0 , minimizing $I_0(\xi) = \text{VAR}(\xi)$ in Ξ , is I-optimal and the design ξ_1 , minimizing $I_1(\xi) = \text{BIAS}(\xi)$ in Ξ , is uniform.

Proof: That ξ_0 is the I-optimal design follows from the definition: $I_0(\xi) = \text{VAR}(\xi)$. By (5), $\text{BIAS}(\xi) \geq 1$. This lower bound is attained by the uniform design, since then

$$\mathbf{b}_{\psi,\xi} = \int_X f(x)\psi(x)\xi(dx) \propto \int_X f(x)\psi(x)\mu(dx) = \mathbf{0},$$

by (3). □

By Lemma 1, the lower bounds of the ranges (6) and (7) are attained by ξ_1 and ξ_0 respectively.

Lemma 2. (a) ξ_ν is a solution to (B) for $b^2(\nu)$. (b) If $b^2 \geq b^2(0) = \text{BIAS}(\xi_0)$ then ξ_0 is a solution to (B) for b^2 .

Proof: (a) For any $\xi \in \Xi_{b(\nu)}$ we must have that $\text{VAR}(\xi) \geq \text{VAR}(\xi_\nu)$, since otherwise

$$I_\nu(\xi) = (1 - \nu) \text{VAR}(\xi) + \nu \text{BIAS}(\xi) < (1 - \nu) \text{VAR}(\xi_\nu) + \nu b^2(\nu) = I_\nu(\xi_\nu),$$

a contradiction. Thus $\xi_\nu \in \Xi_{b(\nu)}$ minimizes $\text{VAR}(\xi)$ in $\Xi_{b(\nu)}$, i.e. is an OBB($b^2(\nu)$) design.

(b) For such b^2 we have that $\text{BIAS}(\xi_0) \leq b^2$ so that $\xi_0 \in \Xi_b$. As well,

$$\text{VAR}(\xi_0) = \min_{\xi \in \Xi} \text{VAR}(\xi) \leq \min_{\xi \in \Xi_b} \text{VAR}(\xi) \leq \text{VAR}(\xi_0), \quad (8)$$

so that we must have equality throughout in (8) and ξ_0 is an OBB(b^2) design. □

Lemma 3. (a) ξ_ν is a solution to (S) for $s^2(\nu)$. (b) If $s^2 \geq s^2(1) = \text{VAR}(\xi_1)$ then ξ_1 is a solution to (S) for s^2 .

The proof of Lemma 3 is identical to that of Lemma 2, apart from the obvious interchanges $\text{BIAS} \leftrightarrow \text{VAR}$, $b \leftrightarrow s$, $\xi_0 \leftrightarrow \xi_1$, and so is omitted. Lemmas 1, 2 and 3 together prove Theorem 1.

Remark: The solutions in Theorem 1 suggest that the maxima of $b^2(\cdot)$ and $s^2(\cdot)$ are unique, with

$$(i) \{0\} = \arg \max_{v \in [0,1]} b^2(v) \text{ and } (ii) \{1\} = \arg \max_{v \in [0,1]} s^2(v). \quad (9)$$

If not, for instance if $b^2(v)$ has multiple maxima or if ‘0’ is not a maximum, then on the set $N_b = \{v^* \in [0, 1] | b^2(v^*) \geq b^2(0)\}$, both ξ_{v^*} and ξ_0 are OBB($b^2(v^*)$), by (a) of Theorem 1 and Lemma 1 respectively, hence furnish the same minimum variance. Similarly, if (ii) fails then the bias is constant on the corresponding set N_s , where $s^2(v^*) \geq s^2(1)$. While counterintuitive if these sets are not singletons – and if the design weights ξ_i vary continuously with v – these events cannot be ruled out without further restrictions. This is shown by the example of regression through the origin – $p = q = 1$, $f(x) = x$, and Ξ the class of designs placing mass $\{\alpha, 1 - 2\alpha, \alpha\}$ on the points of $\chi = \{-1, 0, 1\}$. For any such design we find that $\text{VAR}(\xi) = 1/\alpha$ and $\text{BIAS}(\xi) = 1$, so that $I_v(\xi) = (1 - v)/\alpha + v$ is minimized by $\xi_v = .5\delta_{\pm 1}$ for any v . Thus $I_v(\xi_v) = 2 - v$, (9) fails and in fact $b^2(\cdot)$ and $s^2(\cdot)$ are constant on $[0, 1]$: $b^2(v) = \text{BIAS}(\xi_v) \equiv 1$, $s^2(v) = \text{VAR}(\xi_v) \equiv 2$.

4. Examples

We now assume that the design space is finite: $\mathcal{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$. Let \mathbf{Q} be an $N \times p$ matrix whose orthonormal columns span the column space of $(f(\mathbf{x}_1), \dots, f(\mathbf{x}_N))'$, assumed to have rank p . For a design ξ placing mass ξ_i on \mathbf{x}_i define $\mathbf{D}(\xi) = \text{diag}(\xi_1, \dots, \xi_N)$. Then in terms of

$$\mathbf{R}(\xi) = \mathbf{Q}' \mathbf{D}(\xi) \mathbf{Q}, \quad \mathbf{S}(\xi) = \mathbf{Q}' \mathbf{D}^2(\xi) \mathbf{Q}, \quad \mathbf{U}(\xi) = \mathbf{R}^{-1}(\xi) \mathbf{S}(\xi) \mathbf{R}^{-1}(\xi),$$

it is shown in Wiens (2018) that

$$\text{VAR}(\xi) = \text{tr} \mathbf{R}^{-1}(\xi), \quad \text{BIAS}(\xi) = c h_{\max} \mathbf{U}(\xi).$$

Here tr and h_{\max} denote the trace and maximum eigenvalue, respectively.

The minimization of $I_v(\xi)$ is carried out sequentially, as described in Theorem 5 of Wiens (2018). Briefly, given a current n -point design ξ_n , the loss resulting from the addition of a design point at \mathbf{x}_i is expanded as

$$I_v(\xi_{n+1}^{(i)}) = I_v(\xi_n) - t_{n,i}/n + O(n^{-2}), \quad (10)$$

and then $\mathbf{x}_{(i)}$, with $(i) = \arg \max_i t_{n,i}$, is added to the design. This is carried out to convergence.

We first present output for the case of straight line regression on a symmetric design space of size $N = 40$ in $[-1, 1]$: $\chi = \{x_i | i = 1, \dots, N\}$ with $x_i = -1 + 2(i - 1)/(N - 1) = -x_{N-i+1}$.

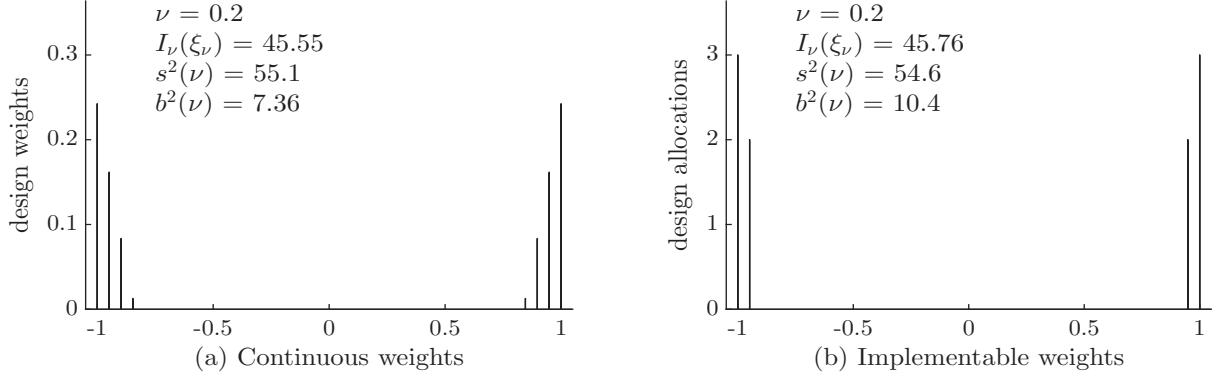


Figure 1: (a) OBB($b^2(.2)$)/OBV($s^2(.2)$) for the values displayed when $\nu = .2$. (b) Implementation of the design in (a); design size $n = 10$.

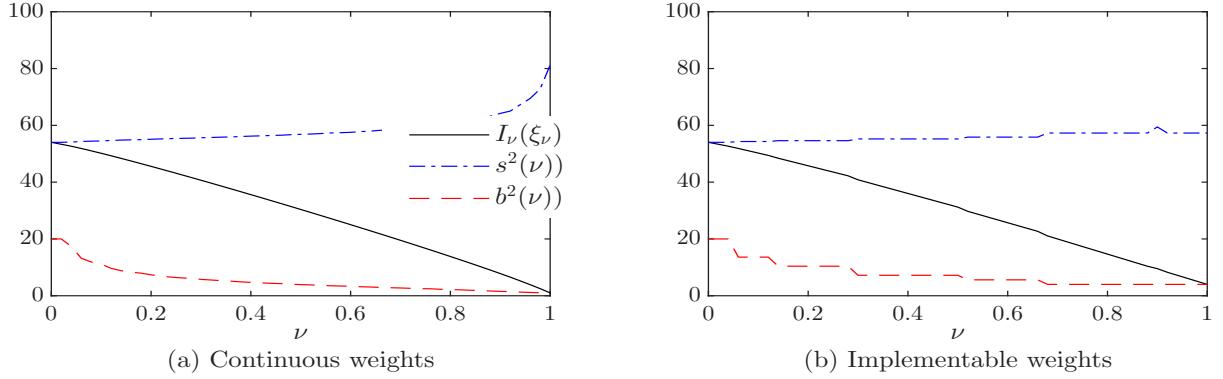


Figure 2: IMSE, VAR and BIAS vs. ν for the continuous optimal designs and their implementable approximations ($n = 10$).

Put $\mathbf{x} = (x_1, \dots, x_N)'$. Then $\mathbf{Q}_{N \times 2} = \left(\mathbf{1}_N / \sqrt{N} : \mathbf{x} / \sqrt{\|\mathbf{x}\|}\right)$. To obtain the OBB and OBV designs we minimize $I_\nu(\xi)$ over unrestricted designs ξ , so that the ξ_i vary freely over the simplex $\mathcal{S} = \{\xi_i \in [0, 1], \sum \xi_i = 1\}$.

The minimax design when $\nu = 1$ is uniform: $\xi_{1,i} \equiv 1/N$, so that $\mathbf{U}(\xi_1) = \mathbf{I}_N$ with $\text{BIAS}(\xi_1) = 1$ and $\text{VAR}(\xi_1) = 2N$. When $\nu = 0$, the minimax design is $\xi_0 = .5\delta_{\pm 1}$, with

$$\text{BIAS}(\xi_0) = \max(N/2, \|\mathbf{x}\|^2/2) = N/2, \quad \text{VAR}(\xi_0) = N + \|\mathbf{x}\|^2.$$

Thus ξ_1 is OBB($b^2 = 1$) and ξ_0 is OBV($s^2 = N + \|\mathbf{x}\|^2$). Representative results are presented in parts (a) of Figure 1 ($\nu = .2$) and Figure 2 – note that (9) holds.

The design in (a) of Figure 1 is not implementable since the allocations $n_i = n\xi_i$ need not be integers. To obtain parts (b) of these figures we first rounded up the n_i to $\lceil n\xi_i \rceil$, whose sum then exceeds n . The excess is decreased stepwise, by removing points whose value of $t_{n,i}$ in (10) is a minimum. This method typically results in only a very small increase in the minimized value of the IMSE.

The behaviour shown in (b) of Figure 2, in particular of the bias and as anticipated in the Remark of §3.1, reflects the lack of continuity of the allocations as functions of ν . This

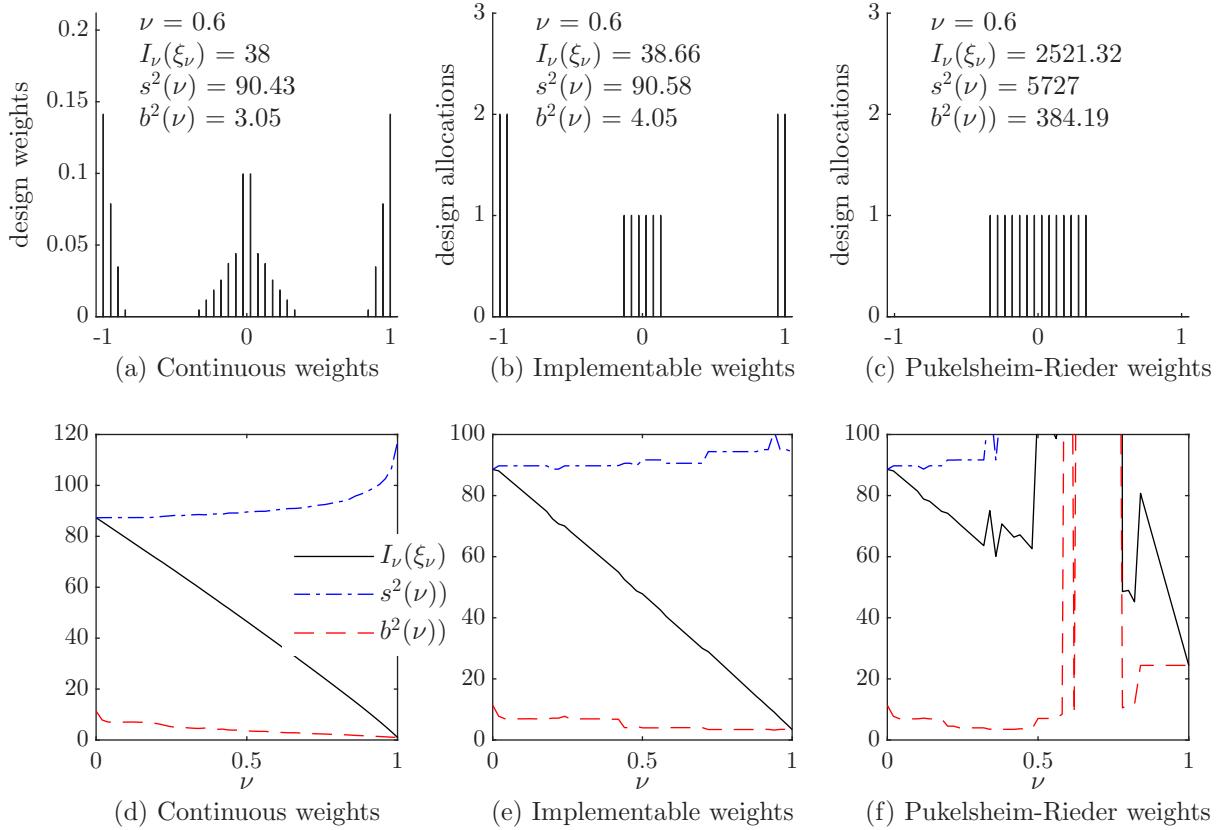


Figure 3: Continuous and implementable designs for quadratic regression; $n = 14$.

plot can serve as a guide to the designer in choosing a value of the bias/variance parameter ν .

Remark: Our method of rounding the design weights so as to obtain implementable designs is somewhat non-standard, and is intended to preserve, as much as possible, the minimized IMSE. A more common method is the ‘efficient design apportionment’ method of Pukelsheim and Rieder (1992). This is a rounding procedure that has, amongst others, the property of ‘sample size monotonicity’ – if a new point is to be added to an existing design, then none of the current allocations will be reduced. Unless this property is required we cannot recommend this method in the current application, as it is too often very unstable, resulting in large increases in the loss. An example is quadratic regression on the same design space as above, with a design size $n = 14$, as illustrated in Figure 3.

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