ROBUST GAUSSIAN PROCESS REGRESSION WITH HUBER LIKELIHOOD

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	SCtMCMC$^{+\text{pw}}$	tLA$^{+\text{pw}}$	HuberMCMC$^{+\text{pw}}$	HuberLA$^{+\text{pw}}$	RCGP$^{+\text{pw}}$	GP$^{+\text{pw}}$	LaplaceMCMC$^{+\text{pw}}$
				$\varepsilon \sim \mathcal{N}(0.01, 0.08)$			
RMSE	2.14 (2.32)	1.26 (0.05)	0.63 (0.14)	1.18 (0.01)	2.04 (0.005)	1.56 (0.01)	0.71 (0.11)
MAE	1.07 (0.62)	0.82 (0.04)	0.47 (0.08)	0.81 (0.01)	1.78 (0.003)	1.38 (0.02)	0.50 (0.07)
				$\varepsilon \sim$ Student-$t(10)$			
RMSE	2.25 (1.56)	1.31 (0.00)	0.61 (0.18)	1.19 (0.00)	2.06 (0.00)	1.58 (0.00)	0.74 (0.16)
MAE	1.11 (0.35)	0.86 (0.00)	0.47 (0.11)	0.83 (0.00)	1.79 (0.00)	1.40 (0.00)	0.53 (0.10)
				$\varepsilon \sim$ Laplace$(0, 0.1)$			
RMSE	1.75 (1.05)	1.31 (0.00)	0.65 (0.15)	1.19 (0.00)	2.06 (0.002)	1.58 (0.00)	0.69 (0.16)
MAE	1.00 (0.24)	0.86 (0.00)	0.49 (0.10)	0.83 (0.00)	1.08 (0.00)	1.40 (0.00)	0.50 (0.09)
				$\varepsilon \sim$ Student-$t(1)$ (Cauchy)			
RMSE	1.33 (0.12)	1.31 (0.00)	0.67 (0.23)	1.19 (0.00)	2.06 (0.00)	1.57 (0.00)	0.71 (0.16)
MAE	0.90 (0.05)	0.86 (0.00)	0.50 (0.15)	0.83 (0.00)	1.05 (0.00)	1.39 (0.00)	0.52 (0.09)

Table 1: RMSE and MAE values on the Neal dataset for the Case 1 (with standard errors in parenthesis). Bold values highlight the best performance with the lowest RMSE and MAE.

	SCtMCMC$^{+\text{pw}}$	tLA$^{+\text{pw}}$	HuberMCMC$^{+\text{pw}}$	HuberLA$^{+\text{pw}}$	RCGP$^{+\text{pw}}$	GP$^{+\text{pw}}$	LaplaceMCMC$^{+\text{pw}}$
				$\varepsilon \sim \mathcal{N}(0.01, 0.08)$			
RMSE	0.91 (0.04)	0.97 (0.14)	1.14 (0.23)	0.84 (0.09)	2.04 (0.004)	0.90 (0.02)	0.90 (0.09)
MAE	0.62 (0.03)	0.59 (0.05)	0.76 (0.16)	0.57 (0.06)	1.68 (0.002)	0.67 (0.02)	0.61 (0.04)
				$\varepsilon \sim$ Student-$t(10)$			
RMSE	0.85 (0.02)	0.81 (0.00)	0.98 (0.12)	0.80 (0.08)	2.05 (0.00)	0.88 (0.00)	0.87 (0.12)
MAE	0.61 (0.01)	0.56 (0.00)	0.67 (0.08)	0.56 (0.06)	1.70 (0.001)	0.66 (0.00)	0.62 (0.08)
				$\varepsilon \sim$ Laplace$(0, 0.1)$			
RMSE	0.85 (0.02)	0.81 (0.00)	0.99 (0.13)	0.83 (0.07)	2.05 (0.002)	0.88 (0.00)	0.84 (0.07)
MAE	0.61 (0.01)	0.55 (0.00)	0.68 (0.10)	0.58 (0.05)	1.69 (0.00)	0.66 (0.00)	0.59 (0.04)
				$\varepsilon \sim$ Student-$t(1)$ (Cauchy)			
RMSE	0.86 (0.04)	0.82 (0.01)	0.91 (0.10)	0.79 (0.06)	2.05 (0.00)	0.88 (0.01)	0.83 (0.07)
MAE	0.62 (0.03)	0.56 (0.01)	0.61 (0.08)	0.55 (0.05)	1.69 (0.00)	0.66 (0.01)	0.58 (0.05)

Table 2: RMSE and MAE values on the Neal dataset for the Case 3 (with standard errors in parenthesis). Bold values highlight the best performance with the lowest RMSE and MAE.

Theorem 1. *Let $\mathcal{D} = (\boldsymbol{x}_i, y_i)_{i=1}^n$ be a dataset with distinct covariates $\boldsymbol{x}_i \in \mathcal{X}$ and response $y_i \in \mathcal{Y}$, where $n < \infty$. The kernel matrix $\mathbf{K} \in \mathbb{R}^{n \times n}$ is positive definite, with elements $K_{ij} = k(\boldsymbol{x}_i, \boldsymbol{x}_j)$ defined by a continuous kernel function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$. Assume the Huber likelihood function $p_H(\mathbf{y}|\mathbf{f}, \boldsymbol{\sigma})$ based on strictly convex and continuous Huber loss $\rho(r_i) : \mathbb{R} \to \mathbb{R}$. Then the posterior distribution $p(\mathbf{f}|\mathcal{D}, \boldsymbol{\theta}, \sigma)$ is unimodal.*

Proof. The GP-Huber posterior distribution is proportional to the expression:

$$p(\mathbf{f}|\mathcal{D}, \boldsymbol{\theta}, \sigma) \propto \exp\left(-\frac{1}{2}\mathbf{f}^\top \mathbf{K}^{-1}\mathbf{f} - \sum_{i=1}^n \rho(y_i - f_i)\right),$$

where ρ denotes the Huber loss function, which is continuous and strictly convex. The derivative of the log-posterior with respect to $\mathbf{f}$ is:

$$\nabla_{\mathbf{f}} \log p(\mathbf{f}|\mathcal{D}, \boldsymbol{\theta}, \sigma) \propto -\mathbf{K}^{-1}\mathbf{f} - \nabla_{\mathbf{f}}\rho(y_i - f_i),$$

	SCtMCMC$^{-\text{pw}}$	tLA$^{-\text{pw}}$	HuberMCMC$^{-\text{pw}}$	HuberLA$^{-\text{pw}}$	RCGP$^{-\text{pw}}$	GP$^{-\text{pw}}$	LaplaceMCMC$^{-\text{pw}}$
				$\varepsilon \sim \mathcal{N}(0.01, 0.08)$			
RMSE	2.74 (1.84)	1.23 (0.10)	1.24 (0.04)	1.30 (0.01)	2.03 (0.01)	1.68 (0.02)	1.29 (0.12)
MAE	1.10 (0.52)	0.75 (0.09)	0.88 (0.03)	0.89 (0.01)	1.69 (0.008)	1.46 (0.02)	0.88 (0.06)
				$\varepsilon \sim$ Student-$t(10)$			
RMSE	1.92 (1.54)	1.18 (0.02)	1.17 (0.04)	1.29 (0.00)	2.07 (0.00)	1.70 (0.00)	1.26 (0.10)
MAE	0.92 (0.39)	0.71 (0.03)	0.84 (0.04)	0.88 (0.00)	1.70 (0.00)	1.48 (0.00)	0.89 (0.06)
				$\varepsilon \sim$ Laplace$(0, 0.1)$			
RMSE	3.26 (1.83)	1.20 (0.04)	1.16 (0.10)	1.29 (0.00)	2.08 (0.00)	1.70 (0.00)	1.17 (0.08)
MAE	1.26 (0.47)	0.74 (0.05)	0.84 (0.06)	0.88 (0.00)	1.70 (0.00)	1.48 (0.00)	0.82 (0.06)
				$\varepsilon \sim$ Student-$t(1)$ (Cauchy)			
RMSE	3.40 (1.82)	1.16 (0.06)	1.12 (0.08)	1.29 (0.00)	2.08 (0.00)	1.70 (0.00)	1.19 (0.10)
MAE	1.31 (0.47)	0.69 (0.06)	0.81 (0.05)	0.89 (0.00)	1.70 (0.00)	1.48 (0.00)	0.84 (0.07)

Table 3: Results for Case 2 (standard errors in parentheses)

	SCtMCMC$^{-\text{pw}}$	tLA$^{-\text{pw}}$	HuberMCMC$^{-\text{pw}}$	HuberLA$^{-\text{pw}}$	RCGP$^{-\text{pw}}$	GP$^{-\text{pw}}$	LaplaceMCMC$^{-\text{pw}}$
				$\varepsilon \sim \mathcal{N}(0.01, 0.08)$			
RMSE	3.45 (1.78)	1.17 (0.06)	1.28 (0.02)	1.18 (0.05)	1.99 (0.003)	1.68 (0.02)	1.13 (0.11)
MAE	1.28 (0.50)	0.67 (0.06)	0.87 (0.02)	0.85 (0.04)	1.74 (0.002)	1.45 (0.02)	0.79 (0.07)
				$\varepsilon \sim$ Student-$t(10)$			
RMSE	2.43 (1.49)	1.21 (0.15)	1.24 (0.00)	1.15 (0.09)	1.99 (0.00)	1.72 (0.00)	1.17 (0.10)
MAE	1.06 (0.45)	0.76 (0.14)	0.91 (0.00)	0.83 (0.06)	1.75 (0.00)	1.47 (0.00)	0.82 (0.07)
				$\varepsilon \sim$ Laplace$(0, 0.1)$			
RMSE	3.53 (1.69)	1.19 (0.10)	1.24 (0.00)	1.14 (0.10)	1.99 (0.00)	1.72 (0.00)	1.17 (0.07)
MAE	1.33 (0.49)	0.74 (0.10)	0.90 (0.00)	0.82 (0.06)	1.75 (0.00)	1.47 (0.00)	0.82 (0.06)
				$\varepsilon \sim$ Student-$t(1)$ (Cauchy)			
RMSE	2.53 (1.82)	1.13 (0.04)	1.21 (0.03)	1.08 (0.09)	2.00 (0.00)	1.71 (0.00)	1.15 (0.08)
MAE	1.04 (0.51)	0.66 (0.05)	0.88 (0.02)	0.78 (0.07)	1.76 (0.00)	1.47 (0.00)	0.81 (0.06)

Table 4: Results for Case 4 (standard errors in parentheses)

and for each component f_i, the derivative becomes:

$$h_i(f_i) = \frac{-(y_i - f_i)}{\sqrt{1 + (y_i - f_i)^2}} - v_i,$$

where v_i represents the i^{th} component of $\mathbf{v} = \mathbf{K}^{-1}\mathbf{f}$. The term $\frac{-(y_i - f_i)}{\sqrt{1+(y_i-f_i)^2}}$ is strictly monotonic in f_i, as its derivative is positive for all f_i. Its behavior at the limits is given by:

$$\frac{-(y_i - f_i)}{\sqrt{1 + (y_i - f_i)^2}} = \begin{cases} 0 & \text{if } f_i \to y_i, \\ -1 & \text{if } f_i \to \infty. \end{cases}$$

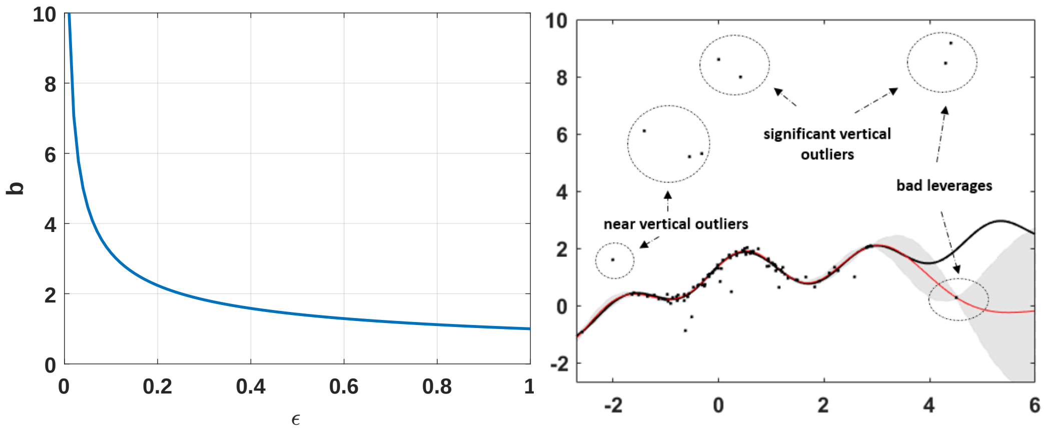
The second term, v_i, arises from the precision matrix $\mathbf{K}^{-1}$, which is symmetric and positive definite. By the spectral theorem, $\mathbf{K}^{-1}$ can be diagonalized as $\mathbf{K}^{-1} = \mathbf{Q}\Lambda\mathbf{Q}^\top$, where Λ is the diagonal matrix of positive eigenvalues, and $\mathbf{Q}$ is an orthogonal matrix. This ensures that v_i is a linear combination of the entries of $\mathbf{f}$ and is therefore continuous and differentiable in f_i. Combining these terms, $h_i(f_i)$ is strictly monotonic because the first term is monotonic and the second term is linear. By the intermediate value theorem, $h_i(f_i)$ crosses zero exactly once because:

$$\lim_{f_i \to y_i} h_i(f_i) = 0 \quad \text{and} \quad \lim_{f_i \to \infty} h_i(f_i) = -1.$$

Thus, $h_i(f_i)$ has a unique root, ensuring that the log-posterior $\log p(\mathbf{f}|\mathcal{D}, \boldsymbol{\theta}, \sigma)$ is strictly concave. The strict concavity of the log-posterior implies that the posterior distribution $p(\mathbf{f}|\mathcal{D}, \boldsymbol{\theta}, \sigma)$ has a unique mode, proving that it is unimodal. □ □

Theorem 2. *Under the same assumptions as Theorem 1, the influence of an individual observation y_i on the posterior mean $\mathbb{E}[f(x) \mid \mathbf{y}]$ is bounded, ensuring robustness to outliers:*

$$\left| \frac{\partial}{\partial y_i} \mathbb{E}[f \mid y] \right| \le \frac{b}{\sigma}.$$



(a) (b)

Figure 1: (a) b vs contamination ε; (b) extreme (significant) outliers, near outliers, and bad leverage points analyzed on the Neal dataset

Proof. The influence function $I(r_i) = -\frac{\partial}{\partial r_i} \log p(y_i \mid f(\boldsymbol{x}_i))$ of the likelihood $p(y_i \mid f(\boldsymbol{x}_i), \sigma^2)$ for inliers ($|r_i| \leq b$) is:

$$I(r_i) = \frac{r_i}{\sigma^2},$$

and for outliers ($|r_i| > b$) becomes:

$$I(r_i) = \frac{\delta \, \mathrm{sign}(r_i)}{\sigma}.$$

We observe that the $I(r_i)$ is bounded i.e. the contribution of any individual observation y_i to $\mathbb{E}[f(x) \mid \mathbf{y}]$ is bounded, ensuring robustness to outliers. $\square$

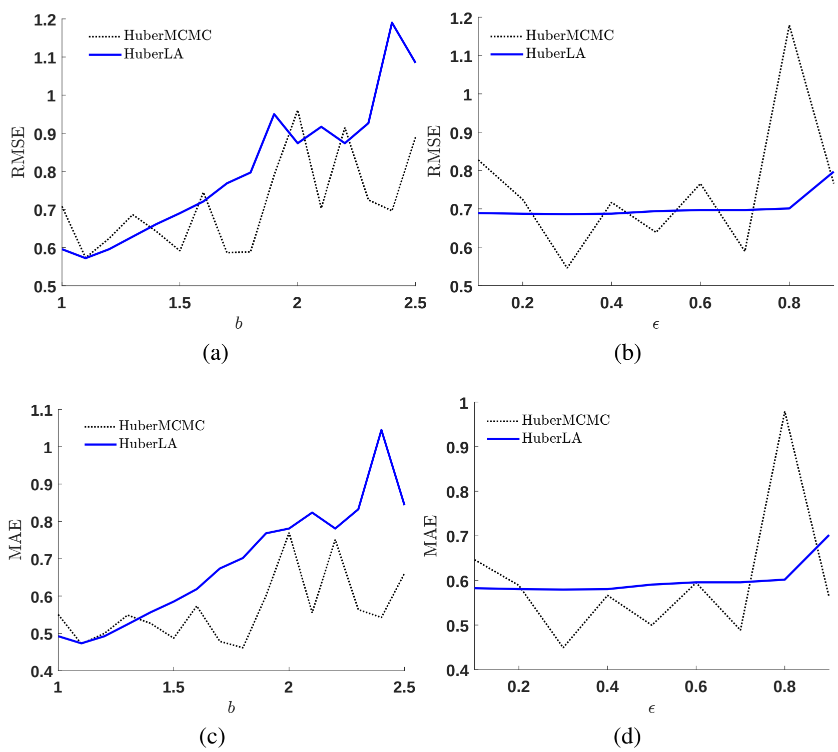


Figure 2: Impact of b and ε on predictions for Neal dataset (case 1 with Student-t noise): (a) RMSE vs b ($\varepsilon = 0.45$); (b) RMSE vs ε ($b = 1.5$); (c) MAE vs b; (d) MAE vs ε.