Approximate General Bayesian Inference via Semiparametric Variational Bayes

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June 29, 2022

Overview

Some background

Risk–based parameter definition

$$
\begin{aligned}
\text{Data distribution}: &\quad y \sim (\mathcal{Y}, \mathcal{F}, \mathbb{P}) \\
\text{Parameter of interest}: &\quad \boldsymbol{\theta} = \operatorname{argmin}\ R(\,\cdot\,; \mathbb{P}) \\
\text{Theoretical risk function}: &\quad R(\boldsymbol{\theta}; \mathbb{P}) = \mathbb{E}\{L(y, \boldsymbol{\theta})\}
\end{aligned}
$$

General belief updating (Bissiri et al., 2016)

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\text{Subjective prior belief}: &\quad \boldsymbol{\theta} \sim p(\boldsymbol{\theta}) \\
\text{Empirical risk function}: &\quad R(\boldsymbol{\theta}; \mathbf{y}) = \textstyle\sum_{i=1}^{n} L(y_i, \boldsymbol{\theta})/n \\
\text{Bayesian belief updating}: &\quad p(\boldsymbol{\theta}|\mathbf{y}) \propto p(\boldsymbol{\theta}) \exp\{-nR(\boldsymbol{\theta}; \mathbf{y})\}
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Bayesian belief updating : $p(\boldsymbol{\theta}|\mathbf{y}) \propto p(\boldsymbol{\theta}) \exp\{-nR(\boldsymbol{\theta}; \mathbf{y})\}$

Overview

Bayesian mixed model

Empirical risk function

$$-nR(\boldsymbol{\theta}; \mathbf{y}) = -\frac{n}{\alpha}\log\sigma_\varepsilon^2 - \frac{1}{\alpha\sigma_\varepsilon^2}\sum_{i=1}^{n}\psi(y_i, \eta_i),$$

- $\{y_i, \mathbf{x}_i, \mathbf{z}_i\} \in \mathcal{Y} \times \mathbb{R}^p \times \mathbb{R}^d$
- $\eta_i = \mathbf{x}_i^\top \boldsymbol{\beta} + \mathbf{z}_i^\top \boldsymbol{u}$
- $\psi(y, \eta)$: loss function
- σ_ε^2: dispersion parameter
- α: calibrating parameter

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Prior distributions

$$\boldsymbol{u}|\sigma_u^2 \sim \mathsf{N}_d(\mathbf{0}_d, \sigma_u^2\mathbf{Q}^{-1}), \qquad \sigma_u^2 \sim \mathsf{IG}(A_u, B_u),$$
$$\boldsymbol{\beta} \sim \mathsf{N}_p(\mathbf{0}_p, \sigma_\beta^2\mathbf{I}_p), \qquad \sigma_\varepsilon^2 \sim \mathsf{IG}(A_\varepsilon, B_\varepsilon),$$

Here, $\sigma_\beta^2, A_\varepsilon, B_\varepsilon, A_u, B_u > 0$ and $\mathbf{Q} \succeq 0$ are fixed prior parameters.

Generalized posterior distribution

$$\underbrace{p(\boldsymbol{\beta}, \boldsymbol{u}, \sigma_u^2, \sigma_\varepsilon^2 \mid \mathbf{y})}_{\text{Generalized posterior}} \propto \underbrace{p(\sigma_\varepsilon^2)\, p(\boldsymbol{\beta})\, p(\sigma_u^2)\, p(\boldsymbol{u}|\sigma_u^2)}_{\text{Prior beliefs}}\ \underbrace{\exp\{-nR(\mathbf{y}, \boldsymbol{\theta})\}}_{\text{Pseudo–likelihood}}$$

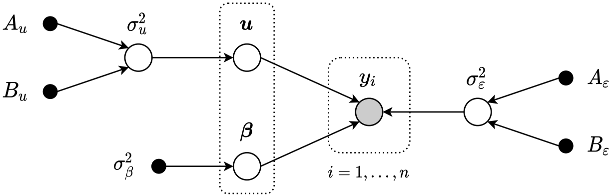

Figure: Direct acyclic graph representing the Bayesian model.

Overview

Semiparametric variational inference

- Variational approximation: $p(\boldsymbol{\theta}|\mathbf{y}) \approx q(\boldsymbol{\theta};\boldsymbol{\xi}) = q_1(\boldsymbol{\theta}_1)\cdots q_K(\boldsymbol{\theta}_K)\, q_\phi(\phi;\boldsymbol{\xi})$
- Variational problem: $(q_1^*, \ldots, q_K^*, q_\phi^*) = \operatorname{argmin}\ \mathsf{KL}(q(\boldsymbol{\theta};\boldsymbol{\xi}) \,\|\, p(\boldsymbol{\theta}|\mathbf{y}))$

Mean field variational Bayes

$$q_k^*(\boldsymbol{\theta}_k) \propto \exp\left[\mathbb{E}_{-k}\{\log p(\boldsymbol{\theta}_k \mid \mathsf{rest})\}\right]$$

Knowles–Minka–Wand recursion

- $q_\phi(\phi;\boldsymbol{\mu},\Sigma) \sim \mathsf{N}(\boldsymbol{\mu},\Sigma)$
- $\hat{\mu} \leftarrow \hat{\mu} - \rho\,\mathbf{H}^{-1}\mathbf{g}$
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- $f(\boldsymbol{\mu},\Sigma) = \mathbb{E}_q\{\log p(\mathbf{y},\boldsymbol{\theta})\}$
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See Ormerod and Wand (2010), Blei et al. (2017) for MFVB.
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Optimal variational distributions

Assumptions:

- mean field factorization: $q(\boldsymbol{\beta}, \boldsymbol{u}, \sigma_u^2, \sigma_\varepsilon^2) = q(\sigma_\varepsilon^2)\, q(\sigma_u^2)\, q(\boldsymbol{\beta}, \boldsymbol{u})$
- parametric restriction: $q(\boldsymbol{\beta}, \boldsymbol{u}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) \sim \mathsf{N}\left(\begin{bmatrix} \boldsymbol{\mu}_\beta \\ \boldsymbol{\mu}_u \end{bmatrix}, \begin{bmatrix} \boldsymbol{\Sigma}_{\beta\beta} & \boldsymbol{\Sigma}_{\beta u} \\ \boldsymbol{\Sigma}_{u\beta} & \boldsymbol{\Sigma}_{uu} \end{bmatrix} \right)$

Closed form solutions:

- $q^*(\sigma_\varepsilon^2) \sim \mathsf{IG}(\hat{A}_\varepsilon, \hat{B}_\varepsilon)$ where $\hat{A}_\varepsilon \leftarrow A_\varepsilon + n/\alpha$ and $\hat{B}_\varepsilon \leftarrow B_\varepsilon + \mathbf{1}_n^\top \boldsymbol{\Psi}^{(0)}/\alpha$
- $q^*(\sigma_u^2) \sim \mathsf{IG}(\hat{A}_u, \hat{B}_u)$ where $\hat{A}_u \leftarrow A_u + d/2$ and $\hat{B}_u \leftarrow B_u + \frac{1}{2}\hat{\boldsymbol{\mu}}_u^\top \mathbf{Q}\, \hat{\boldsymbol{\mu}}_u + \frac{1}{2}\mathrm{trace}\left[\mathbf{Q}\hat{\boldsymbol{\Sigma}}_{uu}\right]$

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Parametric solution:

$$\text{(update)} \qquad \boldsymbol{\mu} \leftarrow \boldsymbol{\mu} - \rho\,\mathbf{H}^{-1}\mathbf{g}, \quad \boldsymbol{\Sigma} \leftarrow -\mathbf{H}^{-1},$$

$$\text{(gradient)} \qquad \mathbf{g}(\boldsymbol{\mu}, \boldsymbol{\Sigma}) = -\begin{bmatrix} \sigma_\beta^{-2}\boldsymbol{\mu}_\beta \\ \mu_{q(1/\sigma_u^2)}\mathbf{Q}\,\boldsymbol{\mu}_u \end{bmatrix} - \mu_{q(1/\sigma_\varepsilon^2)}\mathbf{C}^\top \boldsymbol{\Psi}^{(1)}/\alpha,$$

$$\text{(Hessian)} \qquad \mathbf{H}(\boldsymbol{\mu}, \boldsymbol{\Sigma}) = -\begin{bmatrix} \sigma_\beta^{-2}\mathbf{I}_p & \mathbf{O} \\ \mathbf{O} & \mu_{q(1/\sigma_u^2)}\mathbf{Q} \end{bmatrix} - \mu_{q(1/\sigma_\varepsilon^2)}\mathbf{C}^\top \mathrm{diag}\big[\boldsymbol{\Psi}^{(2)}\big]\,\mathbf{C}/\alpha,$$

where $\mathbf{C} = \big[\mathbf{X},\, \mathbf{Z}\big]$, $\mu_{q(1/\sigma_u^2)} = \mathbb{E}_q(1/\sigma_u^2)$, $\mu_{q(1/\sigma_\varepsilon^2)} = \mathbb{E}_q(1/\sigma_\varepsilon^2)$ and

$$\Psi_i^{(r)} = \Psi^{(r)}(y_i, \mathbf{c}_i^\top\boldsymbol{\mu}, \mathbf{c}_i^\top\boldsymbol{\Sigma}\,\mathbf{c}_i) = \mathbb{E}_q\left\{\frac{\partial^r}{\partial\eta^r}\psi(y_i, \eta_i)\right\}, \qquad r = 0, 1, 2.$$

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Ψ–functions

Proposition

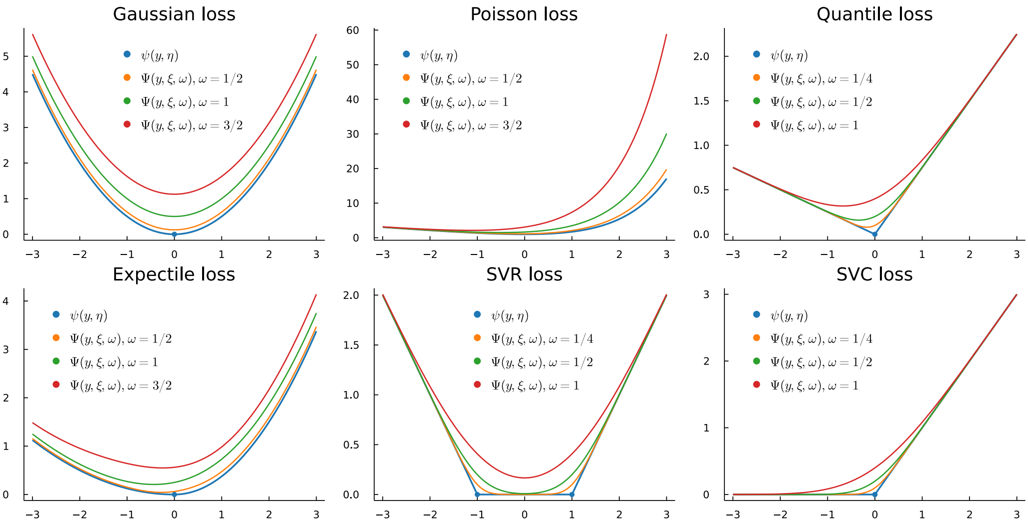
Let $\psi(y, \eta)$ be a **convex**, 2–times **weakly differentiable** function wrt to η, then:

1. $\Psi^{(r)}(y, \mathbf{c}^\top \boldsymbol{\mu}, \mathbf{c}^\top \boldsymbol{\Sigma}\, \mathbf{c})$ has infinitely many derivatives wrt $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$;
2. $\Psi^{(0)}(y, \mathbf{c}^\top \boldsymbol{\mu}, \mathbf{c}^\top \boldsymbol{\Sigma}\, \mathbf{c})$ is jointly convex wrt $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$;
3. $\Psi^{(0)}(y, \mathbf{c}^\top \boldsymbol{\mu}, \mathbf{c}^\top \boldsymbol{\Sigma}\, \mathbf{c}) \geq \psi(y, \mathbf{c}^\top \boldsymbol{\mu})$ for any y and $\mathbf{c}$.

Then

- the optimum of the KL–divergence is unique
- the KMW recursion converges to the optimum

Models


Gaussian loss
$\psi(y,\eta)$
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$\Psi(y,\xi,\omega), \omega = 3/2$
Poisson loss
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Algorithm

Semiparametric variational Bayes algorithm for approximate Bayesian inference

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Initialize $\hat{A}_\varepsilon$, $\hat{B}_\varepsilon$, $\hat{A}_u$, $\hat{B}_u$, $\hat{\boldsymbol{\mu}}$, $\hat{\boldsymbol{\Sigma}}$;

While *convergence is not reached* **do**:

Evaluate $\boldsymbol{\Psi}^{(0)}$, $\boldsymbol{\Psi}^{(1)}$, $\boldsymbol{\Psi}^{(2)}$;

$\hat{A}_u \leftarrow A_u + d/2; \quad \hat{B}_u \leftarrow B_u + \frac{1}{2}\hat{\boldsymbol{\mu}}_u^\top \mathbf{Q}\,\hat{\boldsymbol{\mu}}_u + \frac{1}{2}\mathrm{trace}\big[\mathbf{Q}\,\hat{\boldsymbol{\Sigma}}_{uu}\big];$

$\hat{A}_\varepsilon \leftarrow A_\varepsilon + n/\alpha; \quad \hat{B}_\varepsilon \leftarrow B_\varepsilon + \mathbf{1}_n^\top \boldsymbol{\Psi}^{(0)}/\alpha;$

$\mu_{q(1/\sigma_u^2)} \leftarrow \hat{A}_u/\hat{B}_u; \quad \mu_{q(1/\sigma_\varepsilon^2)} \leftarrow \hat{A}_\varepsilon/\hat{B}_\varepsilon;$

$\mathbf{g} \leftarrow -\,\mathrm{stack}\big[\sigma_\beta^{-2}\hat{\boldsymbol{\mu}}_\beta, \mu_{q(1/\sigma_u^2)}\mathbf{Q}\,\hat{\boldsymbol{\mu}}_u\big] - \mu_{q(1/\sigma_\varepsilon^2)}\mathbf{C}^\top\boldsymbol{\Psi}^{(1)}/\alpha;$

$\mathbf{H} \leftarrow -\,\mathrm{blockdiag}\big[\sigma_\beta^{-2}\mathbf{I}_p, \mu_{q(1/\sigma_u^2)}\mathbf{Q}\big] - \mu_{q(1/\sigma_\varepsilon^2)}\mathbf{C}^\top\mathrm{diag}\big[\boldsymbol{\Psi}^{(2)}\big]\mathbf{C}/\alpha;$

$\rho \leftarrow \mathrm{LineSearch}(f, \mathbf{g}, \mathbf{H}); \quad \hat{\boldsymbol{\Sigma}} \leftarrow -\mathbf{H}^{-1}; \quad \hat{\boldsymbol{\mu}} \leftarrow \hat{\boldsymbol{\mu}} - \rho\,\mathbf{H}^{-1}\mathbf{g};$

End of while

Overview

Simulation setup

1. **Data generating process**:
   - $y_i | x_i \overset{\text{ind.}}{\sim} \begin{cases} \mathsf{N}(f(x_i), \{g(x_i)\}^2) & \text{for regression} \\ \mathsf{Be}(\text{expit}\{f(x_i)\}) & \text{for classification} \end{cases}$
   - mean function: $f(x) = 1.6 \sin(3\pi x^2)$
   - variance function: $g(x) = \exp\{-0.6 + 0.5 \cos(4\pi x)\}$
2. **Linear predictor**:
   - Bayesian penalized semiparametric regression
3. **Loss functions**:
   - quantile regression (MCMC: Kozumi and Kobayashi, 2011; MFVB: Wand et al., 2011)
   - expectile regression (MCMC: Waldmann et al., 2017; Laplace approximation)
   - support vector regression (MCMC: Polson and Scott, 2011; MFVB: Luts and Ormerod, 2014)
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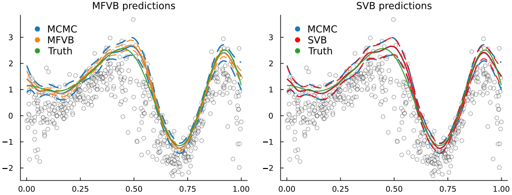
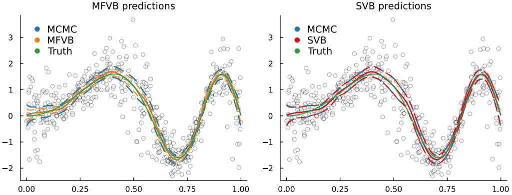
Predictive distributions

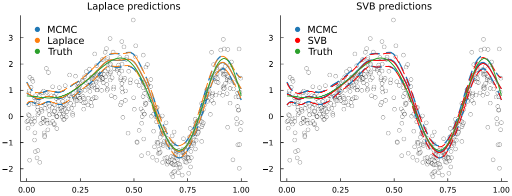
Quantile regression ($\tau = 0.9$)



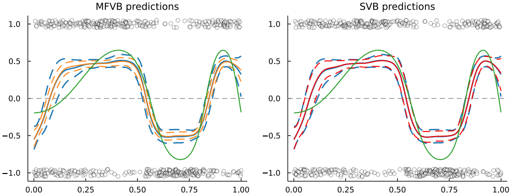
Support vector regression ($\epsilon = 0.01$)



Expectile regression ($\tau = 0.9$)



Support vector classification



Marginal approximations

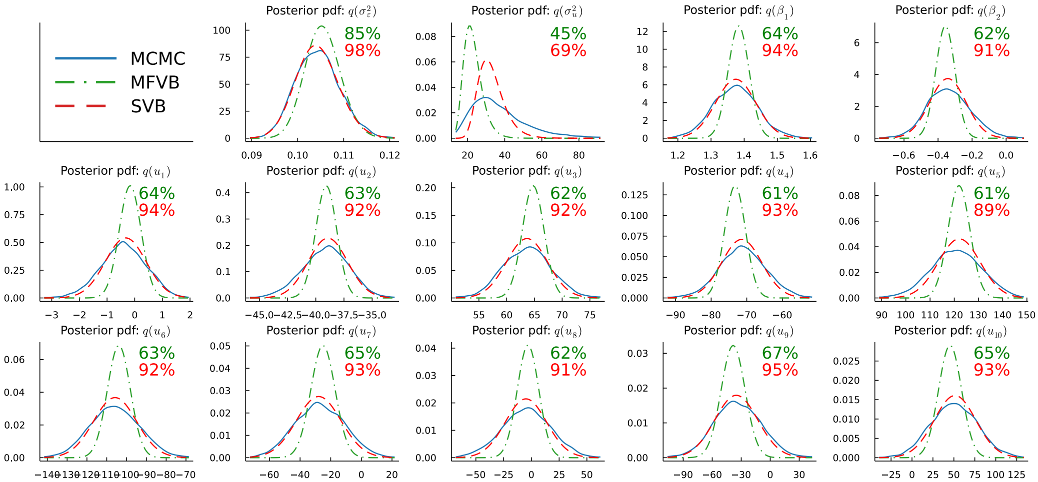


Figure: Marginal posterior density functions for the quantile regression model.

Results

Model	Method	ELBO	Accuracy	Iter.Count	Exe.Time (S.E.)
QReg	MCMC	–	–	10000	4170.000 (32.482) ms
	MFVB	-713.9727	0.8613	47	81.697 (3.463) ms
	SVB	-710.1009	0.9196	27	80.252 (3.761) ms
EReg	MCMC	–	–	10000	3710.000 (33.565) ms
	Laplace	–	0.9669	26	46.734 (3.014) ms
	SVB	153.8963	0.9687	35	62.979 (3.113) ms
SVR	MCMC	–	–	10000	4867.000 (30.114) ms
	MFVB	-637.3713	0.9090	33	61.805 (3.477) ms
	SVB	-634.9547	0.9521	20	75.474 (3.256) ms
SVC	MCMC	–	–	10000	4396.000 (35.974) ms
	MFVB	-537.9229	0.8579	69	118.710 (2.885) ms
	SVB	-536.1095	0.9070	37	129.785 (4.563) ms

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Overview

Conclusions

Methodological innovations:

- we introduced a simplified general algorithm for the estimating risk–based mixed models
- existing algorithms are included into our framework (GLMs)
- new algorithms for Quantile, Expectile and SVM models

Empirical evidences:

- improvement over existing data–augmented MFVB approximations
- good–to–excellent performance in posterior approximation

Possible extensions:

- streamlined algorithms for structured prior distributions (cross–random effects, GMRF)
- hierarchical prior for inducing sparsity and shrinkage on the estimates
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Thank you for your attention!