Bayesian simultaneous credible bands for polynomial regression

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4 July 2025



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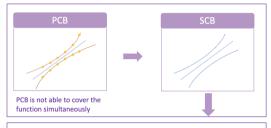
Bayesian simultaneous credible bands for polynomial regression

Motivation



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To assess the plausible range of an unknown function



Bayesian

Frequentist

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)

Bayesian simultaneous credible bands

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Notations

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$Y = X\theta + e, (1)$

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

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Key Property

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Key Property

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

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

- $P\{\cdot\}$, $E(\theta)$, and $\text{Var}(\boldsymbol{x}^T\boldsymbol{\theta})$ are with respect to the posterior distribution of $\boldsymbol{\theta}|\boldsymbol{Y}$
- λ is the critical constant.



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 (2)

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



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Key Property

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The Key Procedure

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

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

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The Conjugate Prior Method

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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 θ and τ .
- Here we assume the prior $\xi({m{ heta}}, au)$ is a normal-gamma prior density,

•
$$\xi(\boldsymbol{\theta}, \tau) = \xi_1(\boldsymbol{\theta}|\tau) \cdot \xi_2(\tau), \quad \boldsymbol{\theta} \in \mathbb{R}^p, \tau > 0,$$

•
$$\theta | \tau \sim \mathcal{N}(\mu, \tau^{-1} \mathcal{P})$$

•
$$\tau \sim \mathsf{Gamma}(\alpha_0, \beta_0)$$

Use a data-driven approach for the hyperparameters in the priors:

•
$$\mu = \hat{\theta}_{GLS} = (X^T V^{-1} X)^{-1} X^T V^{-1} Y$$
,

•
$$\mathcal{P} = c \cdot I_p$$
,

•
$$\alpha_0 = 1$$
,

•
$$\beta_0 = \frac{\hat{e}_{GLS}^T \hat{e}_{GLS}}{n-p}$$



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The Conjugate Prior Method

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The multivariate t distribution

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

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

The Key Procedure

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

- $E(\boldsymbol{\theta}|\boldsymbol{Y}) = \mu^*$,
- $Var(\theta|Y) = \frac{n+2\alpha_0}{n+2\alpha_0-2}(D^*)^{-1}$, 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 .

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

Input: $X, Y, n, \mu, \mathcal{P}, \alpha_0, \beta_0, x \in (a, b), 1 - \alpha$. Output: $\hat{\boldsymbol{\theta}}, \hat{\tau}, \lambda$

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

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



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

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

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

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

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

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The HMC Method

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The HMC Method



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

• $E(\boldsymbol{\theta})$, $Var(\boldsymbol{\theta})$

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The HMC Method

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

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

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

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

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



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The HMC Method

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

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

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 θ . Draw one value of θ .

• b. Derive the $E(\theta) = \mu^*$, and $Var(\theta)$ according to the posterior distribution.

• c. Compute $\lambda^{(l)}$ which is given by

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

• Step 2: Order these $\lambda^{(l)}$ values as $\lambda_{[1]} \leq \cdots \leq \lambda_{[L]}$ and use $\lambda_{[<(1-\alpha)L>]}$ as the λ we want. Here $<(1-\alpha)L>$ denotes the integer part of $(1-\alpha)L$. The simultaneous credible bands for $\boldsymbol{x}^T\boldsymbol{\theta}$ is given by:

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



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Comparison Methods & Evaluation Criterion

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Comparison Methods & Evaluation Criterion



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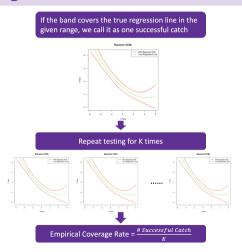
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References

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)

The Empirical Coverage Rate



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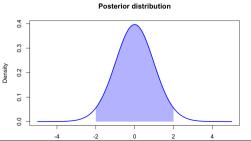
Yet, it is not an appropriate criterion to use in the Bayesian context.

Comparison Methods & Evaluation Criterion

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 $x^T \theta$, $x \in (a, b)$, as \mathcal{I}_A : the posterior coverage probability is defined as

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





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A Toy Example

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A Toy Example

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

- $x_i \sim U(-5,5)$, $e_i \sim N(0,\sigma^2)$, $i = 1, \ldots, n$,
 - Linear Setting: $\theta = (1, 2)^T$
 - n=100
 - $\sigma = 0.25$
 - Quadratic Setting: $\boldsymbol{\theta} = (-6, -3, 0.25)^T$
 - 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.



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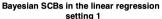


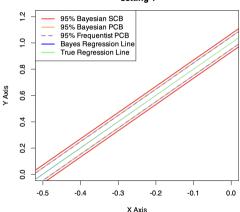
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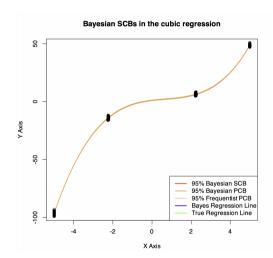
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Figure: The 95% Bayesian SCB, the 95% Bayesian PCB, and the 95% Frequentist PCB for the linear regression line





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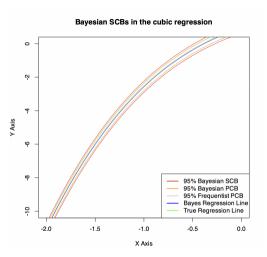
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Figure: The 95% Bayesian SCB, the 95% Bayesian PCB, and the 95% frequentist PCB for the regression curve in the cubic regression example with a D-optimal design matrix





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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

Simulation Results



The Posterior Coverage Probability

_	σ	n	Average Posterior Coverage Probability		
p			95% Bayesian SCB	95% Bayesian PCB	
			Conjugate Prior	3070 Dayesian I CD	
	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	
2		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	
	1	20	0.984	0.950	
3		50	0.987	0.950	
3		100	0.988	0.950	
		200	0.988	0.950	

- 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.

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

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Simulation Results



The HMC Method

p		n			Coverage Rate	Average Posterior Coverage Probability			
P	σ	n	95% Bayesian SCB		95% Bayesian PCB	95% Frequentist PCB		95% Bayesian SCB	95% Bayesian PCB
			Conjugate Prior	HMC			Conjugate Prior	HMC	
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.

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Real Data Example



Dose-response Dataset in a Phase II study

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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.

\mathbf{Dose}	${\bf Sample\ size}$	${\bf Sample\ mean}$	${\bf Sample~SD}$
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



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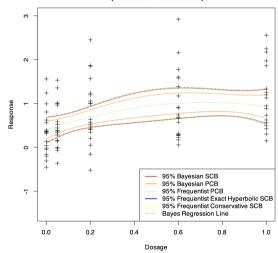


When the covariates are not centered:

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

- λ: 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]

Bayesian SCBs for Bretz et al. (2005) dataset (Covariates Not Centered)



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Summary & Future Work

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Summary

- To assess where lies the true regression function $x^T \theta$, we propose two methods for constructing two-sided hyperbolic Bayesain SCBs over a finite interval on the covariates for the polynomial regression.
- Compared to the Frequentist approach. Bayesian methods are more suitable when data are **limited** or when **domain knowledge** needs to be incorporated.
- Both the conjugate method and the HMC method are computationally convenient. The HMC method is more generally applicable than the conjugate method, as it is **less sensitive** to the hyperparameters.

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Future Work

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

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- [1] Robert J Serfling. *Approximation theorems of mathematical statistics*. John Wiley & Sons, 1980.
- [2] Wei Liu, Sanyu Zhou, and Frank Bretz. Exact simultaneous confidence bands for quadratic and cubic polynomial regression with applications in dose response study. *Australian & New Zealand Journal of Statistics*, 55(4):421–434, 2013.
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- [5] Laurens Sluijterman, Eric Cator, and Tom Heskes. How to evaluate uncertainty estimates in machine learning for regression? *Neural Networks*, 173:106203, 2024

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This is the end of my presentation. Thank you for your attention.

The Conjugate Prior Method

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The multivariate t distribution

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

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

with location vector

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

and precision matrix

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

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

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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 $\boldsymbol{x}^T\boldsymbol{\theta}$ at x is given by:

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

•
$$\hat{\theta} = (X^T V^{-1} X)^{-1} X^T V^{-1} Y$$

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

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Bayesian Pointwise Credible Band

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

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

As μ^* is the posterior mean for θ .

Coverage Probability in the conjugate prior method

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



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

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

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Coverage Probability in the HMC method

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

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

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