

Bayesian simultaneous credible bands for polynomial regression

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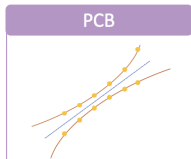
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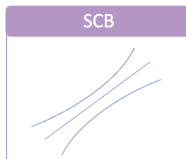
Bayesian simultaneous credible bands for polynomial regression

Motivation

To assess the plausible range of an unknown function



PCB is not able to cover the function simultaneously



Frequentist

Bayesian

Bayesian SCB

Propose two methods

- The Conjugate Prior
- HMC

A new evaluation criterion

Posterior Coverage Probability

Simulations & Real Data Examples

Linear Regression ($p=1$)
Polynomial Regression ($p=2,3$)

Statistics,
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Notations

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\theta} + \mathbf{e}, \quad (1)$$

- $\mathbf{Y} = (y_1, \dots, y_n)^T$
- \mathbf{X} is a $n \times (p+1)$ full column-rank design matrix with the l th ($1 \leq l \leq n$) row given by $(1, x_l, \dots, x_l^p)$. x has been mean-centered.
- $\boldsymbol{\theta} = (\theta_0, \dots, \theta_p)^T$.
- $\mathbf{e} = (e_1, \dots, e_n)^T$ with $e_i \sim N(0, \sigma^2 V)$ where the covariance matrix V is assumed to be a known positive-definite matrix.
- $\boldsymbol{\theta}$ and σ^2 are unknown.

Key Property

Statistics,
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Bayesian simultaneous credible bands for polynomial regression

Methodology

References

For a newly given $x \in (a, b)$, denote $\mathbf{x} = (1, x, \dots, x^p)$, we consider the construction of $1 - \alpha$ level Bayesian simultaneous credible bands for $\mathbf{x}^T \boldsymbol{\theta}$,

$$P\{\mathbf{x}^T \boldsymbol{\theta} \in \mathbf{x}^T E(\boldsymbol{\theta}) \pm \lambda \sqrt{\text{Var}(\mathbf{x}^T \boldsymbol{\theta})} \quad \forall x \in (a, b)\} = 1 - \alpha. \quad (2)$$

$$P\{-\lambda \leq \frac{\mathbf{x}^T (\boldsymbol{\theta} - E(\boldsymbol{\theta}))}{\sqrt{\text{Var}(\mathbf{x}^T \boldsymbol{\theta})}} \leq \lambda, \quad \forall x \in (a, b)\} = 1 - \alpha, \quad (3)$$

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The Key Procedure

Ultimately, we need to evaluate the value of the critical constant λ :

$$\lambda = \sup_{x \in (a, b)} \frac{|\mathbf{x}^T (\boldsymbol{\theta} - E(\boldsymbol{\theta}))|}{\sqrt{\mathbf{x}^T \text{Var}(\boldsymbol{\theta}) \mathbf{x}}}$$

The Conjugate Prior Method

The normal-gamma conjugate prior

- Denote $\tau = \frac{1}{\sigma^2}$, τ is the precision matrix of the random errors e . Now the parameters of interest are $\boldsymbol{\theta}$ and τ .
- Here we assume the prior $\xi(\boldsymbol{\theta}, \tau)$ is a normal-gamma prior density,
 - $\xi(\boldsymbol{\theta}, \tau) = \xi_1(\boldsymbol{\theta}|\tau) \cdot \xi_2(\tau)$, $\boldsymbol{\theta} \in \mathbb{R}^p, \tau > 0$,
 - $\boldsymbol{\theta}|\tau \sim \mathcal{N}(\boldsymbol{\mu}, \tau^{-1}\mathcal{P})$
 - $\tau \sim \text{Gamma}(\alpha_0, \beta_0)$
- Use a data-driven approach for the hyperparameters in the priors:
 - $\boldsymbol{\mu} = \hat{\boldsymbol{\theta}}_{GLS} = (\mathbf{X}^T \mathbf{V}^{-1} \mathbf{X})^{-1} \mathbf{X}^T \mathbf{V}^{-1} \mathbf{Y}$,
 - $\mathcal{P} = c \cdot \mathbf{I}_p$,
 - $\alpha_0 = 1$,
 - $\beta_0 = \frac{\hat{\mathbf{e}}_{GLS}^T \hat{\mathbf{e}}_{GLS}}{n-p}$

The multivariate t distribution

It can be proved that $\boldsymbol{\theta}|\mathbf{Y}$ follows a p -dimensional t distribution with $(n + 2\alpha_0)$ degrees of freedom:

$$(\boldsymbol{\theta}|\mathbf{Y}) \sim t_{(n+2\alpha_0)}(\boldsymbol{\mu}^*, (D^*)^{-1}), \quad (4)$$

The Key Procedure

$$\lambda = \sup_{x \in (a,b)} \frac{|\mathbf{x}^T(\boldsymbol{\theta} - E(\boldsymbol{\theta}))|}{\sqrt{\mathbf{x}^T \text{Var}(\boldsymbol{\theta}) \mathbf{x}}}$$

- $E(\boldsymbol{\theta}|\mathbf{Y}) = \boldsymbol{\mu}^*$,
- $\text{Var}(\boldsymbol{\theta}|\mathbf{Y}) = \frac{n+2\alpha_0}{n+2\alpha_0-2}(D^*)^{-1}$, for $n + 2\alpha_0 > 2$,
- The only numerical optimization step is the monotonic, one-dimensional root finding problem for λ .
- Use a simulation-based method to find λ .

Algorithm Use the conjugate prior method to compute λ by simulation for $\mathbf{x}^T \boldsymbol{\beta}$ where $x \in (a, b)$

Input: $\mathbf{X}, \mathbf{Y}, n, \mu, \mathcal{P}, \alpha_0, \beta_0, x \in (a, b), 1 - \alpha,$

Output: $\hat{\boldsymbol{\theta}}, \hat{\tau}, \lambda$

- Step 1: For $l = 1, 2, \dots, L$, repeat the following:
 - a. Generate one value of $\hat{\boldsymbol{\theta}}^{(l)}$ from (6). That is, generate $\hat{\boldsymbol{\theta}}^{(l)} \sim t_{(n+2\alpha_0)}(\mu^*, D^*)$, where μ^* and D^* is given by (7) and (33).
 - b. Compute $E(\boldsymbol{\theta}) = \mu^*$, and $\text{Var}(\boldsymbol{\theta}) = \frac{n+2\alpha_0}{n+2\alpha_0-2}(D^*)^{-1}$.
 - c. Compute $\lambda^{(l)}$ which is given by

$$\lambda^{(l)} = \sup_{x \in (a, b)} \frac{|\mathbf{x}^T (\boldsymbol{\theta} - \mu^*)|}{\sqrt{\mathbf{x}^T \text{Var}(\boldsymbol{\theta}) \mathbf{x}}},$$

Algorithm Use the conjugate prior method to compute λ by simulation for $\mathbf{x}^T \boldsymbol{\beta}$ where $x \in (a, b)$

Input: $\mathbf{X}, \mathbf{Y}, n, \mu, \mathcal{P}, \alpha_0, \beta_0, x \in (a, b), 1 - \alpha,$

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$$\lambda^{(l)} = \sup_{x \in (a, b)} \frac{|\mathbf{x}^T (\boldsymbol{\theta} - \mu^*)|}{\sqrt{\mathbf{x}^T \text{Var}(\boldsymbol{\theta}) \mathbf{x}}},$$

- Step 2: Order these $\lambda^{(l)}$ values as $\lambda_{[1]} \leq \dots \leq \lambda_{[L]}$ and use $\lambda_{[\langle (1-\alpha)L \rangle]}$ as the λ we want. Here $\langle (1-\alpha)L \rangle$ denotes the integer part of $(1-\alpha)L$. $\lambda_{[\langle (1-\alpha)L \rangle]}$ converges to λ with probability one as $L \rightarrow \infty$ (Serfling, 1980 [1]). The simultaneous credible bands for $\mathbf{x}^T \boldsymbol{\theta}$ is given by:

$$\left[\mathbf{x}^T E(\boldsymbol{\theta}) - \lambda_{[\langle (1-\alpha)L \rangle]} \sqrt{\mathbf{x}^T \text{Var}(\boldsymbol{\theta}) \mathbf{x}}, \quad \mathbf{x}^T E(\boldsymbol{\theta}) + \lambda_{[\langle (1-\alpha)L \rangle]} \sqrt{\mathbf{x}^T \text{Var}(\boldsymbol{\theta}) \mathbf{x}} \right]$$

return $\hat{\lambda}$

The HMC Method

Methodology

- The Hamiltonian Monte Carlo sampler method is originated in the physics literature as an approach uniting MCMC and molecular dynamics approaches
- Hyperparameters:
 - Chains: 4
 - Iterations per chain: 8000
 - Warmup: 4000
- Outputs:
 - Posterior distribution of θ
 - $E(\theta)$, $\text{Var}(\theta)$

Algorithm Use the HMC method to compute λ by simulation for $\mathbf{x}^T \boldsymbol{\beta}$ where $x \in (a, b)$

Input: $\mathbf{X}, \mathbf{Y}, V, n, \mu, \mathcal{P}, \alpha_0, \beta_0, x \in (a, b), 1 - \alpha$

Output: $\hat{\boldsymbol{\theta}}, \lambda$

- Step 1: For $l = 1, 2, \dots, L$, repeat the following:
 - a. Using the HMC to produce the posterior distribution of $\boldsymbol{\theta}$. Draw one value of $\boldsymbol{\theta}$.
 - b. Derive the $E(\boldsymbol{\theta}) = \mu^*$, and $\text{Var}(\boldsymbol{\theta})$ according to the posterior distribution.
 - c. Compute $\lambda^{(l)}$ which is given by

$$\lambda^{(l)} = \sup_{x \in (a, b)} \frac{|\mathbf{x}^T (\boldsymbol{\theta} - \mu^*)|}{\sqrt{\mathbf{x}^T \text{Var}(\boldsymbol{\theta}) \mathbf{x}}},$$

Algorithm Use the HMC method to compute λ by simulation for $\mathbf{x}^T \boldsymbol{\beta}$ where $x \in (a, b)$

Input: $\mathbf{X}, \mathbf{Y}, V, n, \mu, \mathcal{P}, \alpha_0, \beta_0, x \in (a, b), 1 - \alpha$

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- Step 1: For $l = 1, 2, \dots, L$, repeat the following:
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- Step 2: Order these $\lambda^{(l)}$ values as $\lambda_{[1]} \leq \dots \leq \lambda_{[L]}$ and use $\lambda_{[\langle (1-\alpha)L \rangle]}$ as the λ we want. Here $\langle (1-\alpha)L \rangle$ denotes the integer part of $(1-\alpha)L$. The simultaneous credible bands for $\mathbf{x}^T \boldsymbol{\theta}$ is given by:

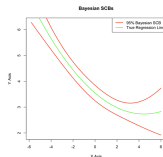
$$\left[\mathbf{x}^T E(\boldsymbol{\theta}) - \lambda_{[\langle (1-\alpha)L \rangle]} \sqrt{\mathbf{x}^T \text{Var}(\boldsymbol{\theta}) \mathbf{x}}, \quad \mathbf{x}^T E(\boldsymbol{\theta}) + \lambda_{[\langle (1-\alpha)L \rangle]} \sqrt{\mathbf{x}^T \text{Var}(\boldsymbol{\theta}) \mathbf{x}} \right]$$

Comparison Methods & Evaluation Criterion

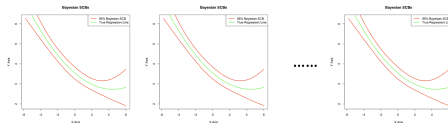
We select the following methods to compare with the proposed method,

- ① The Frequentist simultaneous confidence band (Frequentist SCB)
 - The exact SCB of Liu et al.(2013)[2];
 - The conservative SCB of Naiman (1986)[3]
- ② The Bayesian pointwise credible band (Bayesian PCB)
- ③ The Frequentist pointwise confidence band (Frequentist PCB)

If the band covers the true regression line in the given range, we call it as one successful catch



Repeat testing for K times



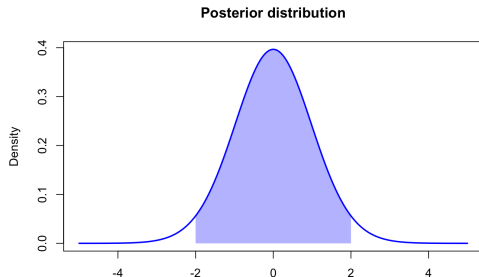
$$\text{Empirical Coverage Rate} = \frac{\# \text{ Successful Catch}}{K}$$

Yet, it is **not an appropriate criterion** to use in the Bayesian context.

The Posterior Coverage Probability

It reflects the probability that the band contains the true regression function under the posterior distribution. Denote the Bayesian SCB for $\mathbf{x}^T \boldsymbol{\theta}$, $x \in (a, b)$, as \mathcal{I}_A : the posterior coverage probability is defined as

$$\inf P_{\boldsymbol{\theta}|Y} \{ \{ \mathbf{x}^T \boldsymbol{\theta} \in \mathcal{I}_A \} \quad \forall x \in (a, b) \}, \quad (5)$$



A Toy Example

Simulation

A Toy Example

$$Y = X^T \theta + e,$$

- $x_i \sim U(-5, 5)$, $e_i \sim N(0, \sigma^2)$, $i = 1, \dots, n$,
 - Linear Setting: $\theta = (1, 2)^T$
 - $n=100$
 - $\sigma = 0.25$
 - Quadratic Setting: $\theta = (-6, -3, 0.25)^T$
 - $n = 20, 50, 100, 200$
 - $\sigma = 0.2, 0.5, 1$
 - Cubic Setting: $\theta = (1, 2, -1, 0.5)^T$
 - $n = 200$
 - $\sigma = 1$
- For the polynomial model, we use D-optimal design to construct the design matrix.
 - e.g. The optimal design for $x \in [-5, 5]$ is:
 $x = -5, -2.237447, -2.235447, 2.235447, 2.237447, 5$.

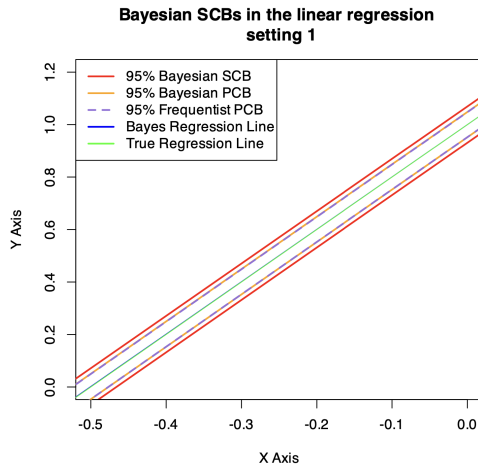


Figure: The 95% Bayesian SCB, the 95% Bayesian PCB, and the 95% Frequentist PCB for the linear regression line

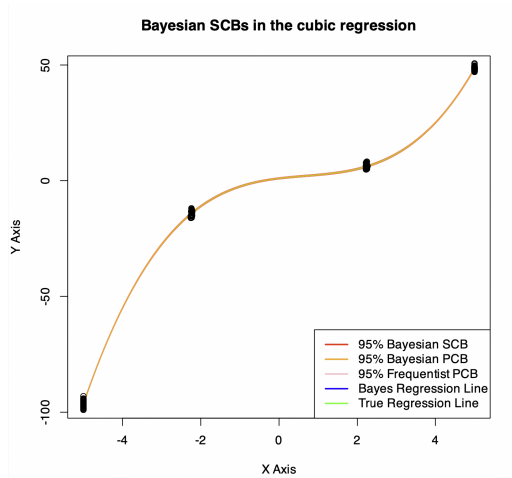


Figure: The 95% Bayesian SCB, the 95% Bayesian PCB, and the 95% frequentist PCB for the regression curve in the cubic regression example with a D-optimal design matrix

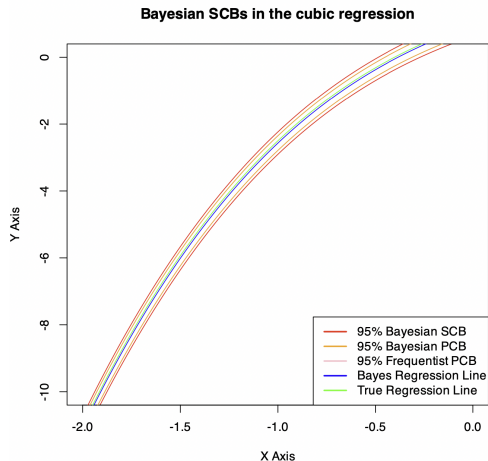


Figure: A zoomed-in look when $x \in [-2, 2]$ for the 95% Bayesian SCB, the 95% Bayesian PCB, and the 95% frequentist PCB in the cubic regression example

The Posterior Coverage Probability

p	σ	n	Average Posterior Coverage Probability	
			95% Bayesian SCB Conjugate Prior	95% Bayesian PCB
2	0.2	20	0.981	0.950
		50	0.984	0.950
		100	0.985	0.950
		200	0.986	0.950
	0.5	20	0.981	0.950
		50	0.984	0.950
		100	0.985	0.950
		200	0.986	0.950
	1	20	0.981	0.950
		50	0.984	0.950
		100	0.985	0.950
		200	0.986	0.950
3	1	20	0.984	0.950
		50	0.987	0.950
		100	0.988	0.950
		200	0.988	0.950

Figure: The posterior coverage probability of the 95 % Bayesian SCB, and the 95 % Bayesian PCB for the quadratic and cubic regression

- The average posterior coverage probability (APCP) is the mean average under 1000 repetitions.
- APCP increases as n increases
- APCP is not sensitive to the changes of the noise level σ .

The HMC Method

p	σ	n	Empirical Coverage Rate				Average Posterior Coverage Probability		
			95% Bayesian SCB Conjugate Prior	95% Bayesian SCB HMC	95% Bayesian PCB	95% Frequentist PCB	95% Bayesian SCB Conjugate Prior	95% Bayesian SCB HMC	95% Bayesian PCB
2	0.2	20	0.901	0.949	0.766	0.814	0.981	0.985	0.950
2	0.2	50	0.917	0.932	0.787	0.799	0.984	0.986	0.950
2	0.2	100	0.937	0.941	0.804	0.810	0.985	0.986	0.950
2	0.2	200	0.933	0.938	0.811	0.814	0.986	0.986	0.950

Figure: The posterior coverage probability of the 95 % Bayesian SCB, and the 95 % Bayesian PCB for the HMC method in the quadratic regression

The HMC method is less sensitive to the choice of initial hyperparameters, making it more flexible and easier to use than the conjugate prior approach.

Real Data Example

Dose-response Dataset in a Phase II study

Real Data Example

Dose-response Dataset in a Phase II study (Bretz et al., 2005)[4]

- Goal: To accurately finding the dose-response relationship in a a randomized double-blind parallel group trial involving 100 patients who were randomly assigned, with equal probability, to receive either placebo or one of four active doses, coded as $x = 0.05, 0.2, 0.6, 1$.
- Y: The response to the doses of treatment.
- x: The doses of the drug.

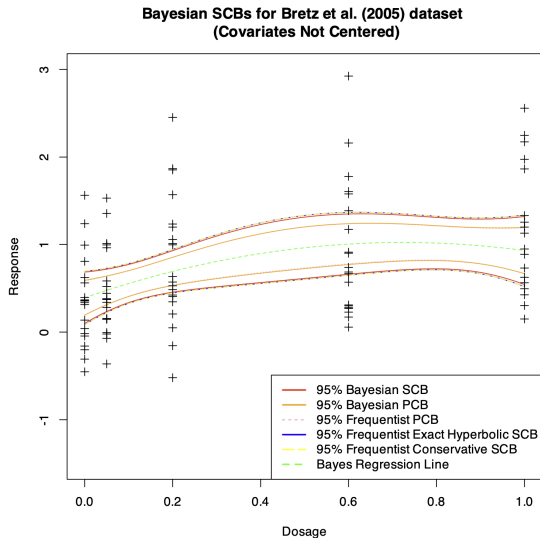
Dose	Sample size	Sample mean	Sample SD
0	20	0.34	0.52
0.05	20	0.46	0.49
0.2	20	0.81	0.74
0.6	20	0.93	0.76
1	20	0.95	0.95

Real Data Example

- When the covariates are not centered:

$$Y = 0.392 + 1.743x - 1.205x^2,$$

- $\lambda : 2.442347$, the same as the one when covariates are centered.
- Compared with:
 - The exact Frequentist SCB of Liu et al.(2013)[2];
 - The conservative Frequentist SCB of Naiman (1986)[3]



Summary & Future Work

Statistics,
Dept of Math,
Manchester

Bayesian simultaneous credible bands for polynomial regression

Real Data Example

Discussion

References

- Fei Yang – Statistics, Dept of Math, Manchester

Future Work

- ① Extend the Bayesian approach into other models:
 - ① The GLM,
 - ② Random effects linear model,
 - ③ Quantile regression model
- ② Combine with the machine learning algorithms (Sluijterman et al., 2024 [5]).

- Statistics,
Dept of Math,
Manchester
- Fei Yang
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This is the end of my presentation.
Thank you for your attention.

The multivariate t distribution

It can be proved that $\boldsymbol{\theta}|\mathbf{Y}$ follows a p -dimensional t distribution with $(n + 2\alpha_0)$ degrees of freedom:

$$(\boldsymbol{\theta}|\mathbf{Y}) \sim t_{(n+2\alpha_0)}(\boldsymbol{\mu}^*, (D^*)^{-1}), \quad (6)$$

with location vector

$$\boldsymbol{\mu}^*(\boldsymbol{\theta}|\mathbf{Y}) = (\mathbf{X}^T V^{-1} \mathbf{X} + \mathcal{P})^{-1} (\mathbf{X}^T V^{-1} \mathbf{Y} + \mathcal{P} \boldsymbol{\mu}), \quad (7)$$

and precision matrix

$$D^*(\boldsymbol{\theta}|\mathbf{Y}) = (n + 2\alpha_0)(\mathbf{X}^T V^{-1} \mathbf{X} + \mathcal{P}).$$

$$\left[2\beta_0 + \mathbf{Y}^T V^{-1} \mathbf{Y} + \boldsymbol{\mu}^T \mathcal{P} \boldsymbol{\mu} - (\mathbf{X}^T V^{-1} \mathbf{Y} + \mathcal{P} \boldsymbol{\mu})^T (\mathbf{X}^T V^{-1} \mathbf{X} + \mathcal{P})^{-1} (\mathbf{X}^T V^{-1} \mathbf{Y} + \mathcal{P} \boldsymbol{\mu}) \right]^{-1} \quad (8)$$

For the comparison methods, we choose the frequentist pointwise confidence band (frequentist PCB) and the Bayesian pointwise credible band (Bayesian PCB):

Frequentist Pointwise Confidence Band

A $1 - \alpha$ pointwise confidence band for the regression curve $\mathbf{x}^T \boldsymbol{\theta}$ at \mathbf{x} is given by:

$$P \left\{ \mathbf{x}^T \boldsymbol{\theta} \in \mathbf{x}^T \hat{\boldsymbol{\theta}} \pm t_{n-p-1}^{\alpha/2} \hat{\sigma} \sqrt{\mathbf{x}^T (\mathbf{X}V^{-1}\mathbf{X})^{-1} \mathbf{x}} \right\} = 1 - \alpha, \quad (9)$$

where $t_{n-p-1}^{\alpha/2}$ is the upper $\alpha/2$ point of the t distribution with $n - p - 1$ degrees of freedom.

- $\hat{\boldsymbol{\theta}} = (\mathbf{X}^T V^{-1} \mathbf{X})^{-1} \mathbf{X}^T V^{-1} \mathbf{Y}$
- $\hat{\sigma}^2 = \frac{(\mathbf{Y} - \mathbf{X} \hat{\boldsymbol{\theta}})^T V^{-1} (\mathbf{Y} - \mathbf{X} \hat{\boldsymbol{\theta}})}{n - p - 1}$

Bayesian Pointwise Credible Band

A $1 - \alpha$ pointwise Bayesian credible band for the regression curve is given by:

$$P\{\mathbf{x}^T \boldsymbol{\theta} \in \mathbf{x}^T \mu^* \pm t_{\nu, \alpha/2} \sqrt{\mathbf{x}^T \text{Var}(\boldsymbol{\theta}) \mathbf{x}}\} = 1 - \alpha, \quad (10)$$

As μ^* is the posterior mean for $\boldsymbol{\theta}$.

Denote $T = \mathbf{x}^T \boldsymbol{\theta}$, then $T \sim t_\nu(\mu_t, \sigma_t)$, $\mu_t = \mathbf{x}^T \mu^*$, $\sigma_t = \mathbf{x}^T \text{Cov}(\boldsymbol{\theta}) \mathbf{x}$, $\nu = n + 2\alpha$.
Thus $T_\nu := \frac{T - \mu_t}{\sigma_t} \sim t_\nu$.

$$\begin{aligned} & P_{\mathbf{x}^T \boldsymbol{\theta} | \mathbf{Y}} \{ \mathbf{x}^T \boldsymbol{\theta} \in \mathcal{I}_A \quad \forall x \in (a, b) \} \\ &= P_{\mathbf{x}^T \boldsymbol{\theta} | \mathbf{Y}} \{ L(x) \leq \mathbf{x}^T \boldsymbol{\theta} \leq U(x) \quad \forall x \in (a, b) \}, \\ &= P_{\mathbf{x}^T \boldsymbol{\theta} | \mathbf{Y}} \left\{ \frac{L(x) - \mu_t}{\sigma_t} \leq T_\nu \leq \frac{U(x) - \mu_t}{\sigma_t} \quad \forall x \in (a, b) \right\} \\ &= \int_a^b \left[F_\nu \left(\frac{U(x) - \mu_t}{\sigma_t} \right) - F_\nu \left(\frac{L(x) - \mu_t}{\sigma_t} \right) \right] dF(x), \\ &= \int_a^b \left[F_\nu \left(\frac{U(x) - \mu_t}{\sigma_t} \right) - F_\nu \left(\frac{L(x) - \mu_t}{\sigma_t} \right) \right] f(x | a \leq x \leq b) dx, \\ &= \int_a^b \left[F_\nu \left(\frac{U(x) - \mu_t}{\sigma_t} \right) - F_\nu \left(\frac{L(x) - \mu_t}{\sigma_t} \right) \right] \frac{1}{\sqrt{2\pi}(\Phi(b) - \Phi(a))} \exp(-x^2/2) dx. \end{aligned}$$

Obtain large discretized samples $x^{(i)} \in [a, b], i = 1, \dots, n_x$. For each $x^{(i)}$, we have large number of $\theta_j, j = 1, \dots, n_\theta$. Denote $f_j^{(i)} = \mathbf{x}^{(i)T} \boldsymbol{\theta}_j$, which is a random variable, $\mathbf{f}^{(i)}$ as the distribution of $f_j^{(i)}$, $F^{(i)}$ as the CDF. The posterior coverage probability is approximated by the following equation:

$$\begin{aligned} & P_{\mathbf{x}^T \boldsymbol{\theta} | \mathbf{Y}} \{ \mathbf{x}^T \boldsymbol{\theta} \in \mathcal{I}_A \quad \forall x \in (a, b) \} \\ &= P_{\mathbf{x}^T \boldsymbol{\theta} | \mathbf{Y}} \{ L(x) \leq \mathbf{x}^T \boldsymbol{\theta} \leq U(x) \quad \forall x \in (a, b) \}, \\ &= \int_a^b \{ F(U(x)) - F(L(x)) \} dF(x), \\ &\approx \sum_{i=1}^{n_x} \left\{ F^{(i)}(U(x^{(i)})) - F^{(i)}(L(x^{(i)})) \right\} \end{aligned}$$