Spatial importance weighted cross validation

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Collaborators

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Focusing on a spatial setting

- Dataset: $\mathcal{X} = \{(s_1, y_1), \ldots, (s_n, y_n)\}$
- Spatial locations: $s_1, \ldots, s_n \overset{iid}{\sim} g(s)$ on spatial domain $\mathcal{D}$
- Response model:

$$y_i = h(s_i) + \epsilon_i, \;\; i = 1, \ldots, n.$$

- 'True signal' h is unknown but fixed, sufficiently well-behaved
- $\epsilon_1, \ldots, \epsilon_n$: independent, mean zero, $\text{Var}(\epsilon_i) = \sigma^2(s_i)$

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Often LOOCV or K-fold CV are used

LOOCV in space: Basics

If $Y(s)$ is an observation depending on spatial location $s \subset \mathcal{D}$:

$$\begin{aligned} \text{LOOCV} &= \frac{1}{n}\sum_{i=1}^{n} \mathcal{S}(y_i; P_{\mathcal{X}_{-i}}) \\ &\approx E_{\hat{g},\hat{g}}[\mathcal{S}(Y(s); P_{\mathcal{X}})] \\ &\approx E_{g,g}[\mathcal{S}(Y(s); P_{\mathcal{X}})], \end{aligned}$$

for:

- $\mathcal{S}$: scoring rule
- $\mathcal{X}$: dataset
- $g(s)$: spatial density of data locations
- $E_{f,g}$: prediction locations from f, data locations from g

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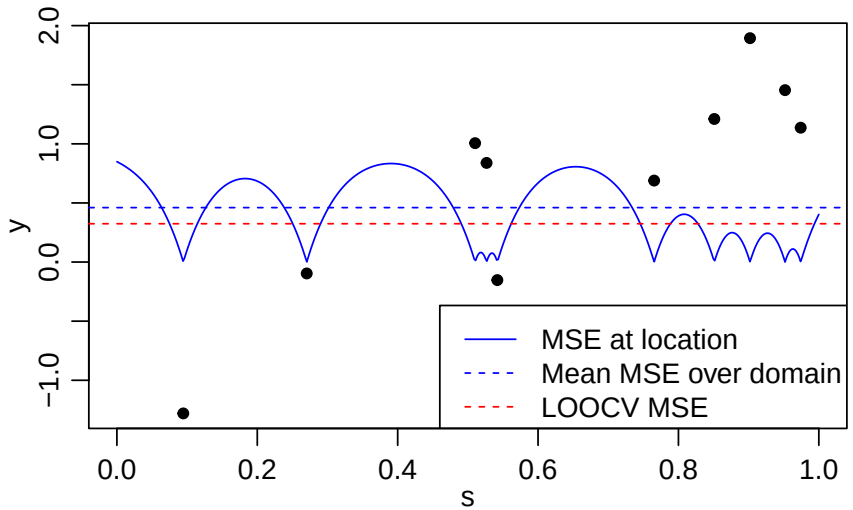
LOOCV in space: Thinking about nonrepresentativeness



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- the data will tend to be in areas we oversample, and so

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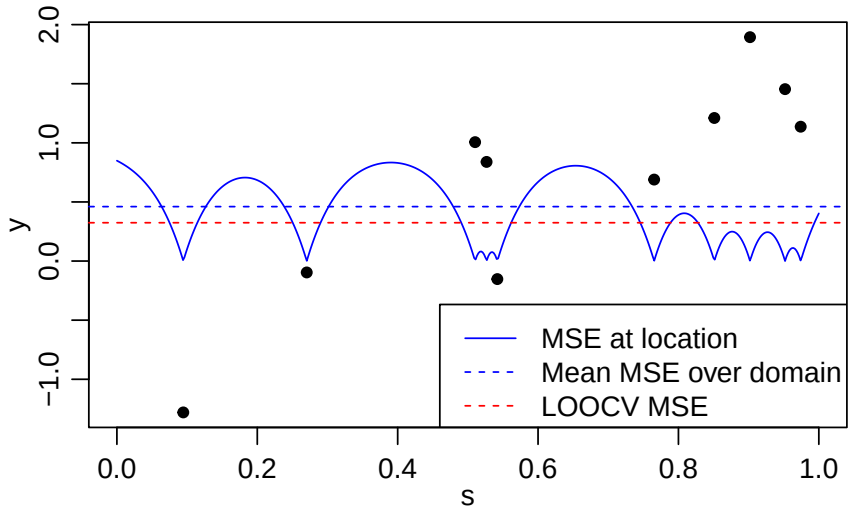

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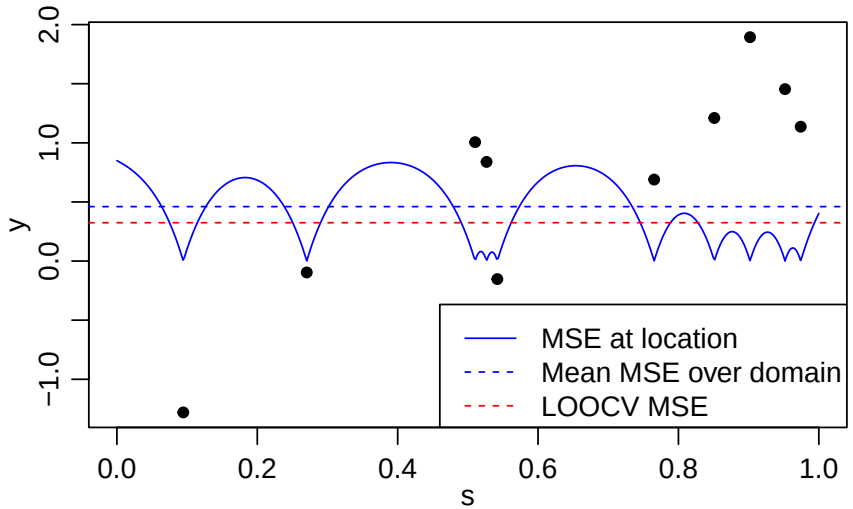

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- LOOCV will be overly optimistic.

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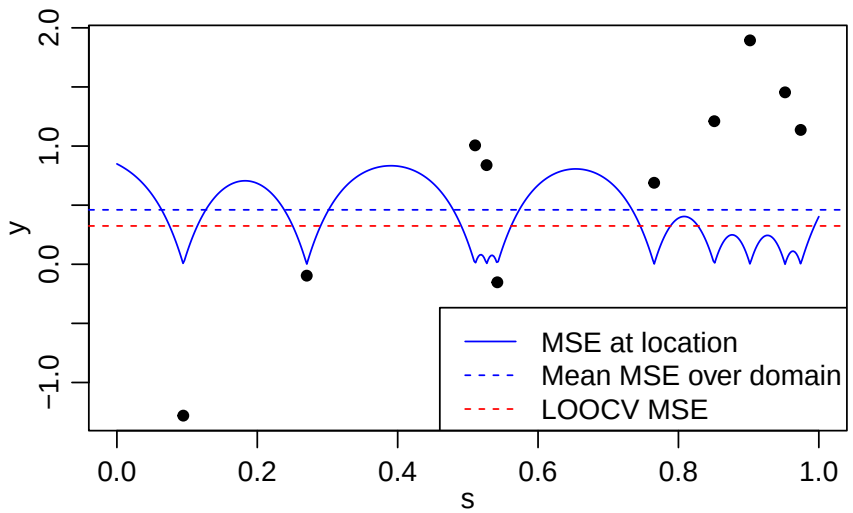

- If we oversample parts of the spatial domain, then LOOCV is overly optimistic.
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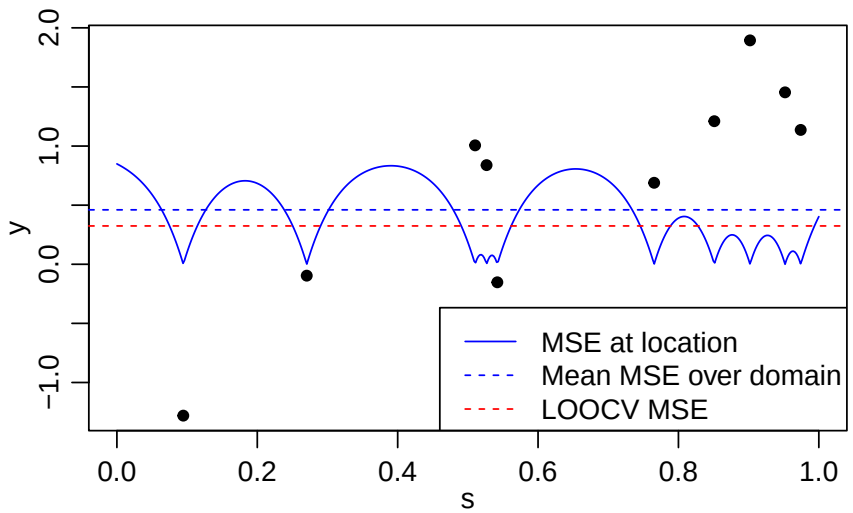

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- **How can we account for nonrepresentativeness in CV methods in space?**

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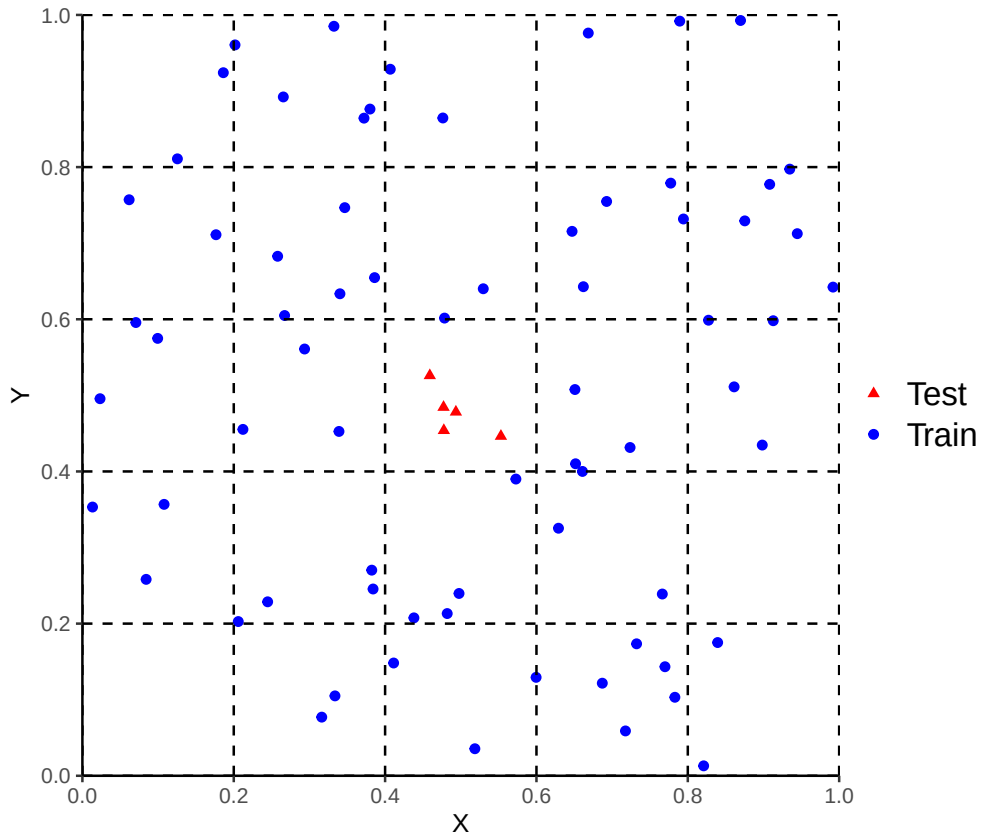

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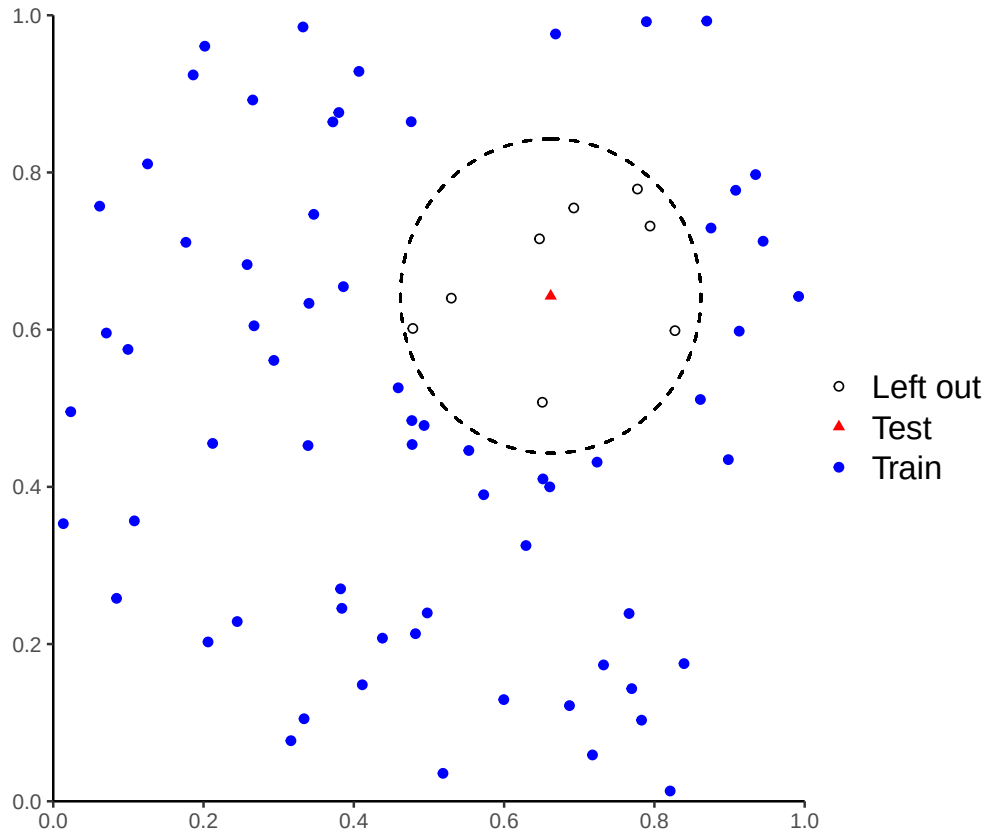
  - Block CV
  - **Buffered CV**



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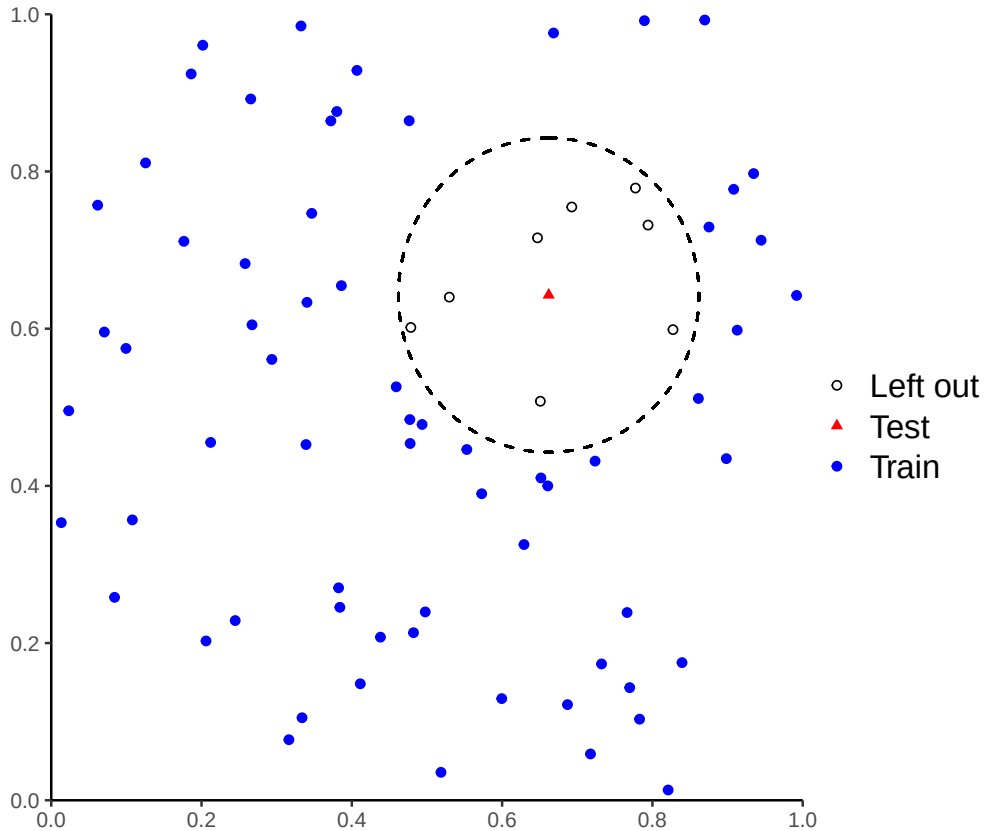
- **Leave group out CV (LGOCV)** Adin et al. (2024)



Defining interpolation error

Let $f(s) = \mathcal{U}(\mathcal{D})$ be the uniform distribution on $\mathcal{D}$. Then the expected interpolation error can be defined as:

$$E_{f,g}[\mathcal{S}(Y(s);\ P_{\mathcal{X}})] = \int_{\mathcal{D}} E[\mathcal{S}(Y(\tilde{s}); P_{\mathcal{X}})|s = \tilde{s}] \cdot f(\tilde{s})\ \mathrm{d}\tilde{s}$$
$$\neq E_{g,g}[\mathcal{S}(Y(s);\ P_{\mathcal{X}})] \qquad \text{(LOOCV)}$$

Rethinking block CV

Block CV with K grid cells, $G_1, \ldots, G_K$ of size $\delta > 0$ can be written:

$$\begin{aligned}
&\frac{1}{K} \sum_{k=1}^{K} \frac{1}{n_k} \sum_{i \in \mathcal{I}^k} \mathcal{S}(y_i; P_{\mathcal{X}_{-\mathcal{I}^k}}) \\
&\approx \frac{1}{K} \sum_{k=1}^{K} \int_{G_k} E_g[\mathcal{S}(Y(\tilde{s}); P_{\mathcal{X}}) | s = \tilde{s}] \cdot \frac{1}{|G_k|} \, \mathrm{d}\tilde{s} \\
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Problems:

- What if some grid cells have no samples?
- How do you choose the grid resolution? Too small $\rightarrow$ LOOCV, too large $\rightarrow$ too much extrapolation

Re-Rethinking block CV: Voronoi Cell CV

Let $V_1, \ldots, V_n \subset \mathcal{D}$ be Voronoi cells generated by observation locations $s_1, \ldots, s_n$. Then:

$$E_{f,g}[\mathcal{S}(Y(s); P_{\mathcal{X}})]$$

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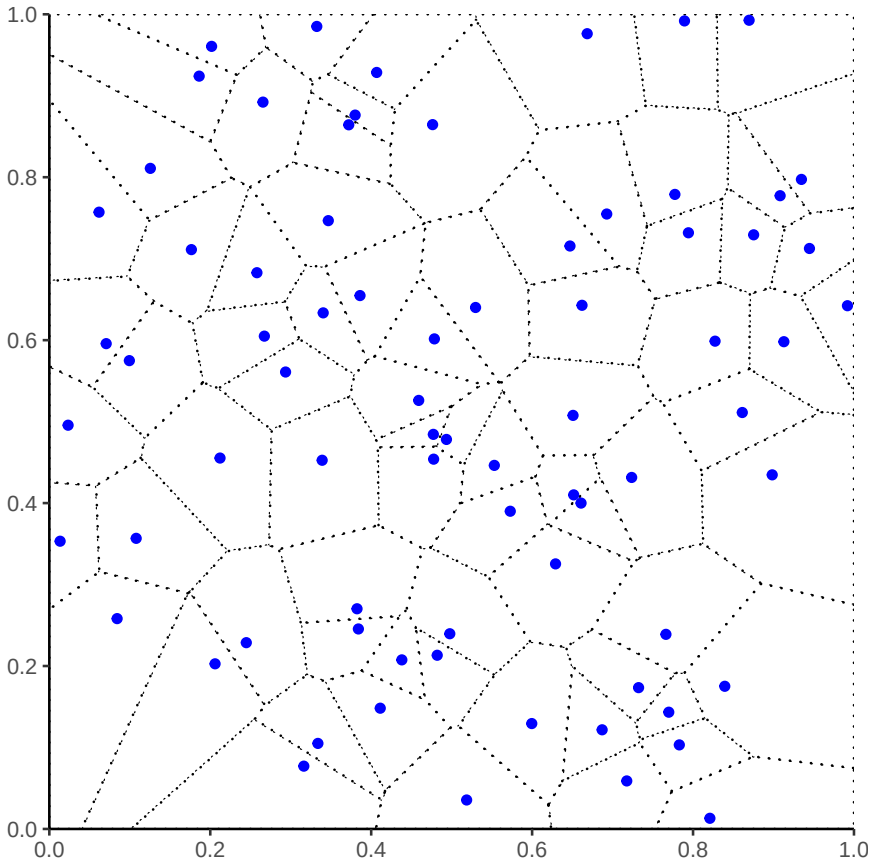
- $|V_i|/|\mathcal{D}|$ is asymptotically unbiased for $f(s_i)/g(s_i)$, an importance weight (Barr and Schoenberg, 2010)
- This is importance weighted CV (IWCV, Sugiyama et al. 2007), domain adaptation (Farahani et al., 2021)

Voronoi Cell CV

$$\text{VCCV} = \sum_{i=1}^{n} \frac{|V_i|}{|\mathcal{D}|} \mathcal{S}(y_i; P_{\mathcal{X}_{-i}}).$$



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$$\text{Var}(\sigma^2_\epsilon(s)) = \begin{cases} 1 & s \text{ in mountains,} \\ 0.1^2 & s \text{ in plains.} \end{cases}$$

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- R: level of oversampling in the mountains

Interval score

- The interval score (Gneiting and Raftery, 2007) at significance level $\alpha \in (0, 1)$ is:

$$\begin{aligned} \mathsf{IS}_\alpha(Y_i; P_i) &= (u_i - l_i) + \frac{2}{\alpha}(l_i - Y_i) I\{Y_i < l_i\} \\ &\quad + \frac{2}{\alpha}(Y_i - u_i) I\{Y_i > u_i\} \\ \mathsf{LOO} &= \frac{1}{n} \sum_{i=1}^{n} \mathsf{IS}_\alpha(Y_i; P_i) \\ \mathsf{IW} &= \sum_{i=1}^{n} w_i \mathsf{IS}_\alpha(Y_i; P_i) \end{aligned}$$

Scoring models

Let

$$\Delta^{\text{LOO}} = \text{LOO}_1 - \text{LOO}_2, \qquad \Delta^{\text{IW}} = \text{IW}_1 - \text{IW}_2, \qquad \text{and}$$

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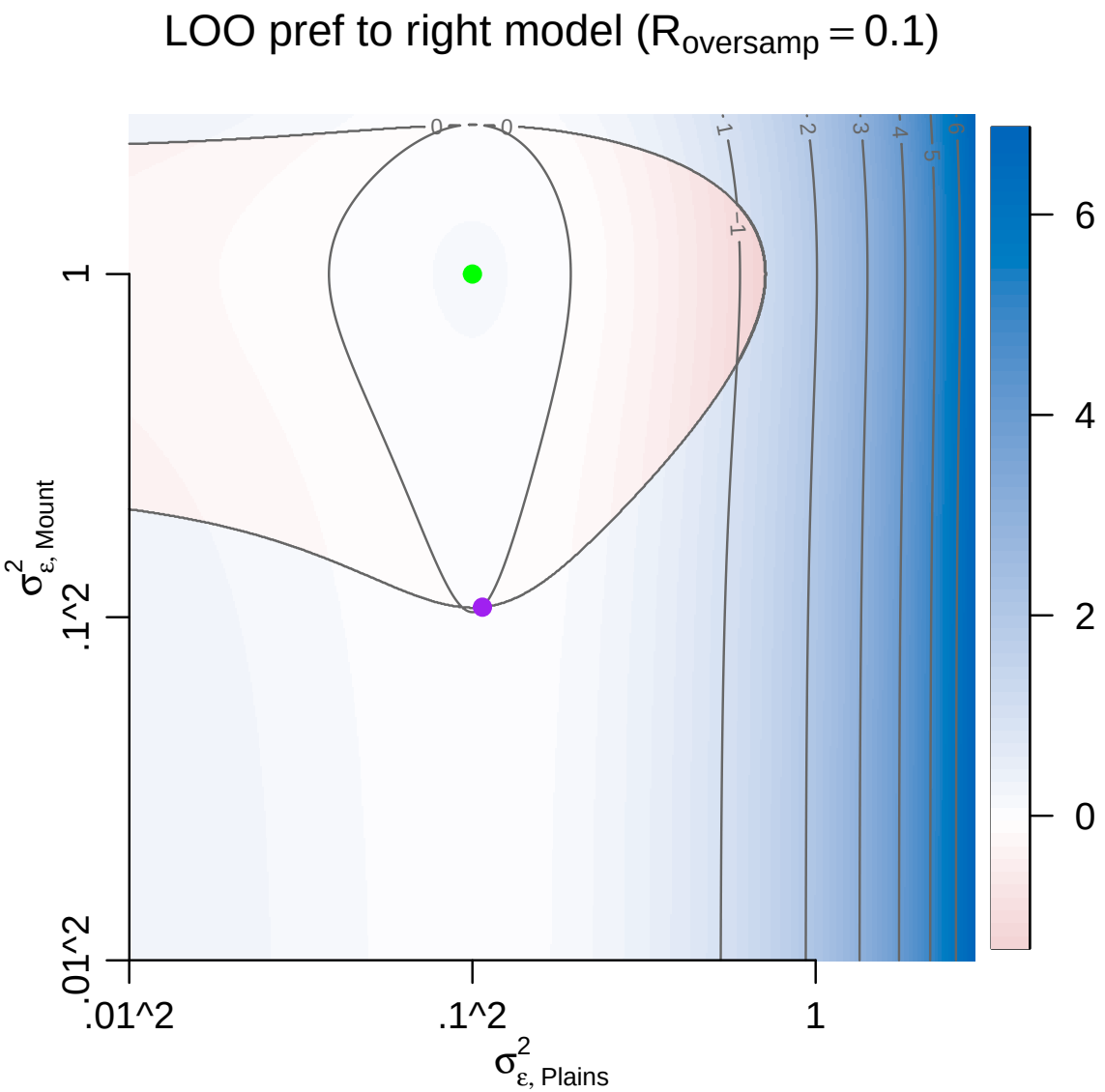
Under infill asymptotics, use the scores/metrics:

- Probability of selecting the best model
- Mean preference towards best model:

$$|E[\Delta^{\text{LOO}}]|\text{sign}\{E[\Delta^{\text{LOO}}] \cdot E[\Delta^{\mathcal{D}}]\}$$

LOO preference of best model vs nonrepresentativeness



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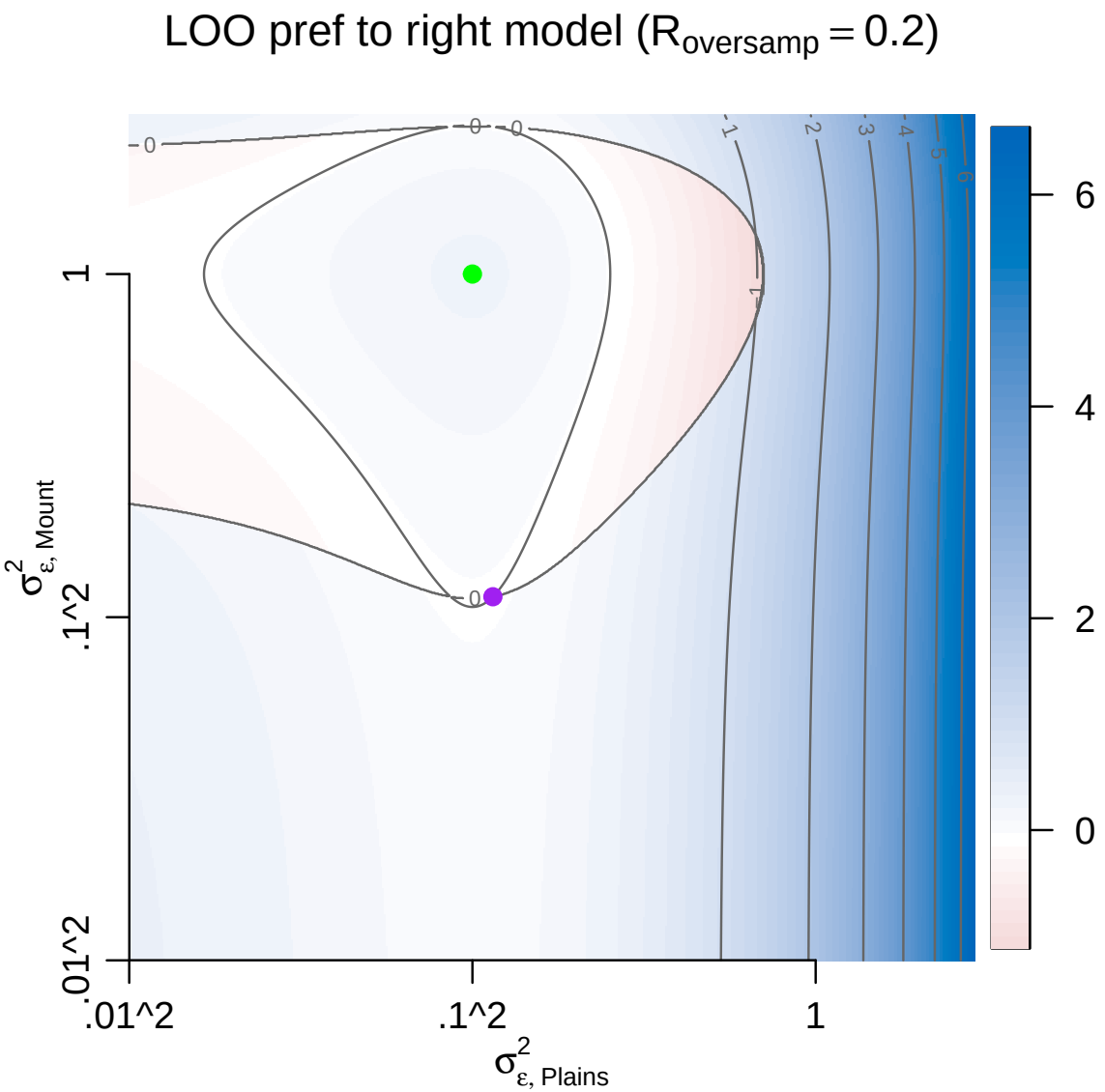

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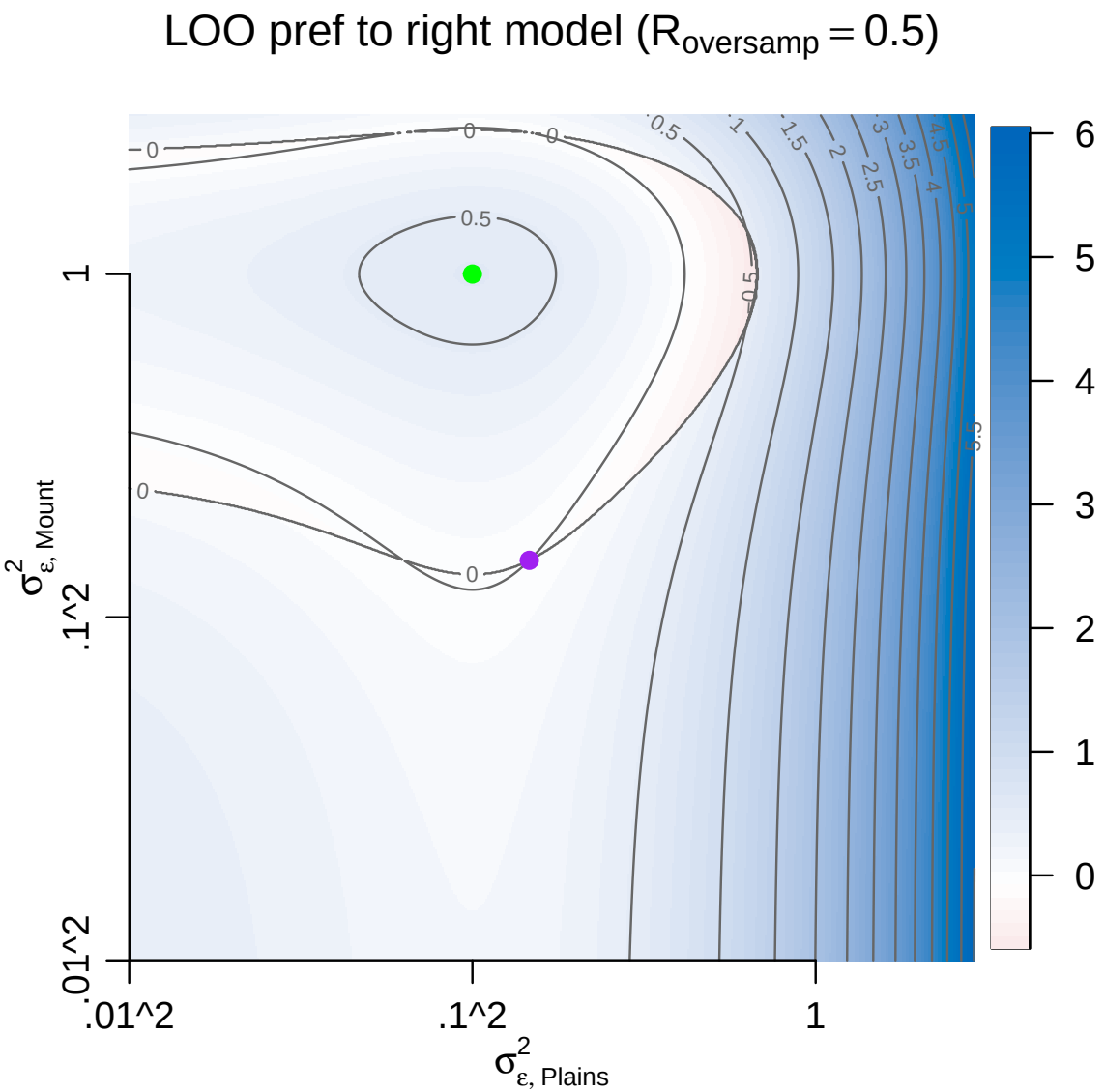

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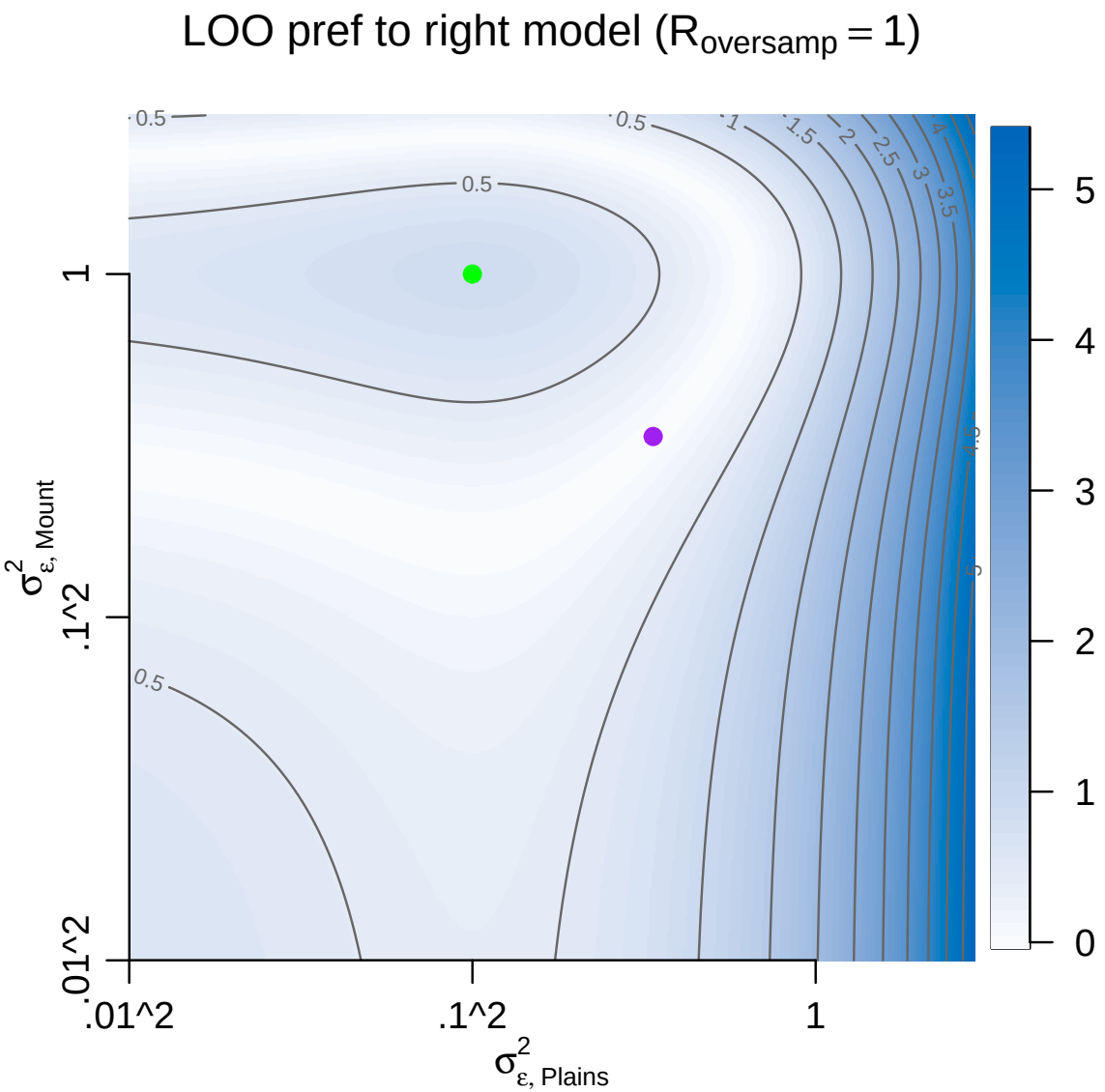

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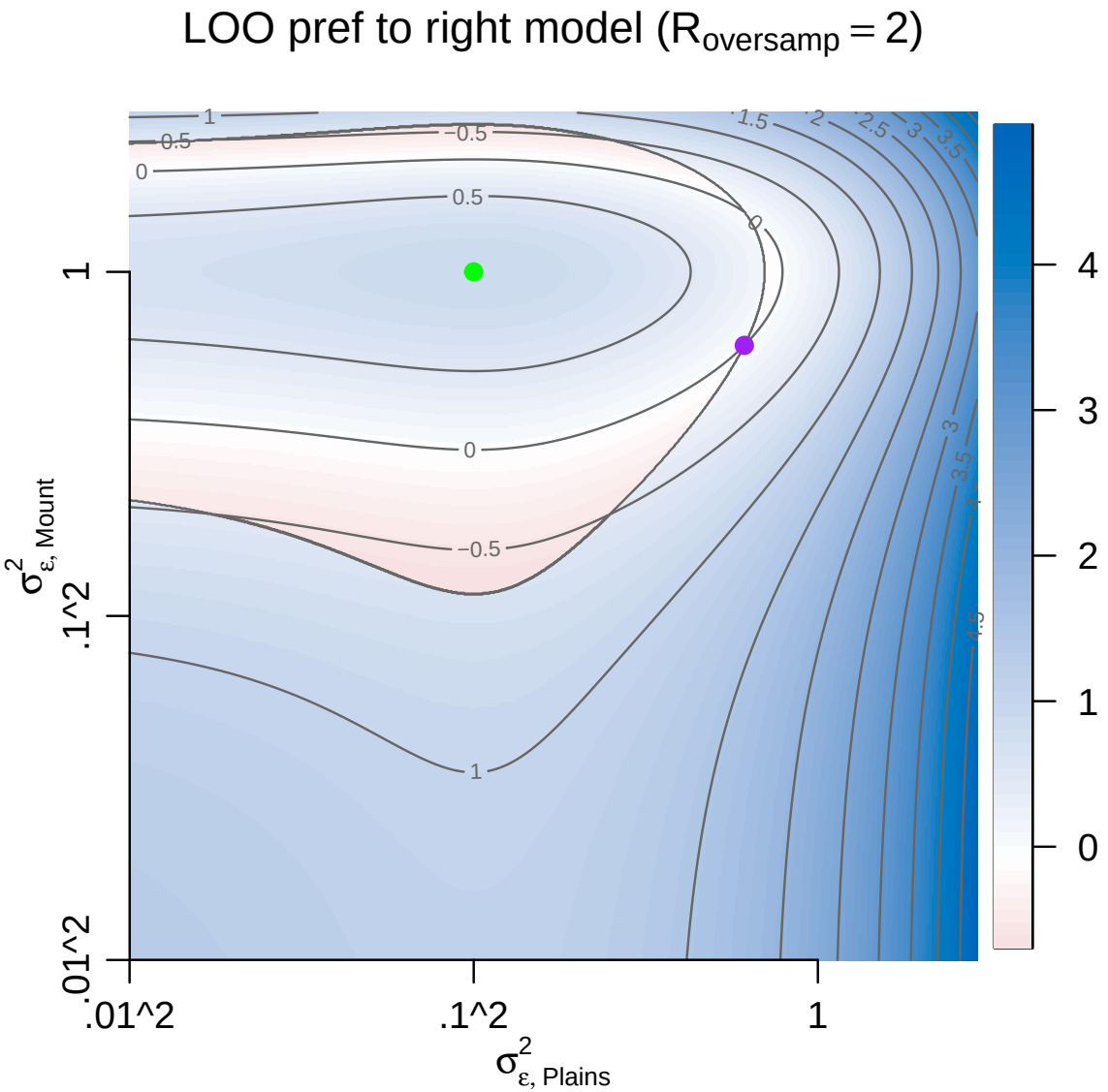

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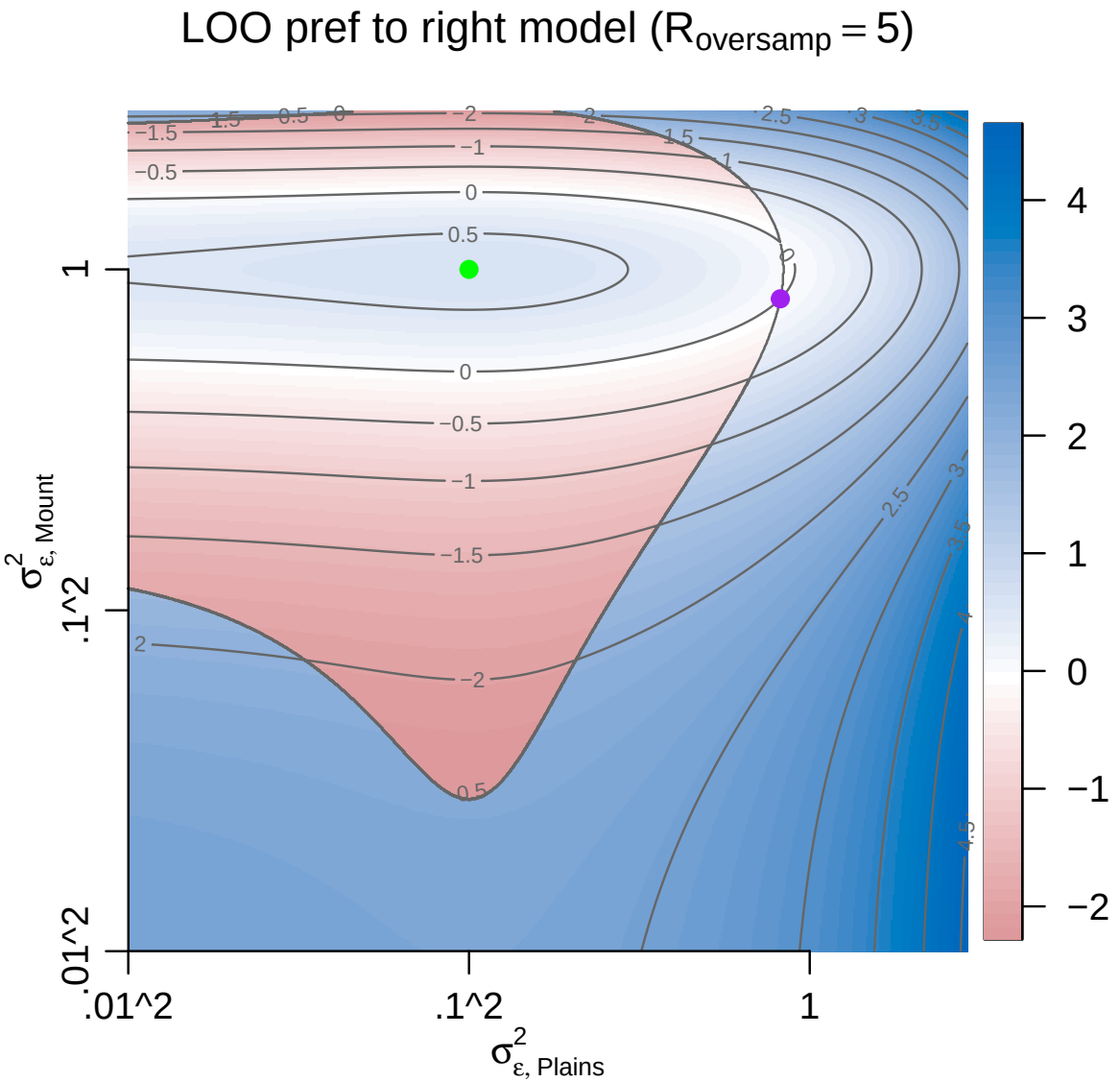

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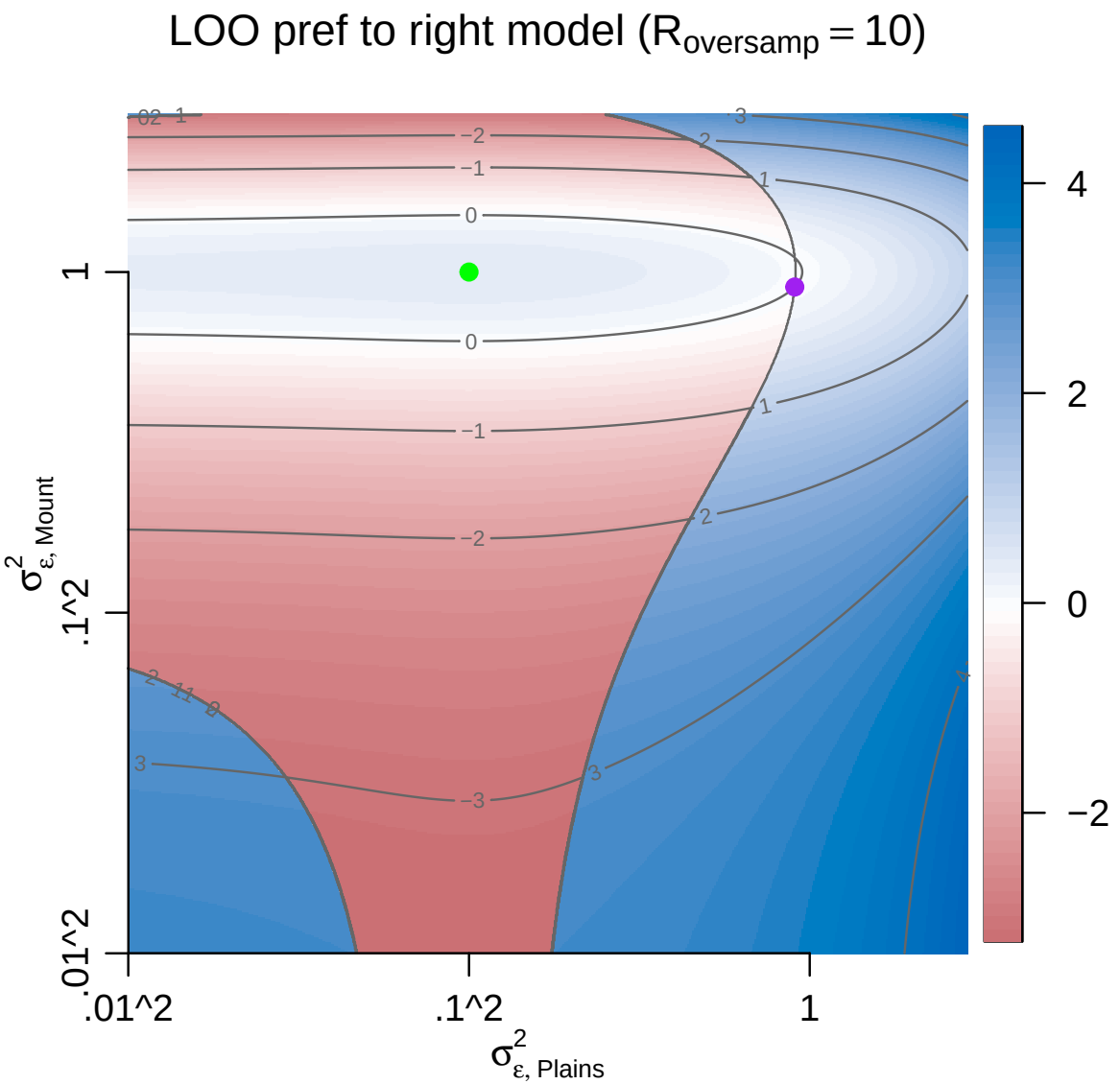
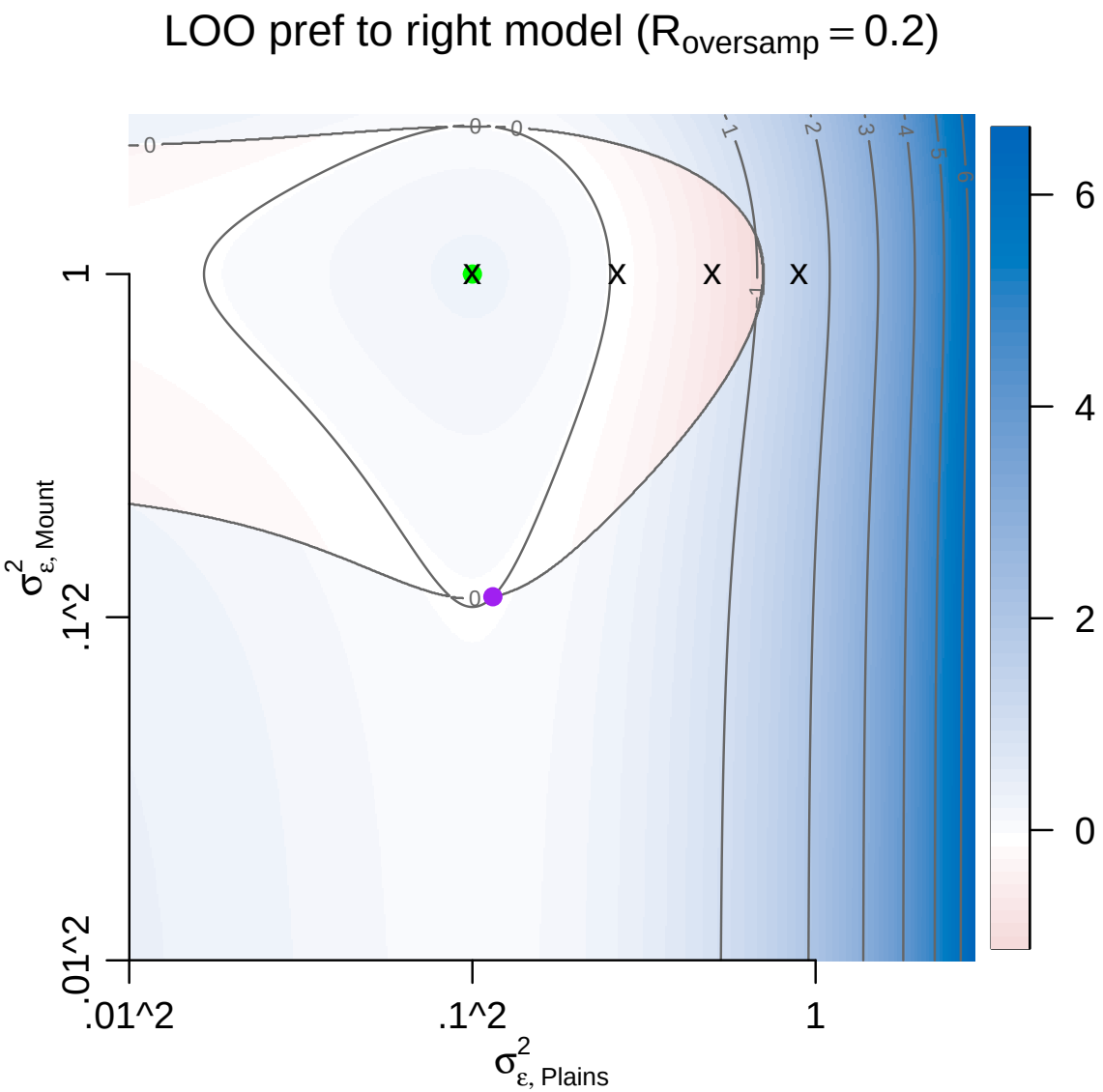
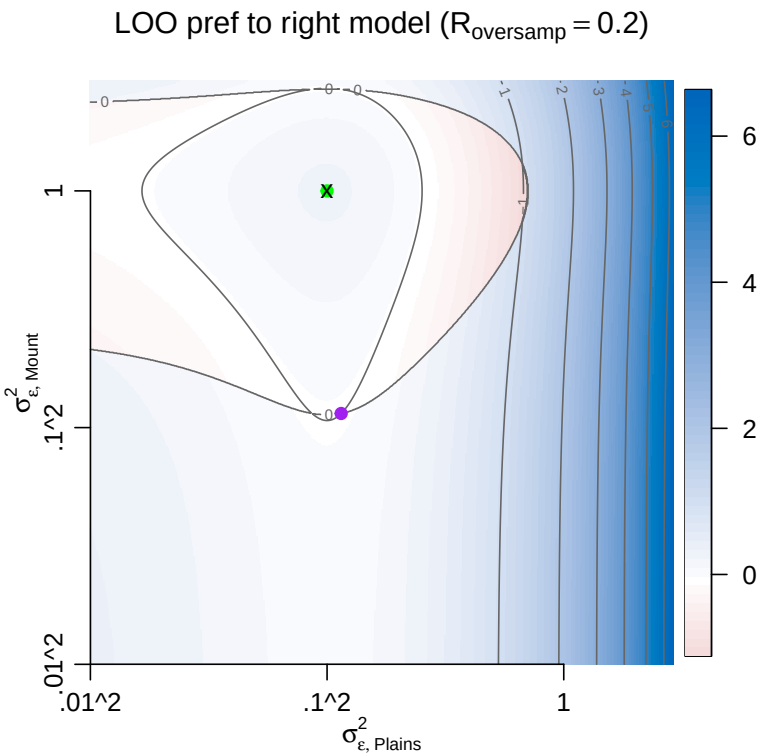
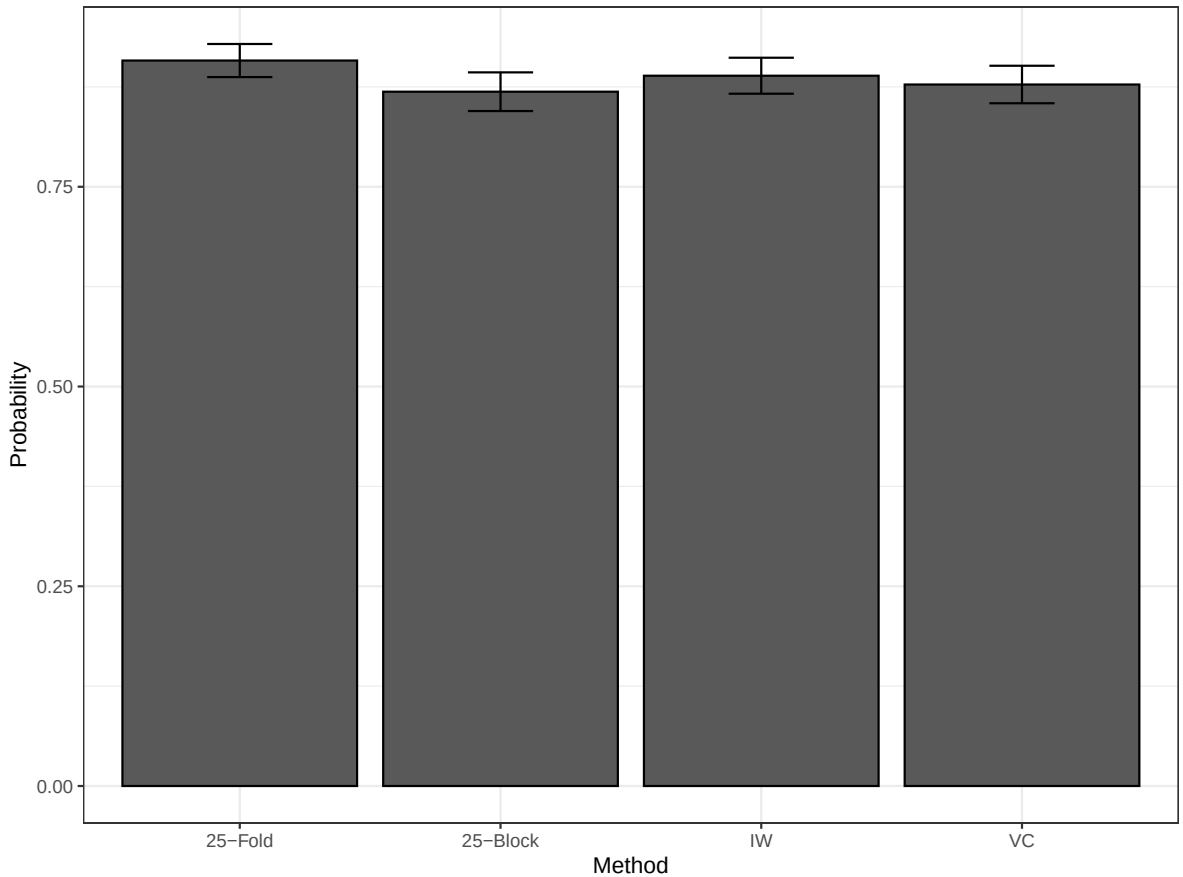


Nonstationary error variance: Simulations

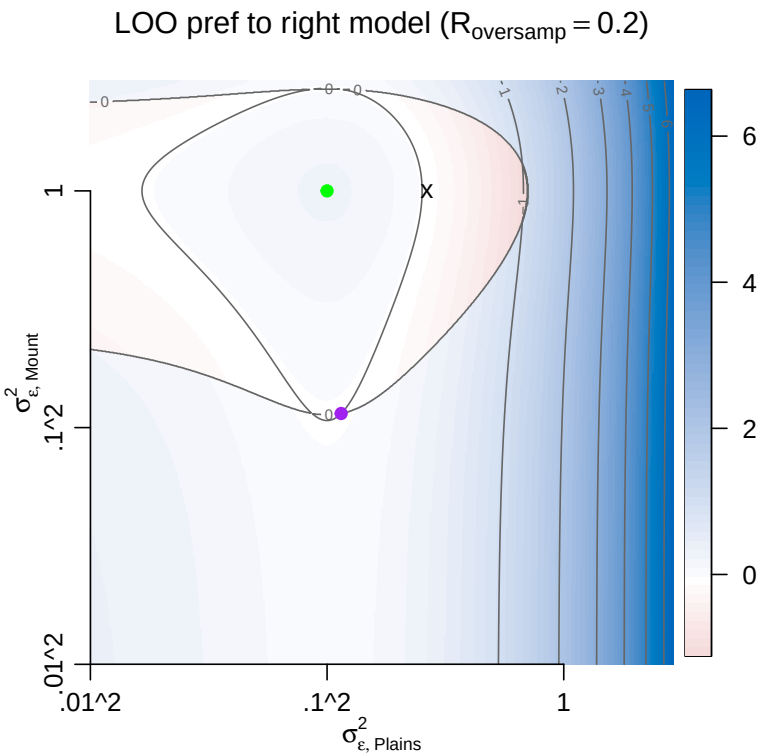


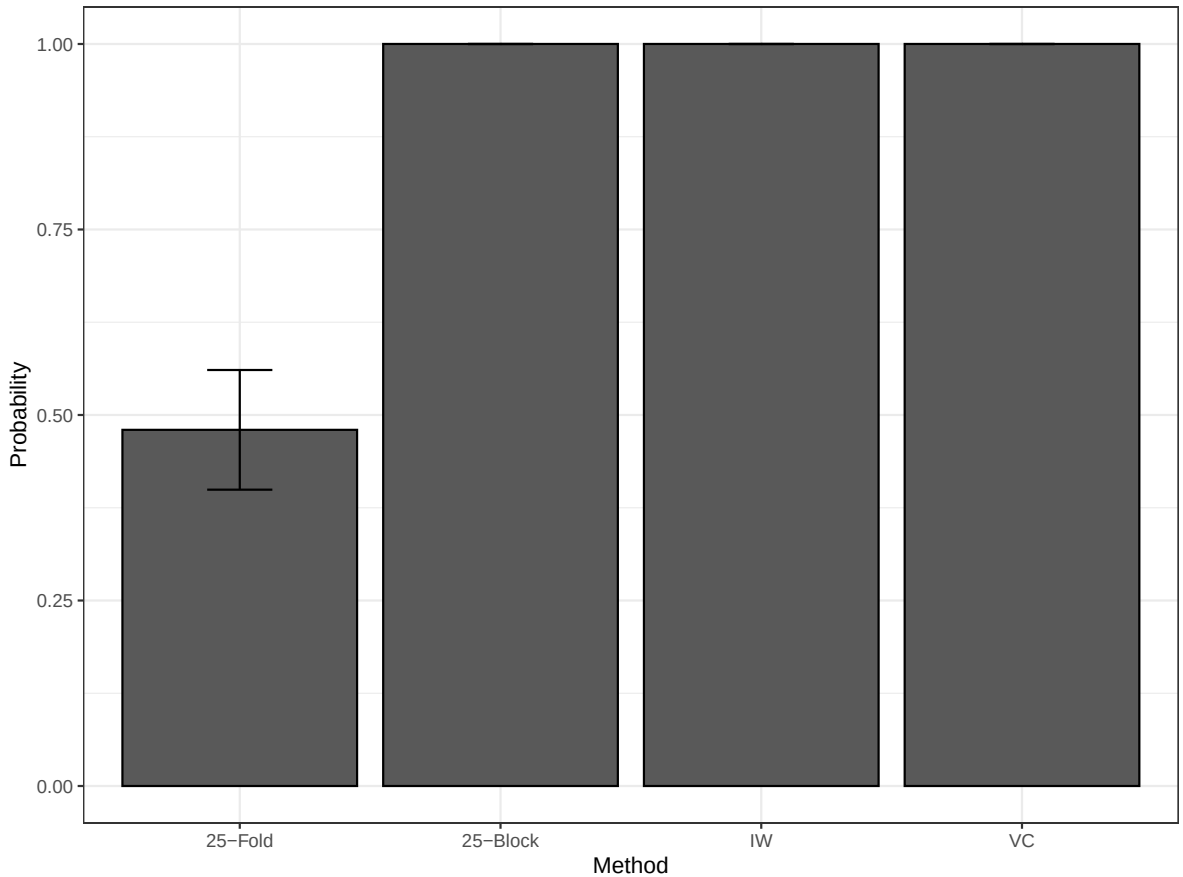
Scenario 1: Comparison vs true model
$n = 50$, 25-fold CV





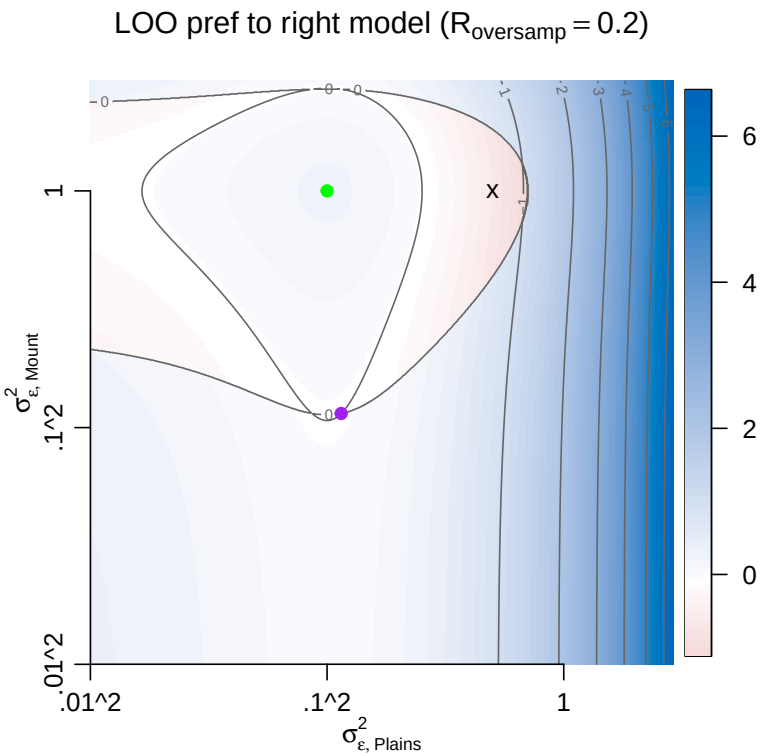
Scenario 2: Equivalent LOO models
$n = 2000$, 25-fold CV

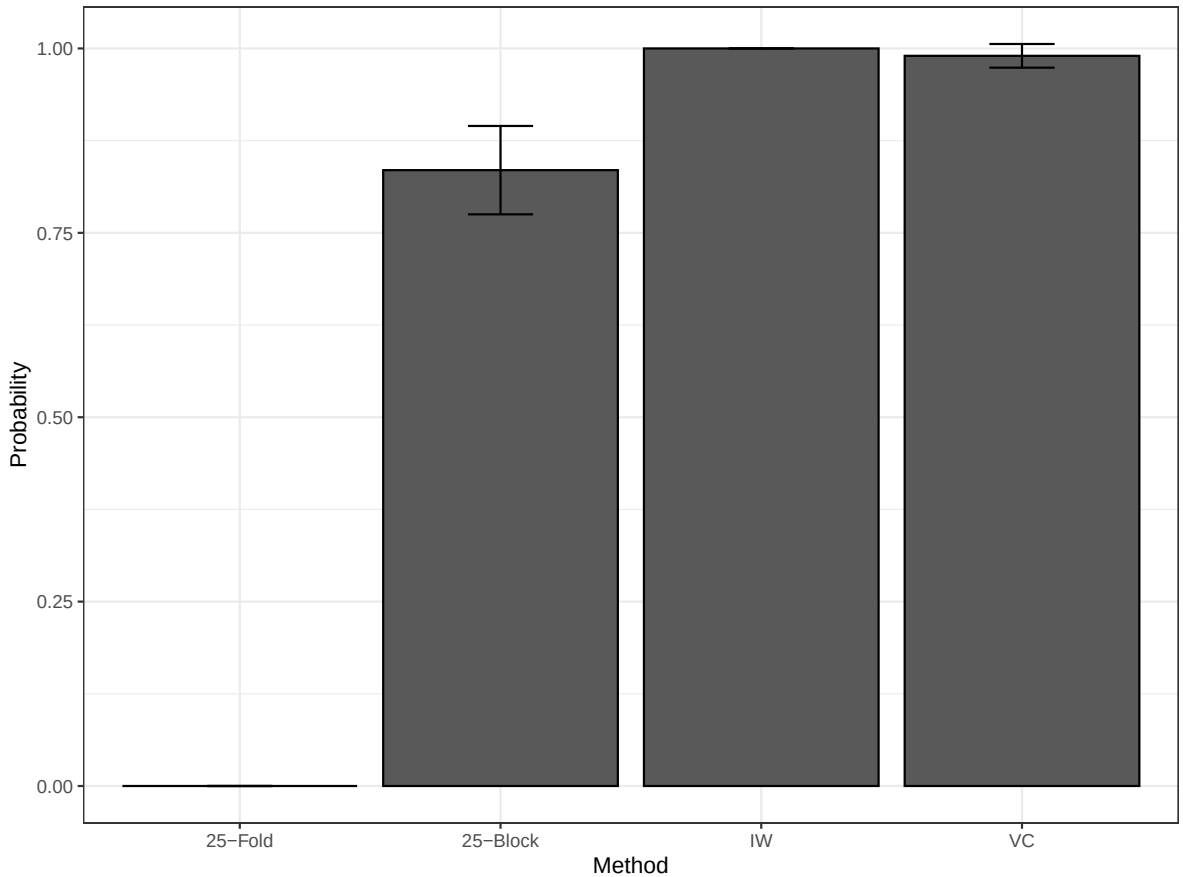




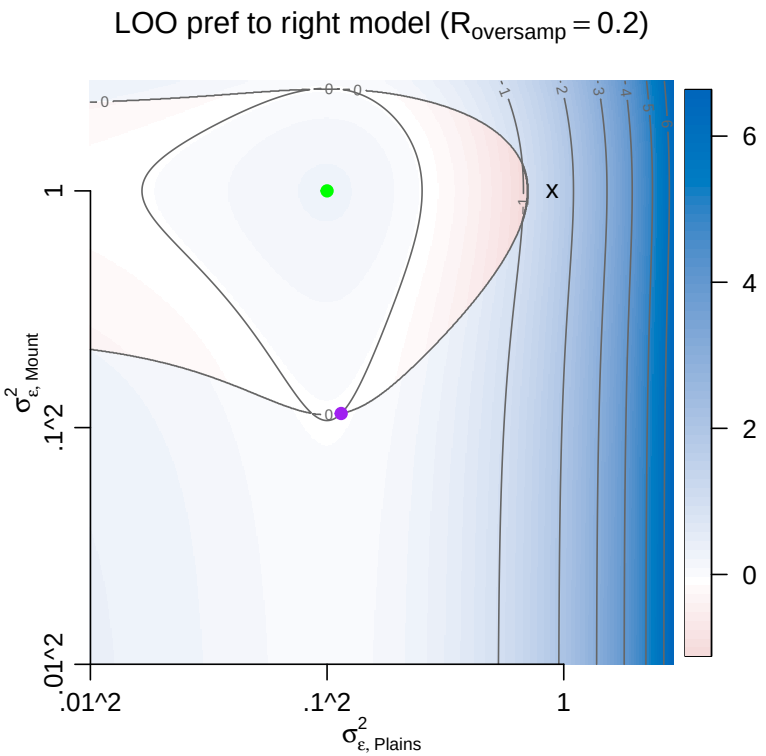
Scenario 3: Better model, worse under LOO

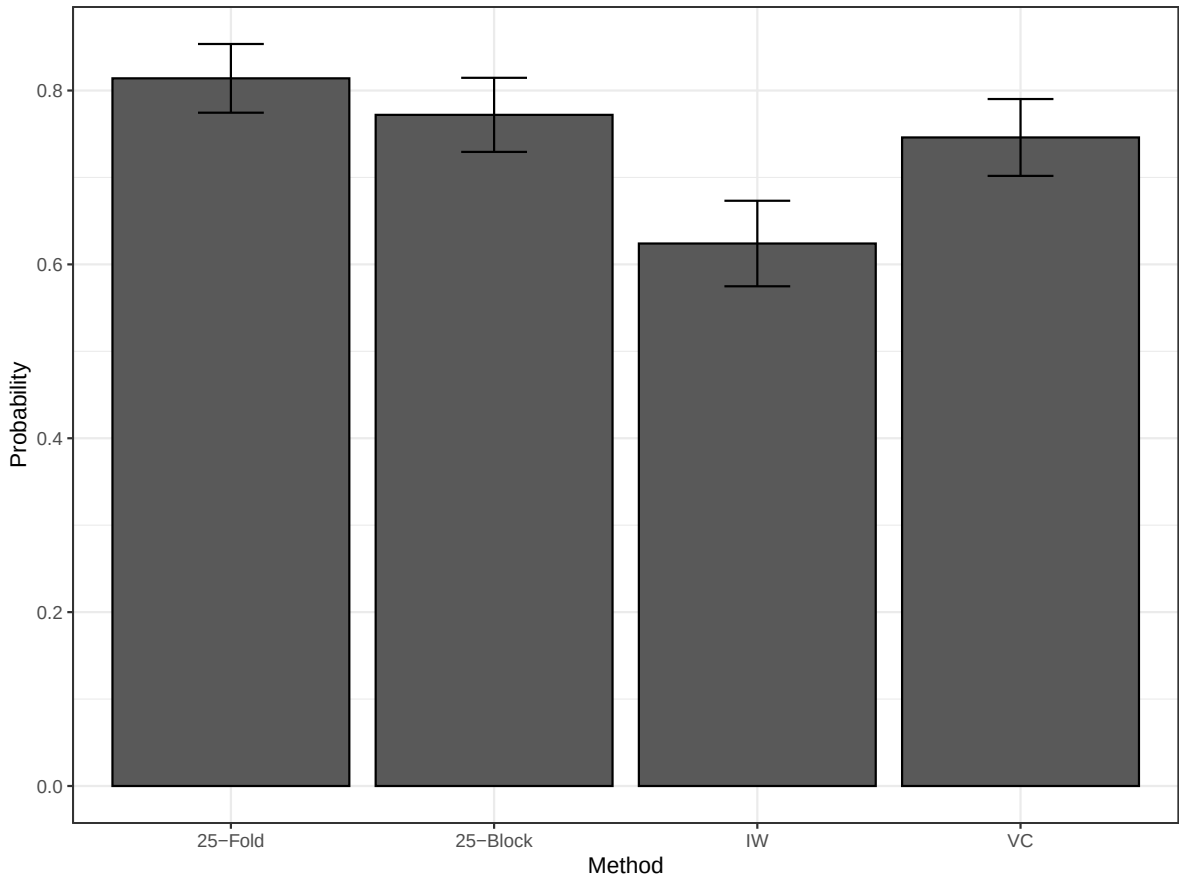
$n = 2000$, 25-fold CV





Scenario 4: Advantage of LOO's lower variance
$n = 200$, 25-fold CV





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- VC CV at times performs better than IW CV due to its accounting for sampling variability
- VC CV is simple and requires no tuning parameters

Limitations, potential future work

- No ‘one size fits all’ solution
- Extension to space-time
- Methods for variance reduction, weight smoothing

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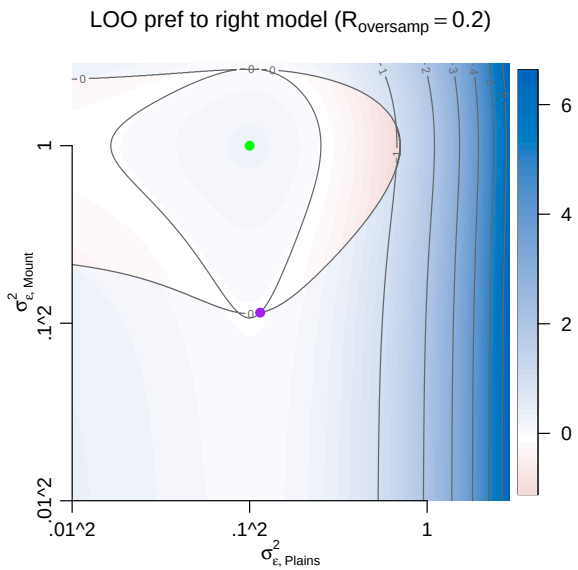
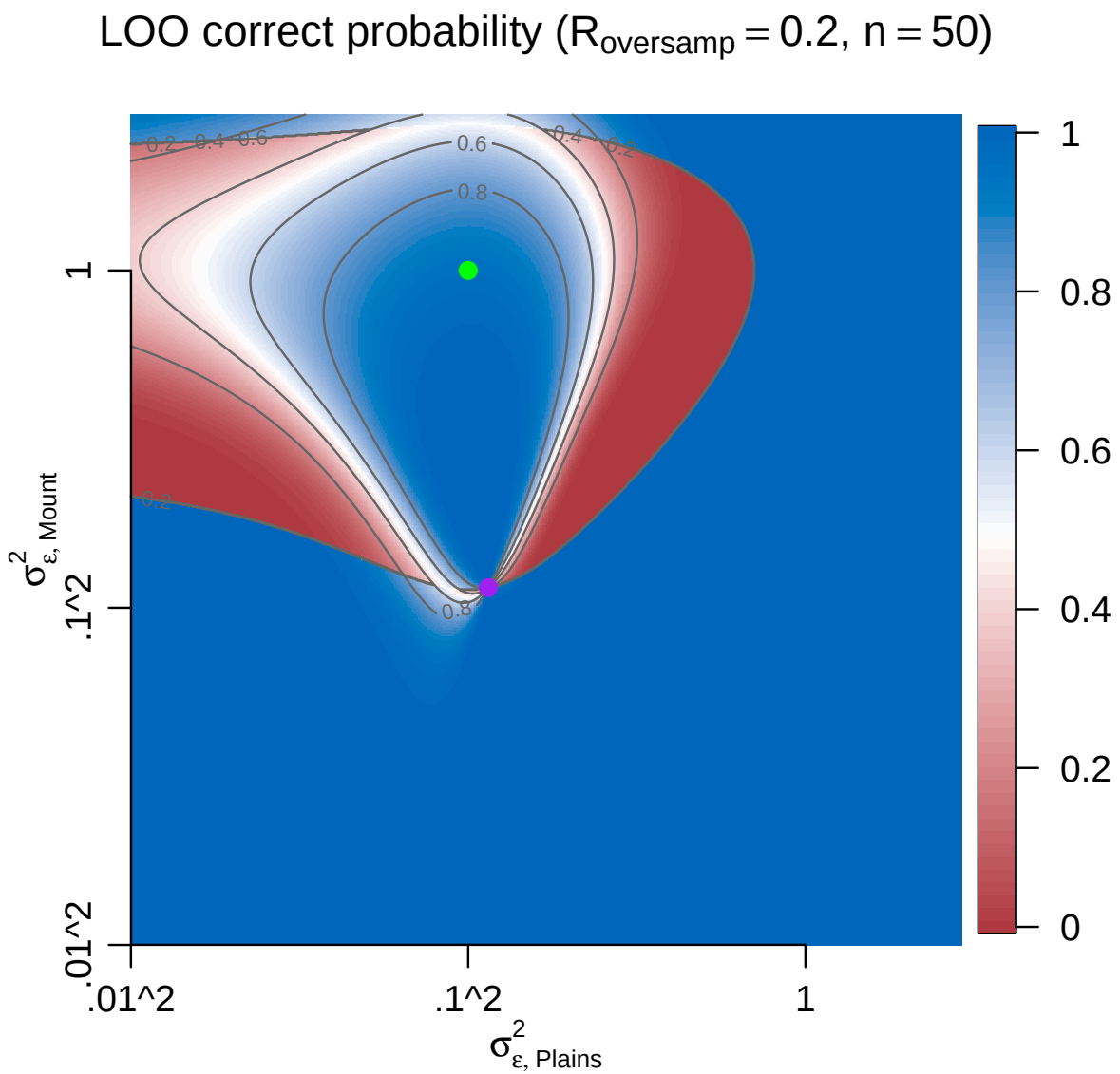
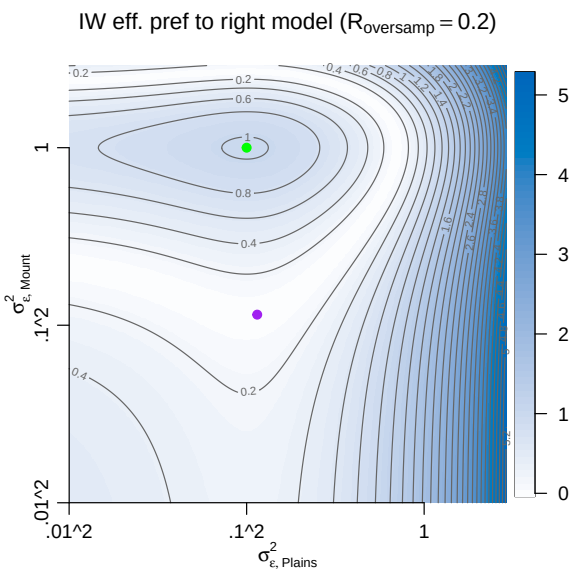
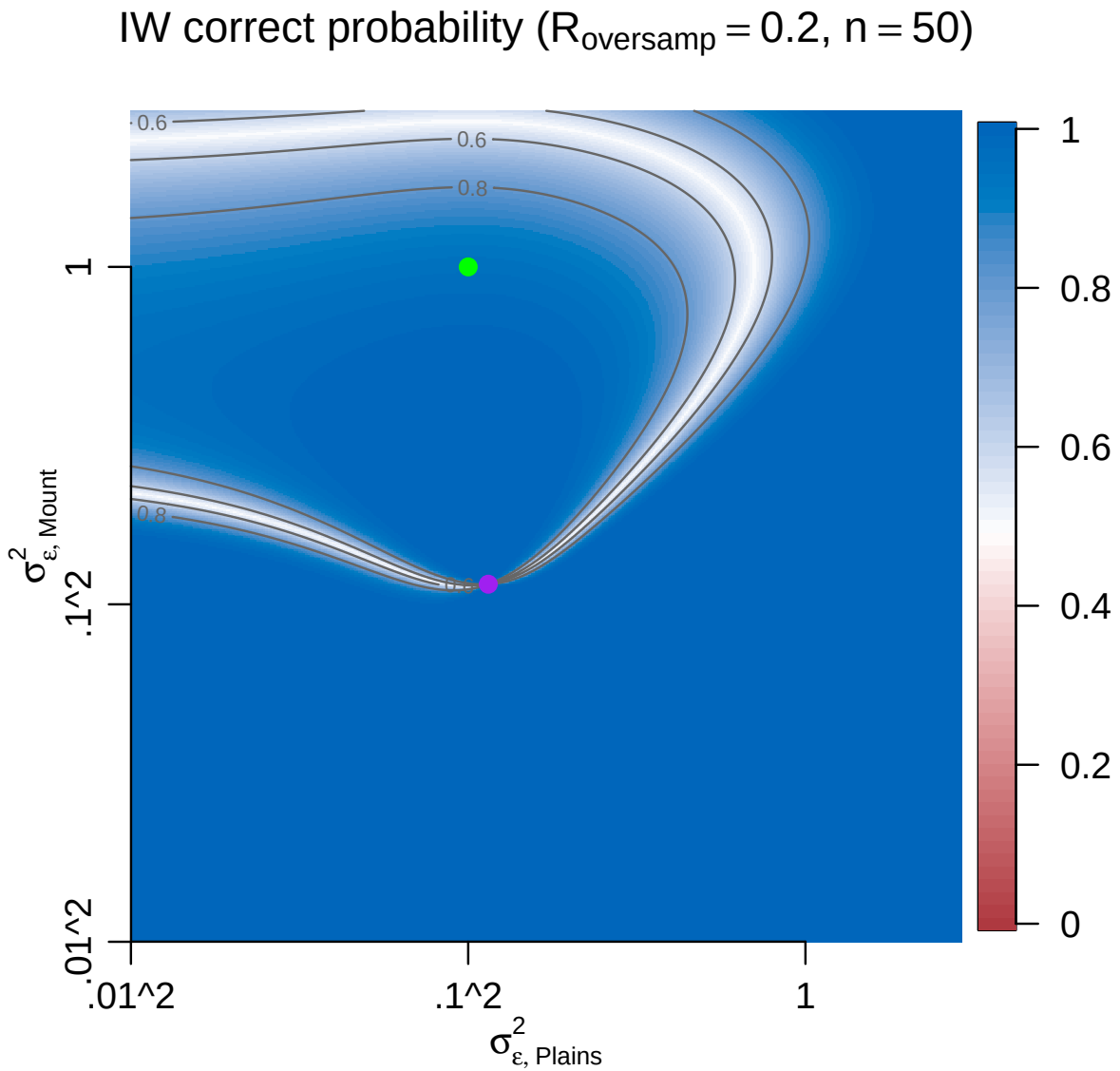
LOO correct model selection probability, $R = 0.2$, $n = 50$



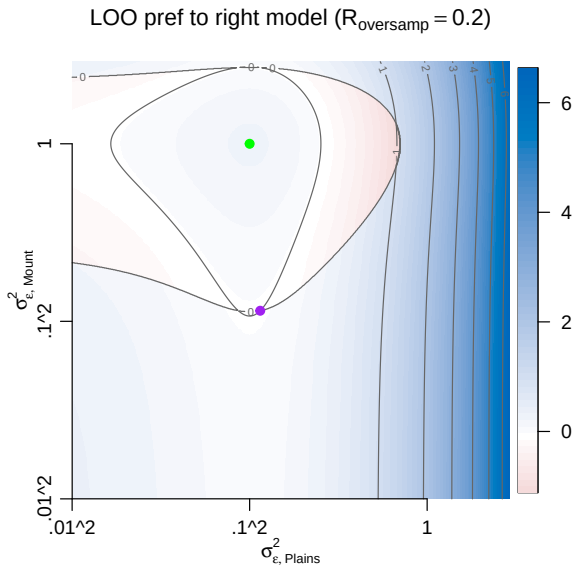


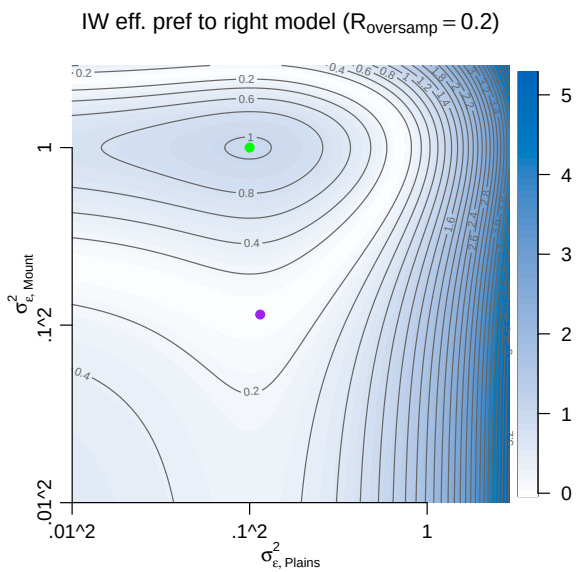
IW correct model selection probability, $R = 0.2$, $n = 50$

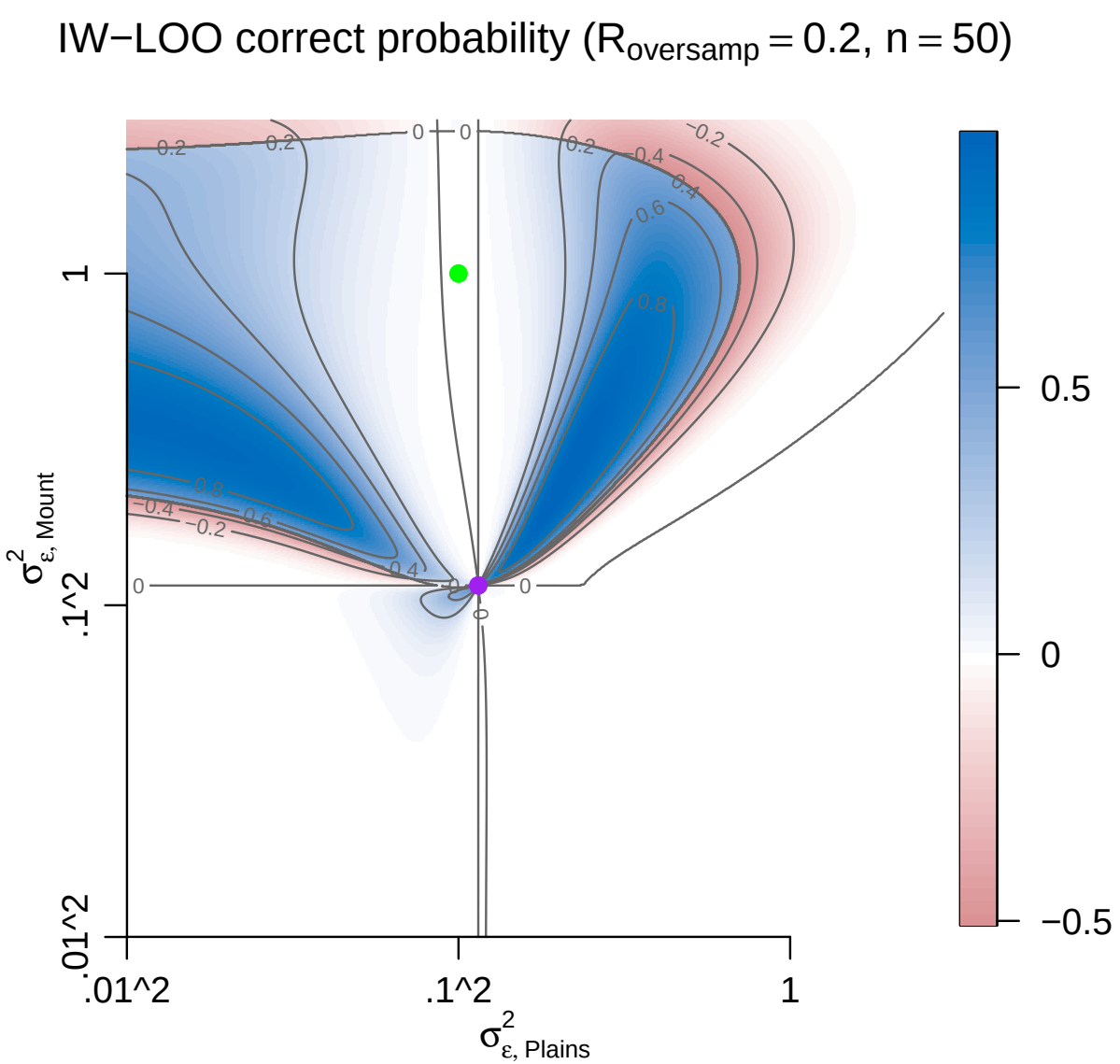




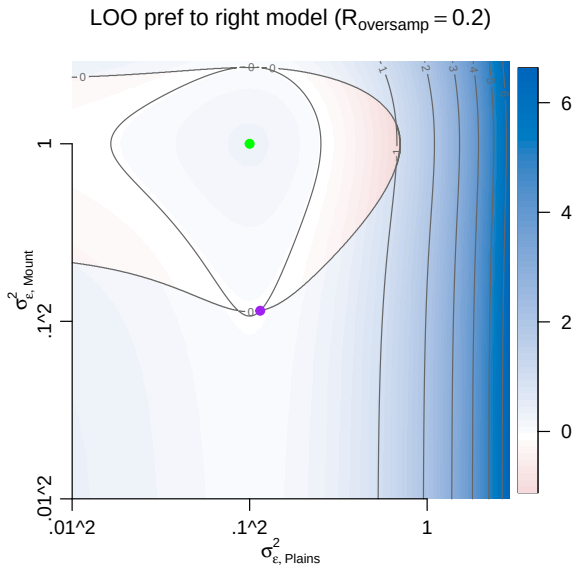
IW-LOO correct selection probability, $R = 0.2$, $n = 50$

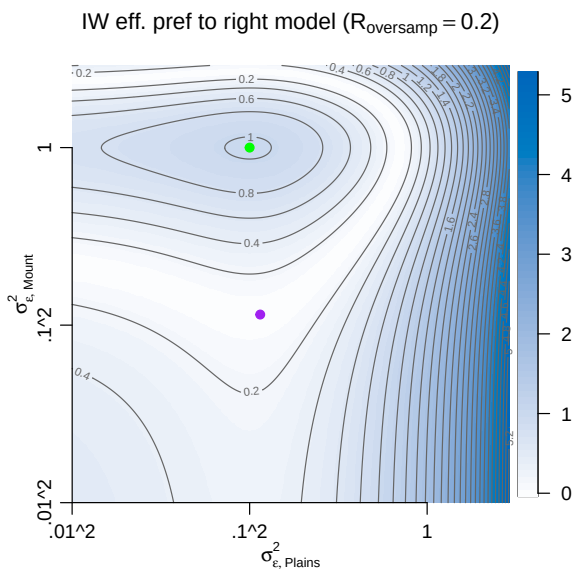


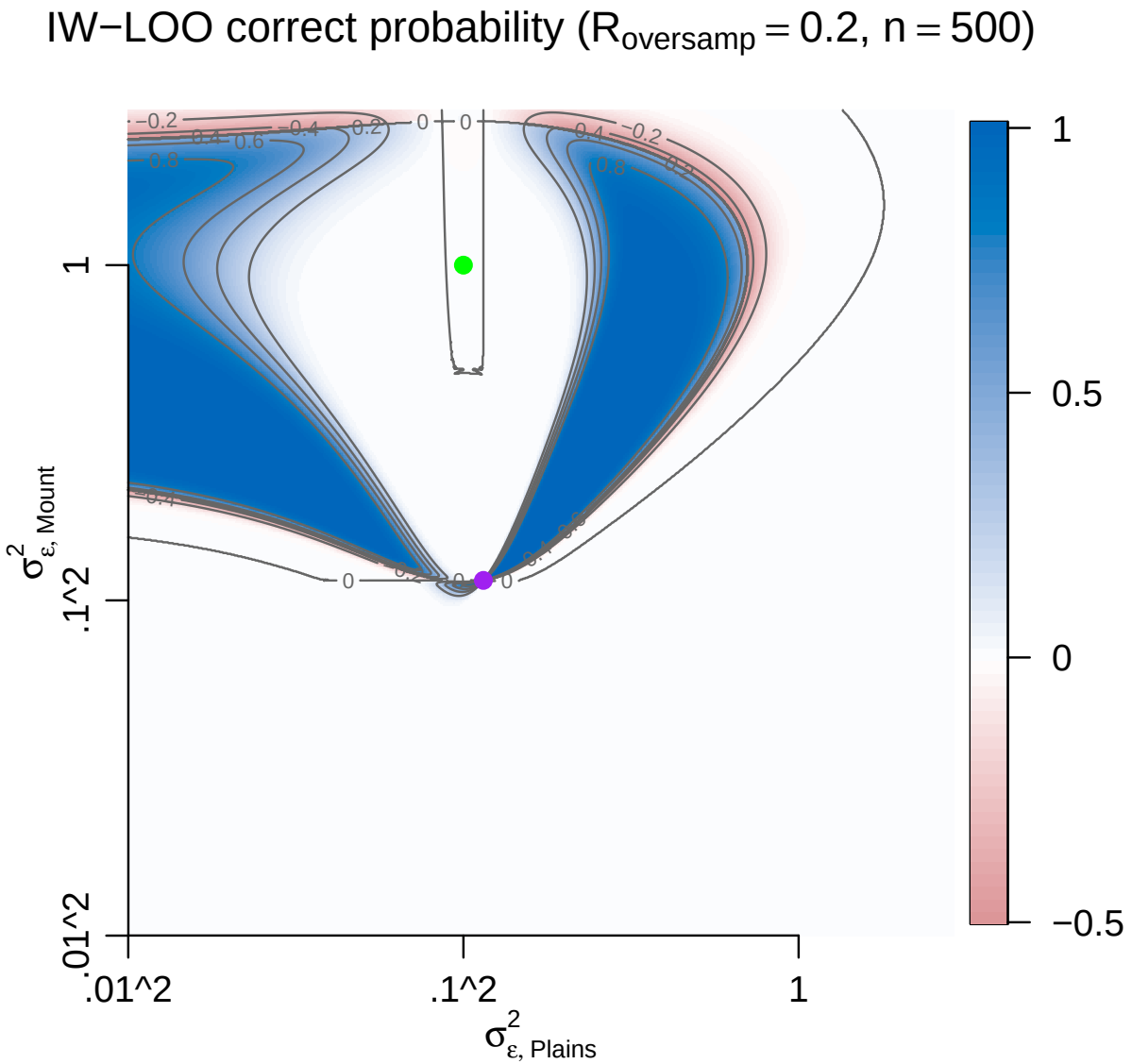




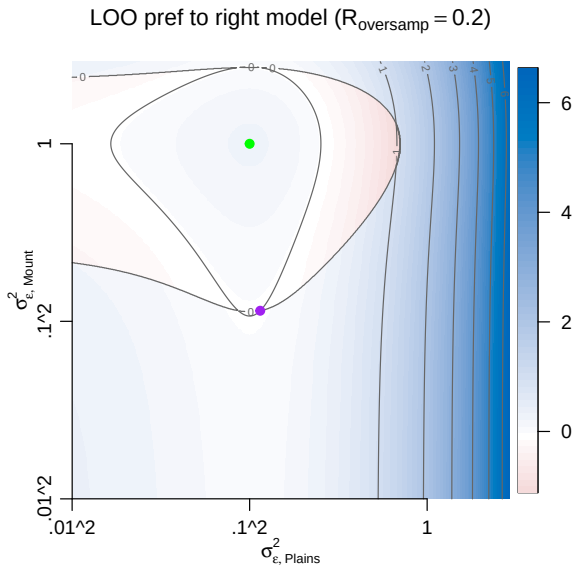
IW-LOO correct selection probability, $R = 0.2$, $n = 500$

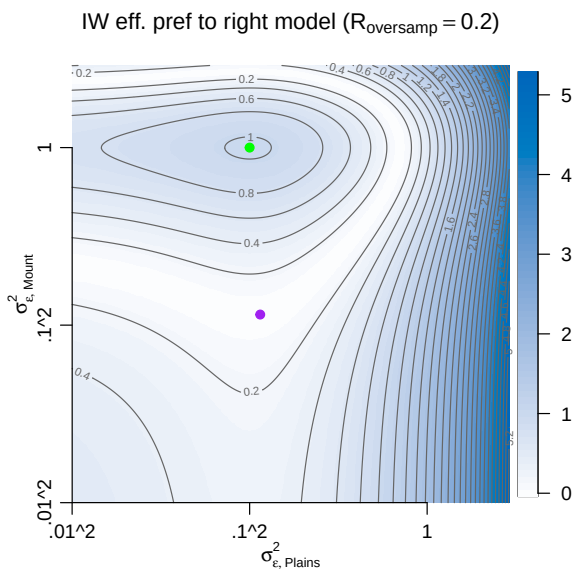


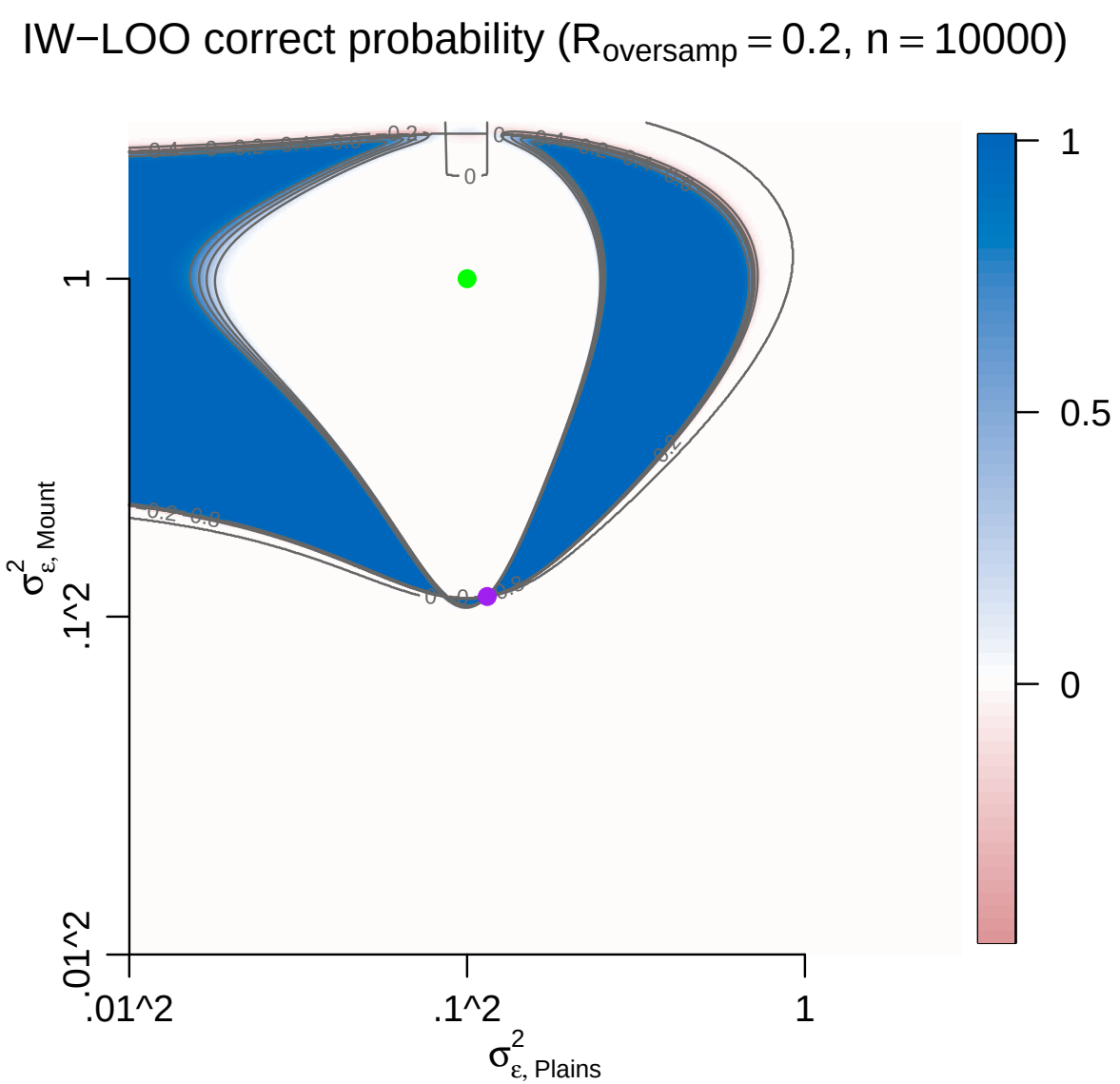




IW-LOO correct selection probability, $R = 0.2$, $n = 10000$







Scoring models

Let

$$\Delta^{\text{LOO}} = \text{LOO}_1 - \text{LOO}_2, \qquad \Delta^{\text{IW}} = \text{IW}_1 - \text{IW}_2, \qquad \text{and}$$

$$\Delta^{\mathcal{D}} = E_{g,g}[\Delta^{\text{IW}}] = E_{f,f}[\Delta^{\text{LOO}}].$$

Under infill asymptotics, use the scores/metrics:

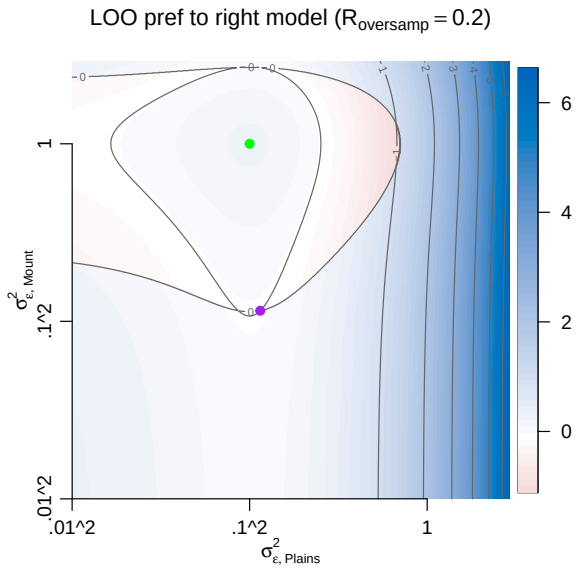
- Probability of selecting the best model
- Mean preference towards best model:

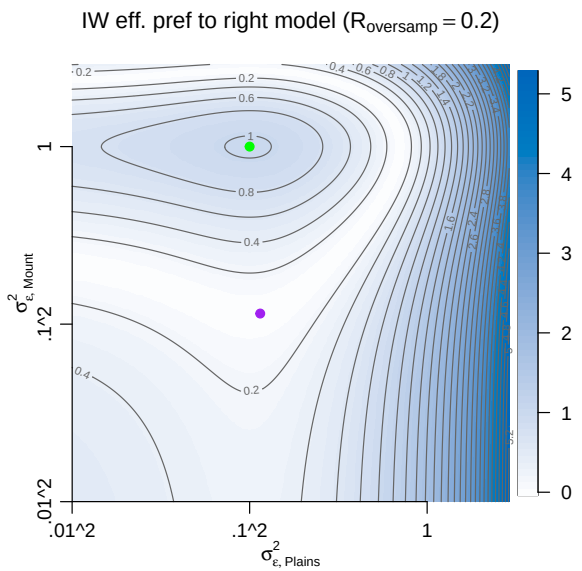
$$|E[\Delta^{\text{LOO}}]|\text{sign}\{E[\Delta^{\text{LOO}}] \cdot E[\Delta^{\mathcal{D}}]\}$$

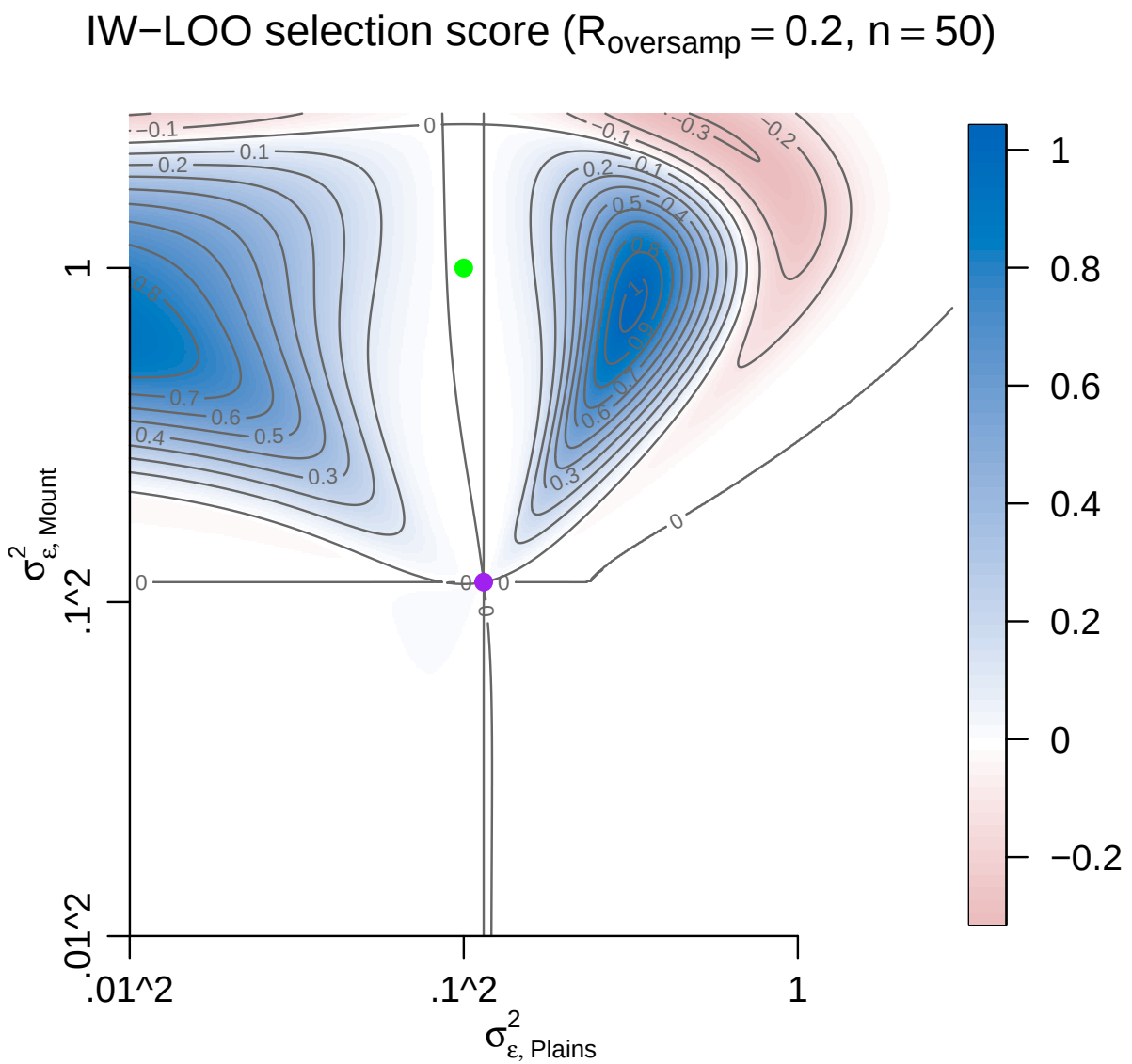
- Expected selection score:

$$E[|\Delta^{\mathcal{D}}|(I_{\text{correct}} - I_{\text{wrong}})]$$

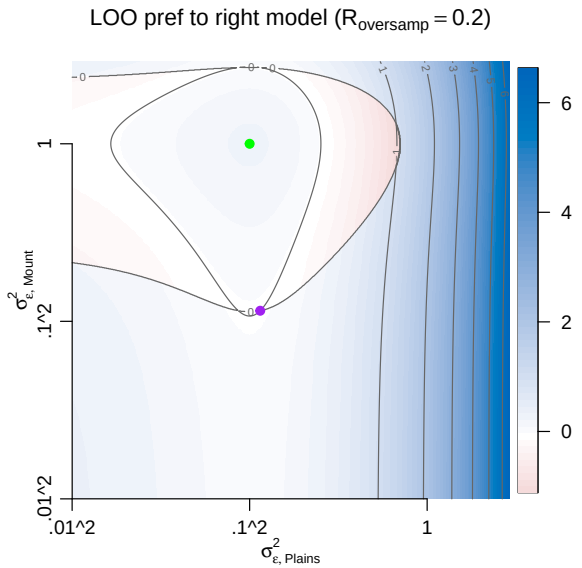
IW-LOO expected selection score, $R = 0.2$, $n = 50$

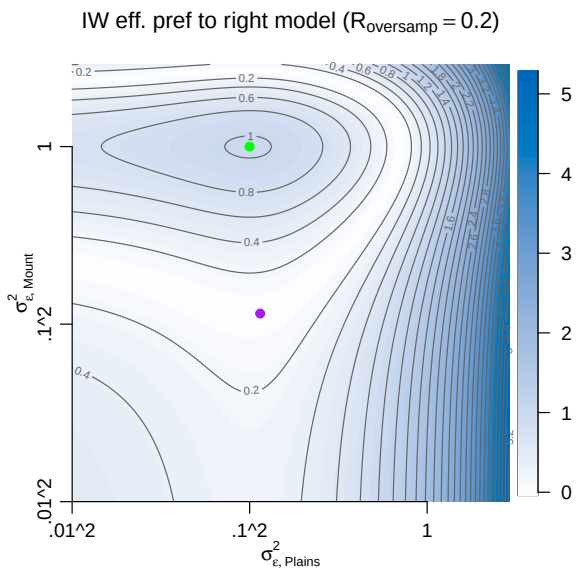


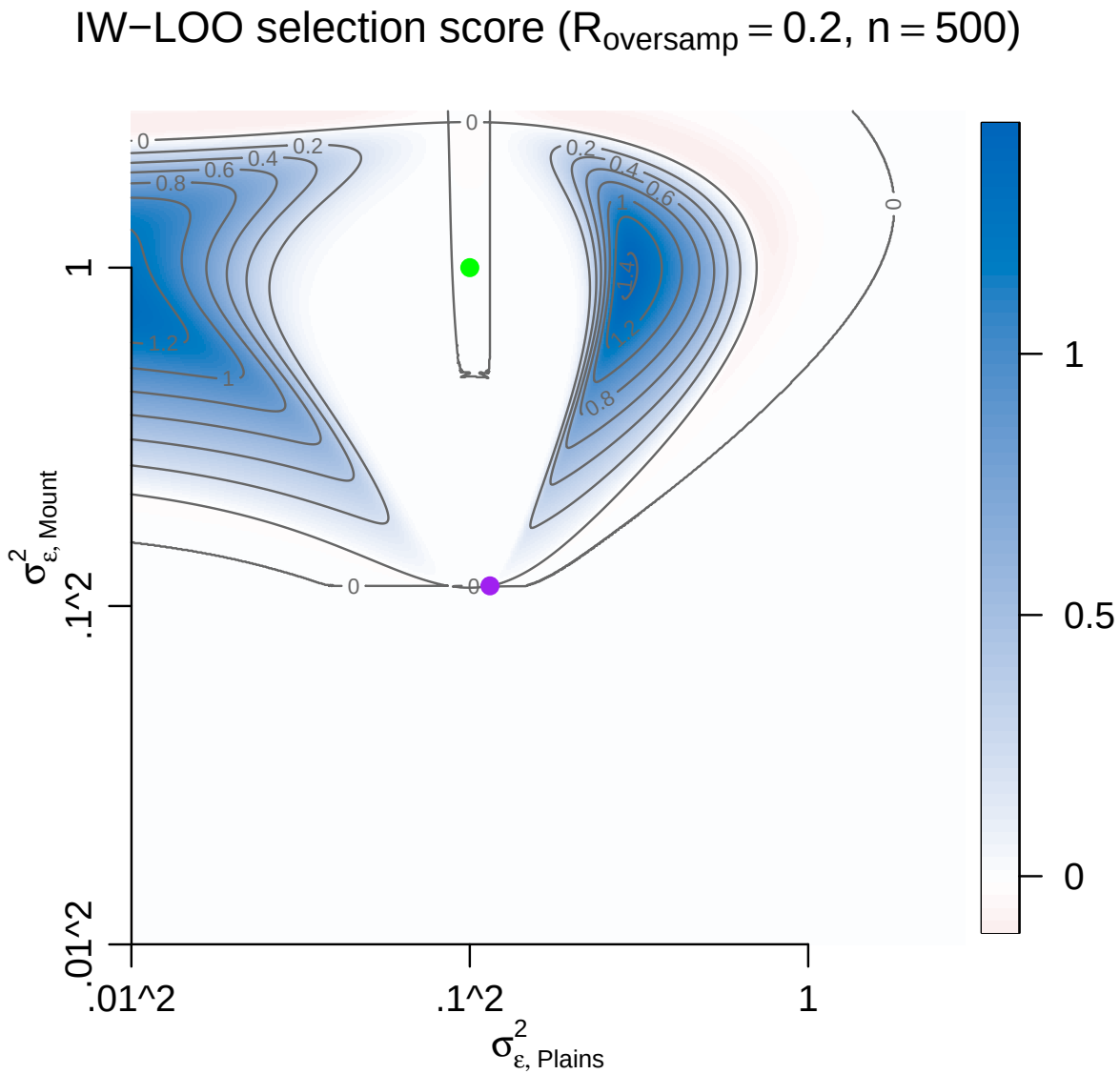




IW-LOO expected selection score, $R = 0.2$, $n = 500$







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