

# Zig-zag computational bounds and further implementation details

## Abstract

Full implementation details for zig-zag algorithms used in “Exact Sampling of Gibbs Measures with Estimated Losses” by Frazier, Knoblauch, Jewson and Drovandi.

## 1 Preliminaries

Firstly we recall Cinlar’s Algorithm ([Cinlar, 1975](#)) for sampling from inhomogeneous Poisson process.

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**Algorithm 1:** Cinlar’s Algorithm ([Cinlar, 1975](#)) to sample  $\mathbb{P}(\tau_j \geq t) = \exp(-\Lambda(t))$

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- 1 Initialisation:  $s = 0$ .
  - 2 Generate  $u \sim U(0, 1)$
  - 3 Set  $s \mapsto s - \log(u)$
  - 4 Return  $t \mapsto \inf \{v : \Lambda(v) \geq s\}$
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We also recall Poisson superposition which helps to implement Cinlar’s Algorithm for some of the applications to come

**Theorem 1** (Poisson superposition ). *Let  $\Lambda^{(1)} : \mathbb{R}_+ \mapsto \mathbb{R}_+$  and  $\Lambda^{(2)} : \mathbb{R}_+ \mapsto \mathbb{R}_+$  be continuous for  $t \geq 0$ . Let  $\tau_1^{(1)}, \tau_2^{(1)}, \dots$  be a increasing finite or infinite sequence of points of a Poisson process with rate function  $(\Lambda^{(1)}(t))_{t \geq 0}$ , and  $\tau_1^{(2)}, \tau_2^{(2)}, \dots$  be another increasing finite or infinite sequence of points of a Poisson process with rate function  $(\Lambda^{(2)}(t))_{t \geq 0}$ .*

Then the ordered infinite sequence obtained from the union of  $\tau_1^{(1)}, \tau_2^{(1)}, \dots$  and  $\tau_1^{(2)}, \tau_2^{(2)}, \dots$ , say,  $\tilde{\tau}_1, \tilde{\tau}_2, \dots$  say, form a nonhomogeneous Poisson process with rate function  $(\Lambda^{(1)}(t) + \Lambda^{(2)}(t))_{t \geq 0}$ .

## 2 Implementation Details

This section contains additional implementation details for the experiments presented in Section 5 of the paper. We start with an additional example where the zig-zag computational bounds are simple to derive.

### 2.1 Student's- $t$ location model with the MMD

Consider estimating the location parameter  $\theta = \{\mu\}$  of a Student's- $t$  likelihood model with fixed scale  $\sigma$  and degree of freedom  $\nu$ . We place a Gaussian prior on  $\theta$  with mean  $\mu_0 = 0$  and variance  $s_0^2 = 25$  and consider sampling from the MMD-Bayes posterior using the RBF kernel with hyperparameter  $\gamma = 1$ . We *indirectly* sample  $u_{1:b} \sim t_\nu(\mu, \sigma^2)$  by first sampling  $v_{1:b}$  with  $v_k = \{v_{k1}, v_{k2}, v_{k3}\} \sim p_v$  and  $p_v(v) = \text{unif}(v_1; 0, 1)\text{unif}(v_2; 0, 1)\mathcal{G}(v_3; \nu/2, \nu/2)$  and setting

$$u_k = G_\mu(v; \eta, \sigma^2) = \mu + \sqrt{\sigma^2/v_3} \sqrt{-2 \log(v_1)} \cos(2\pi v_2).$$

Lemma 1 provides computational bounds for this example and Corollary 1 shows how these can be sampled from.

**Lemma 1** (Computational Bounds for MMD-Bayes for Student's- $t$  location model). *Consider the MMD-Bayes posterior for a Student's- $t$  location model with Gaussian priors with mean  $\mu_0$  and variance  $s_0^2$  on unknown location parameter  $\theta = \{\mu\}$  and fixed degrees of*

freedom  $\nu$  and scale parameter  $\sigma$ . The zig-zag switching rate is given by

$$\hat{\lambda}(\mu, \nu) := \max \left( 0, \nu \frac{\mu - \mu_0}{s_0^2} + 2\nu \frac{\omega}{n} \sum_{i=1}^n \frac{1}{b} \sum_{k=1}^b \frac{(G_\mu(v_k; \eta, \sigma^2) - y_i)}{\sqrt{2\pi}\gamma^{3/2}} \exp \left( -\frac{(G_\mu(v_k; \eta, \sigma^2) - y_i)^2}{2\gamma} \right) \right)$$

where  $v_1, \dots, v_m \sim p_v$ ,

$$G_\mu(v; \eta, \sigma^2) = \mu + \sqrt{\sigma^2/v_3} \sqrt{-2 \log(v_1)} \cos(2\pi v_2),$$

and  $p_v(v) = \text{unif}(v_1; 0, 1) \text{unif}(v_2; 0, 1) \mathcal{G}(v_3; \eta/2, \eta/2)$ .

Computational bounds are given by

$$\hat{\Lambda}_j(\mu + \nu \cdot t, \nu) = \frac{|\mu - \mu_0|}{s_0^2} + \frac{2\omega}{\sqrt{2\pi}\gamma} \exp \left( -\frac{1}{2} \right) + \frac{1}{s_0^2} t.$$

*Proof.* Firstly, we can *indirectly* sample  $u_{1:b} \sim t_\nu(\mu, \sigma^2)$  by first sampling  $v_{1:b}$  with  $v_k = \{v_{k1}, v_{k2}, v_{k3}\} \sim p_v$  and  $p_v(v) = \text{unif}(v_1; 0, 1) \text{unif}(v_2; 0, 1) \mathcal{G}(v_3; \eta/2, \eta/2)$  and setting  $u_k = G_\mu(v_k; \eta, \sigma^2)$

$$G_\mu(v; \eta, \sigma^2) = \mu + \sqrt{\sigma^2/v_3} \sqrt{-2 \log(v_1)} \cos(2\pi v_2).$$

As a result, for the MMD-Bayes posterior with RBF kernel with hyperparameter  $\gamma$  and

Gaussian prior has

$$\begin{aligned}
\Psi_n(\mu) &:= -\log \pi(\mu) + w\mathbf{L}_n^\gamma(\mu) \\
&= \frac{(\mu - \mu_0)^2}{2s_0^2} - 2\frac{w}{n} \sum_{i=1}^n \mathbb{E}_{v \sim p(\cdot)} [\mathcal{K}_\gamma(y_i, G_\mu(v; \eta, \sigma^2))] + \omega \mathbb{E}_{v, v' \sim p(\cdot)} [\mathcal{K}_\gamma(G_\mu(v; \eta, \sigma^2), F_{\eta, \sigma^2}(v'; \mu))] \\
&= \frac{(\mu - \mu_0)^2}{2s_0^2} - 2\frac{w}{n} \sum_{i=1}^n \mathbb{E}_{v \sim p(\cdot)} \left[ \frac{1}{\sqrt{2\pi\gamma}} \exp \left( -\frac{(y_i - G_\mu(v; \eta, \sigma^2))^2}{2\gamma} \right) \right] \\
&\quad + \omega \mathbb{E}_{v, v' \sim p(\cdot)} \left[ \frac{1}{\sqrt{2\pi\gamma}} \exp \left( -\frac{(G_\mu(v; \eta, \sigma^2) - F_{\eta, \sigma^2}(v'; \mu))^2}{2\gamma} \right) \right]
\end{aligned}$$

The zig-zag requires the evaluation of

$$\hat{\lambda}(\mu, \nu) := \max \left( 0, \nu \left( -\frac{\partial}{\partial \mu} \log(\pi(\mu)) + \omega \varphi_{b,n}(\mu) \right) \right)$$

and bounding of  $\hat{\lambda}(\mu + \nu \cdot t, \nu)$ , where

$$\begin{aligned}
\varphi_{b,n}(\mu) &:= 2\frac{1}{n} \sum_{i=1}^n \frac{1}{b} \sum_{k=1}^b \frac{(G_\mu(v_k; \eta, \sigma^2) - y_i)}{\sqrt{2\pi\gamma^{3/2}}} \exp \left( -\frac{(G_\mu(v_k; \eta, \sigma^2) - y_i)^2}{2\gamma} \right) \\
&\quad - \frac{1}{b(b-1)} \sum_{k=1}^b \sum_{k' \neq k} \left( \frac{(G_\mu(v_k; \eta, \sigma^2) - G_\mu(v_{k'}; \eta, \sigma^2))}{\sqrt{2\pi\gamma^{3/2}}} \exp \left( -\frac{(G_\mu(v_k; \eta, \sigma^2) - G_\mu(v_{k'}; \eta, \sigma^2))^2}{2\gamma} \right) \right. \\
&\quad \left. - \frac{(G_\mu(v_{k'}; \eta, \sigma^2) - G_\mu(v_k; \eta, \sigma^2))}{\sqrt{2\pi\gamma^{3/2}}} \exp \left( -\frac{(G_\mu(v_{k'}; \eta, \sigma^2) - G_\mu(v_k; \eta, \sigma^2))^2}{2\gamma} \right) \right) \\
&= \frac{\mu - \mu_0}{s_0^2} + 2\frac{1}{n} \sum_{i=1}^n \frac{1}{b} \sum_{k=1}^b \frac{(G_\mu(v_k; \eta, \sigma^2) - y_i)}{\sqrt{2\pi\gamma^{3/2}}} \exp \left( -\frac{(G_\mu(v_k; \eta, \sigma^2) - y_i)^2}{2\gamma} \right)
\end{aligned}$$

with  $v_1, \dots, v_N \sim p_v$ . Above uses the fact that

$$\begin{aligned}
\frac{\partial}{\partial z} \mathcal{K}_\gamma(z, x) &= -\frac{(z - x)}{\sqrt{2\pi\gamma^{3/2}}} \exp \left( -\frac{(z - x)^2}{2\gamma} \right) \\
\frac{\partial}{\partial \mu} G_\mu(v; \eta, \sigma^2) &= 1
\end{aligned}$$

and the cancellation of the second MMD term happens as  $\frac{\partial}{\partial \mu} G_\mu(v; \eta, \sigma^2)$  does not depend

on  $v$ .

Now, using the fact that for the RBF kernel  $\left| \frac{\partial}{\partial z} \mathcal{K}_\gamma(y, y') \right| \leq \frac{1}{\sqrt{2\pi\gamma}} \exp\left(-\frac{1}{2}\right)$  for any value of  $y$  or  $y'$  we can bound

$$\begin{aligned} \hat{\lambda}(\mu + \nu \cdot t, \nu) &= \max \left( 0, \nu \left( -\frac{\partial}{\partial \mu} \log(\pi(\mu + \nu \cdot t)) + \omega \varphi_{b,n}(\mu + \nu \cdot t) \right) \right) \\ &\leq \frac{|\mu - \mu_0|}{s_0^2} + \frac{2\omega}{\sqrt{2\pi\gamma}} \exp\left(-\frac{1}{2}\right) + \frac{1}{s_0^2} t \\ &= \hat{\Lambda}(\mu + \nu \cdot t, \nu). \end{aligned}$$

□

**Corollary 1.** *Sampling stopping times according to the computational bound in Lemma 1 is achieved by sampling  $u \sim U[0, 1]$  and setting*

$$\tau^* := \frac{\sqrt{a^2 - 2\log(u)b} - a}{b}$$

with

$$\begin{aligned} a &:= \frac{|\mu - \mu_0|}{s_0^2} + \frac{2\omega}{\sqrt{2\pi\gamma}} \exp\left(-\frac{1}{2}\right) \\ b &:= \frac{1}{s_0^2}. \end{aligned}$$

*Proof.* Sampling stopping times according to the computational bounds in Lemma 1 require

the evaluation of

$$\begin{aligned}
\int_0^t \hat{\Lambda}(\mu + \nu \cdot s, \nu) ds &= \int_0^t a + b s ds \\
&= \left[ as + \frac{b}{2} s^2 \right]_0^t \\
&= at + \frac{b}{2} t^2
\end{aligned}$$

with

$$\begin{aligned}
a &:= \frac{|\mu - \mu_0|}{s_0^2} + \frac{2\omega}{\sqrt{2\pi\gamma}} \exp\left(-\frac{1}{2}\right) \\
b &:= \frac{1}{s_0^2}
\end{aligned}$$

and therefore the stopping times can be simulated following Cinlar's Algorithm ([Cinlar, 1975](#)) (Algorithm 1) by sampling  $u \sim U[0, 1]$  and solving

$$\begin{aligned}
t &:= \inf \left\{ \nu : a\nu + \frac{b}{2}\nu^2 \geq -\log(u) \right\} \\
&= \inf \left\{ \nu : \frac{b}{2}\nu^2 + a\nu + \log(u) \geq 0 \right\} \\
&= \frac{-a \pm \sqrt{a^2 - 4\log(u)\frac{b}{2}}}{b_j} \\
&= \frac{\sqrt{a^2 - 2\log(u)b} - a}{b}.
\end{aligned}$$

□

## 2.2 Outlier Robust linear regression with the MMD

Here we provide implementation details for Section 5.2.1 of the paper.

Firstly, the Gaussian regression model has an implicit representation as:

$$G_\theta(v; x) = \beta^\top x + \sqrt{\sigma^2} \sqrt{-2 \log(v_1)} \cos(2\pi v_2).$$

This representation makes clear that we can *indirectly* sample  $u_{1:b} \sim \mathcal{N}(x^\top \beta, \sigma^2)$  by first sampling  $v_{1:b}$  with  $u_k = \{v_{k1}, v_{k2}\} \sim p_v$  and  $p_v(v) = \text{unif}(v_1; 0, 1) \text{unif}(v_2; 0, 1)$  and setting  $u_k = G_\theta(v_k; x)$

Given this, we can conduct implicit sampling based on the following implicit representation of the MMD, which was referred to by [Alquier and Gerber \(2024\)](#) as the ‘tilde’-type estimator (their Eq. (5) and (6)):

$$\begin{aligned} \mathbb{L}_{m,n}(\theta, u_{1:b}) &= \mathbb{L}_{m,n}^{\mathcal{K}_\gamma}(y_{1:n}, G_\theta(v_{1:b}; x)) \\ &= - \sum_{i=1}^n \left\{ 2 \frac{1}{b} \sum_{j=1}^b \mathcal{K}_\gamma(y_i, G_\theta(v_j; x_i)) \right. \\ &\quad \left. - \frac{1}{b(b-1)} \sum_{k=1}^b \sum_{k' \neq k}^b \mathcal{K}_\gamma(G_\theta(v_k; x_i), G_\theta(v_{k'}; x_i)) \right\} \end{aligned}$$

where  $\mathcal{K}_\gamma(y, y') = \frac{1}{\sqrt{2\pi\gamma}} \exp\left(-\frac{(y-y')^2}{2\gamma}\right)$  is the radial basis function (RBF) kernel. We place Gaussian priors with mean  $\mu_0 = 0$  and variance  $s_0^2 = 25$  on each  $\beta_j$ ,  $j = 1, \dots, d$  and an inverse-gamma prior on  $\sigma^2$  with shape  $a_0 = 2$  and scale  $b_0 = 0.5$ . We reparametrise  $\sigma^2 \mapsto \log(\sigma)$  so that the zig-zag can sample from  $\theta = \{\beta, \log(\sigma)\} \in \mathbb{R}^{p+1}$ .

Lemma 2 provides computational bounds for this example and Corollary 2 shows how sampling from these is implemented.

**Lemma 2** (Computational Bounds for MMD-Bayes for Gaussian regression model). *Consider the MMD-Bayes posterior for a Gaussian regression model with Gaussian priors with mean  $\mu_0$  and variance  $s_0^2$  on each regression coefficient  $\beta_j$ ,  $j = 1, \dots, d$  and an inverse-gamma prior on scale parameters  $\sigma^2$  with shape  $a_0$  and scale  $b_0$ . We reparametrise*

$\sigma^2 \mapsto \log(\sigma)$  so that the zig-zag can sample from  $\theta = \{\beta, \log(\sigma)\} \in \mathbb{R}^{p+1}$ . The zig-zag switching rates are given by

$$\hat{\lambda}_j(\theta, \nu) := \max \left( 0, \nu_j \frac{\beta_j - \mu_0}{s_0^2} + 2\nu_j \frac{w}{n} \sum_{i=1}^n \frac{1}{b} \sum_{k=1}^b \frac{(G_\theta(v_k; x_i) - y_i)}{\sqrt{2\pi}\gamma^{3/2}} \exp \left( -\frac{(G_\theta(v_k; x_i) - y_i)^2}{2\gamma} \right) x_{ij} \right)$$

$j = 1, \dots, d$  and

$$\begin{aligned} \hat{\lambda}_{d,d+1}(t; \theta, \nu) &:= \max(0, 2\nu_{p+1}a_0 - 2\nu_{p+1}b_0 \exp(-2\log(\sigma)) \\ &\quad - \nu_{p+1} \frac{w}{n} \sum_{i=1}^n \left\{ -2 \frac{1}{b} \sum_{k=1}^b \frac{(G_\theta(v_k; x_i) - y_i)}{\sqrt{2\pi}\gamma^{3/2}} \exp \left( -\frac{(G_\theta(v_k; x_i) - y_i)^2}{2\gamma} \right) \right. \\ &\quad \times \exp(\log(\sigma)) \sqrt{-2\log(v_{k1})} \cos(2\pi v_{k2}) \\ &\quad + \frac{1}{b(b-1)} \sum_{k=1}^b \sum_{k' \neq k} \exp(\log(\sigma)) \left( \sqrt{-2\log(v_{k1})} \cos(2\pi v_{k2}) - \sqrt{-2\log(u_{k'1})} \cos(2\pi u_{k'2}) \right) \\ &\quad \times \left. \frac{(G_\theta(v_k; x_i) - G_\theta(v_{k'}; x_i))}{\sqrt{2\pi}\gamma^{3/2}} \exp \left( -\frac{(G_\theta(v_k; x_i) - G_\theta(v_{k'}; x_i))^2}{2\gamma} \right) \right\} \end{aligned}$$

where  $v_1, \dots, v_m \sim p_v$  and

$$G_\theta(v; x) = x^\top \beta + \sqrt{\sigma^2} \sqrt{-2\log(v_1)} \cos(2\pi v_2).$$

and  $p_v(v) = \text{unif}(v_1; 0, 1) \text{unif}(v_2; 0, 1)$ .

Computational bounds are given by

$$\hat{\Lambda}_j(\theta + \nu \cdot t, \nu) := \frac{|\beta_j - \mu_0|}{s_0^2} + \frac{2\omega}{\sqrt{2\pi}\gamma} \frac{\sum_{i=1}^n |x_{ij}|}{\sqrt{2\pi}\gamma} \exp \left( -\frac{1}{2} \right) + \frac{1}{s_0^2} t$$

for  $j = 1, \dots, d$  and

$$\hat{\Lambda}_{p+1}(\theta + \nu \cdot t, \nu) := a_0 + 2b_0 \exp(-2(\log(\sigma) + \nu_{p+1}t)) + \frac{2\omega}{\sqrt{2\pi}\sigma^2} \exp \left( -\frac{1}{2} \right) \exp(\log(\sigma) + \nu_{p+1}t) R$$



where  $R$  is an assumed upper bound on  $\max_{v_1} \{\sqrt{-2\log(v_1)}\}$

The bounds in Lemma 2 are slightly different for  $\theta_{p+1} = \log(\sigma)$  from those in Corollary 3 of the main paper. While Corollary 3 proves that an upper bound exists, obtaining those bounds requires solving an intractable optimisation. Lemma 2 is therefore an approximation of Corollary 3. As  $v_1$  has support arbitrarily close to 0  $\sqrt{-2\log(v_1)}$  is in principle unbounded. However, Corollary 3 guarantees that as long as we take  $R$  big enough this will in fact be an upper bound, i.e. looser than the bounds in Corollary 3. We find that setting  $R = \sqrt{-2\log 10^{-6/N}}$  provides a bound that is never exceeded. This bound comes from letting  $10^{-6}$  be a tolerated probability that all  $N$  observations simulated observations be such that  $\sqrt{-2\log v_1} > R$ . We keep track of the maximum value of  $\hat{\lambda}_{p+1}(\theta + \nu \cdot t, \nu) / \Lambda_{p+1}(\theta + \nu \cdot t, \nu)$  throughout the sampling and check that this is always less than 1.

*Proof.* Firstly, we can *indirectly* sample  $u_{1:b} \sim \mathcal{N}(x^\top \beta, \sigma^2)$  by first sampling  $v_{1:b}$  with  $v_k = \{v_{k1}, v_{k2}\} \sim p_v$  and  $p_0(v) = \text{unif}(v_1; 0, 1) \text{unif}(v_2; 0, 1)$  and setting  $u_k = G_\theta(v_k; x)$

$$G_\theta(v; x) = x^\top \beta + \sqrt{\sigma^2} \sqrt{-2\log(v_1)} \cos(2\pi v_2).$$

As a result, for the MMD-Bayes posterior

$$\begin{aligned}
\Psi_n(\theta) &:= - \sum_{j=1}^p \log \pi(\beta_j) - \log \pi(\log(\sigma)) + w \mathbf{L}_n^{\mathcal{K}_\gamma}(\theta) \\
&= \sum_{j=1}^p \frac{(\beta_j - \mu_0)^2}{2s_0^2} + 2a_0 \log(\sigma) + b_0 \exp(-2 \log(\sigma)) \\
&\quad - \frac{w}{n} \sum_{i=1}^n \{2\mathbb{E}_{v \sim p_v} [\mathcal{K}_\gamma(y_i, G_\theta(v; x_i))] - \mathbb{E}_{v, v' \sim p_v} [\mathcal{K}_\gamma(G_\theta(v; x_i), G_\theta(v'; x_i))]\} \\
&= \sum_{j=1}^p \frac{(\beta_j - \mu_0)^2}{2s_0^2} + 2a_0 \log(\sigma) + b_0 \exp(-2 \log(\sigma)) \\
&\quad - \frac{w}{n} \sum_{i=1}^n \left\{ 2\mathbb{E}_{v \sim p_v} \left[ \frac{1}{\sqrt{2\pi\gamma}} \exp \left( -\frac{(y_i - G_\theta(v; x_i))^2}{2\gamma} \right) \right] \right. \\
&\quad \left. - \mathbb{E}_{v, v' \sim p_v} \left[ \frac{1}{\sqrt{2\pi\gamma}} \exp \left( -\frac{(G_\theta(v; x_i) - G_\theta(v'; x_i))^2}{2\gamma} \right) \right] \right\}
\end{aligned}$$

The zig-zag requires the evaluation of

$$\hat{\lambda}_j(\theta, \nu) := \max \left( 0, \nu \left( -\frac{\partial}{\partial \theta_j} \log(\pi(\theta)) + \omega \varphi_{b,n}(\theta) \right) \right)$$

and bounding of  $\hat{\lambda}_j(\theta + \nu \cdot t, \nu)$  for  $j = 1, \dots, p+1$ .

**For the regression coefficients:** For  $j = 1, \dots, p$  we have that

$$\begin{aligned}
[\varphi_{m,n}(\theta)]_j &= -\frac{1}{n} \sum_{i=1}^n \left\{ -2\frac{1}{b} \sum_{k=1}^b \frac{(G_\theta(v_k; x_i) - y_i)}{\sqrt{2\pi\gamma^{3/2}}} \exp \left( -\frac{(G_\theta(v_k; x_i) - y_i)^2}{2\gamma} \right) x_{ij} \right. \\
&\quad + \frac{1}{b(b-1)} \sum_{k=1}^b \sum_{k' \neq k}^b \left( \frac{(G_\theta(v_k; x_i) - G_\theta(v_{k'}; x_i))}{\sqrt{2\pi\gamma^{3/2}}} \exp \left( -\frac{(G_\theta(v_k; x_i) - G_\theta(v_{k'}; x_i))^2}{2\gamma} \right) x_{ij} \right. \\
&\quad \left. \left. - \frac{(G_\theta(v_k; x_i) - G_\theta(v_{k'}; x_i))}{\sqrt{2\pi\gamma^{3/2}}} \exp \left( -\frac{(G_\theta(v_k; x_i) - G_\theta(v_{k'}; x_i))^2}{2\gamma} \right) x_{ij} \right) \right\} \\
&= \frac{1}{n} \sum_{i=1}^n \left\{ 2\frac{1}{b} \sum_{k=1}^b \frac{(G_\theta(v_k; x_i) - y_i)}{\sqrt{2\pi\gamma^{3/2}}} \exp \left( -\frac{(G_\theta(v_k; x_i) - y_i)^2}{2\gamma} \right) x_{ij} \right\}.
\end{aligned}$$

with  $v_1, \dots, v_N \sim p_v$ . Above uses the fact that

$$\begin{aligned}\frac{\partial}{\partial z} \mathcal{K}_\gamma(z, x) &= -\frac{(z-x)}{\sqrt{2\pi}\gamma^{3/2}} \exp\left(-\frac{(z-x)^2}{2\gamma}\right) \\ \frac{\partial}{\partial \beta_j} G_\theta(v; x) &= x_j\end{aligned}$$

and the cancellation of the second MMD term happens as  $\frac{\partial}{\partial \beta_j} G_\theta(v; x)$  doesn't depend on  $v$ .

We can then use the fact that  $\left| \frac{\partial}{\partial y} \mathcal{K}_\gamma(y, y') \right| \leq \frac{1}{\sqrt{2\pi}\gamma} \exp(-\frac{1}{2})$  for any value of  $y$  or  $y'$  and bound

$$\begin{aligned}\hat{\lambda}_j(\theta + \nu \cdot t, \nu) &= \max\left(0, \nu \left(-\frac{\partial}{\partial \theta_j} \log(\pi(\theta + \nu \cdot t)) + \omega[\varphi_{b,n}(\theta + \nu \cdot t)]_j\right)\right) \\ &\leq \frac{|\beta_j - \mu_0|}{s_0^2} + \frac{2w \frac{1}{n} \sum_{i=1}^n |x_{ij}|}{\sqrt{2\pi}\gamma} \exp\left(-\frac{1}{2}\right) + \frac{1}{s_0^2} t \\ &= \hat{\Lambda}_j(\theta + \nu \cdot t, \nu)\end{aligned}$$

**For the residual variance:**

$$\begin{aligned}[\varphi_{b,n}(\theta)]_{d+1} &:= \\ &- \frac{1}{n} \sum_{i=1}^n \left\{ -2 \frac{1}{b} \sum_{k=1}^b \frac{(G_\theta(v_k; x_i) - y_i)}{\sqrt{2\pi}\gamma^{3/2}} \exp\left(-\frac{(G_\theta(v_k; x_i) - y_i)^2}{2\gamma}\right) \exp(\log(\sigma)) \sqrt{-2 \log(v_{k1})} \cos(2\pi v_{k2}) \right. \\ &+ \frac{1}{b(b-1)} \sum_{k=1}^b \sum_{k' \neq k} \left( \frac{(G_\theta(v_k; x_i) - G_\theta(v_{k'}; x_i))}{\sqrt{2\pi}\gamma^{3/2}} \exp\left(-\frac{(G_\theta(v_k; x_i) - G_\theta(v_{k'}; x_i))^2}{2\gamma}\right) \exp(\log(\sigma)) \sqrt{-2 \log(v_{k1})} \cos(2\pi v_{k2}) \right. \\ &\left. \left. - \frac{(G_\theta(v_k; x_i) - G_\theta(v_{k'}; x_i))}{\sqrt{2\pi}\gamma^{3/2}} \exp\left(-\frac{(G_\theta(v_k; x_i) - G_\theta(v_{k'}; x_i))^2}{2\gamma}\right) \exp(\log(\sigma)) \sqrt{-2 \log(u_{k'1})} \cos(2\pi u_{k'2}) \right) \right\} \\ &= -\frac{1}{n} \sum_{i=1}^n \left\{ -2 \frac{1}{b} \sum_{k=1}^b \frac{(G_\theta(v_k; x_i) - y_i)}{\sqrt{2\pi}\gamma^{3/2}} \exp\left(-\frac{(G_\theta(v_k; x_i) - y_i)^2}{2\gamma}\right) \exp(\log(\sigma)) \sqrt{-2 \log(v_{k1})} \cos(2\pi v_{k2}) \right. \\ &+ \frac{1}{b(b-1)} \sum_{k=1}^b \sum_{k' \neq k} \exp(\log(\sigma)) \left( \sqrt{-2 \log(v_{k1})} \cos(2\pi v_{k2}) - \sqrt{-2 \log(u_{k'1})} \cos(2\pi u_{k'2}) \right) \\ &\left. \times \frac{(G_\theta(v_k; x_i) - G_\theta(v_{k'}; x_i))}{\sqrt{2\pi}\gamma^{3/2}} \exp\left(-\frac{(G_\theta(v_k; x_i) - G_\theta(v_{k'}; x_i))^2}{2\gamma}\right) \right\}\end{aligned}$$

as

$$\frac{\partial}{\partial \log(\sigma)} G_\theta(v; x) = \exp(\log(\sigma)) \sqrt{-2 \log(u_1)} \cos(2\pi u_2).$$

While Corollary 4 proves that a finite bound on this exists, the bounds derived in Corollary 4 are intractable to use in practice. Instead, we use the following *approximate* bound

$$\begin{aligned} \hat{\lambda}_{m,p+1}(\theta + \nu \cdot t, \nu) &:= \max \left( 0, \nu \left( -\frac{\partial}{\partial \theta_{d+1}} \log(\pi(\theta + \nu \cdot t)) + \omega[\varphi_{b,n}(\theta + \nu \cdot t)]_{d+1} \right) \right) \\ &\leq a_0 + 2b_0 \exp(-2(\log(\sigma) + \nu_{p+1}t)) + \frac{2\omega}{\sqrt{2\pi}\sigma^2} \exp\left(-\frac{1}{2}\right) \exp(\log(\sigma) + \nu_{p+1}t) R \\ &= \Lambda_{p+1}(\theta + \nu \cdot t, \nu) \end{aligned}$$

where  $R$  is an assumed upper bound on  $\max_{v_1} \{\sqrt{-2 \log(v_1)}\}$ . □

**Corollary 2.** *Sampling stopping times according to the computational bound in Lemma 2 is achieved for  $j = 1, \dots, d$  by sampling  $u_j \sim U[0, 1]$  and setting*

$$\tau_j^* := \frac{\sqrt{a_j^2 - 2 \log(u_j) b_j} - a_j}{b_j}$$

with

$$\begin{aligned} a_j &:= \frac{|\beta_j - \mu_0|}{s_0^2} + \frac{2w \frac{1}{n} \sum_{i=1}^n |x_{ij}|}{\sqrt{2\pi}\gamma} \exp\left(-\frac{1}{2}\right) \\ b_j &:= \frac{1}{s_0^2} \end{aligned}$$

and

$$\tau_{p+1}^* = \min\{\tau_{p+1}^{(1)}, \tau_{p+1}^{(2)}, \tau_{p+1}^{(3)}\}$$

with

$$\begin{aligned}\tau_{p+1}^{(1)} &= \frac{-\log(u_{p+1}^{(1)})}{a_0} \\ \tau_{p+1}^{(2)} &= \begin{cases} -\frac{1}{2\nu_{p+1}} \log \left( 1 + \frac{\log(u_{p+1}^{(2)})\nu_{p+1} \exp(2\log(\sigma))}{b_0} \right) & \text{if } -\log(u_{p+1}^{(2)}) < \frac{b_0}{\nu_{p+1} \exp(2\log(\sigma))} \\ \infty & \text{otherwise} \end{cases} \\ \tau_{p+1}^{(3)} &= \begin{cases} \frac{1}{\nu_{p+1}} \log \left( 1 - \frac{\log(u_{p+1}^{(3)})\nu_{p+1} \exp(-\log(\sigma))}{\left(\frac{2n}{\sqrt{2\pi}\gamma} \exp(-\frac{1}{2})R\right)} \right) & \text{if } -\log(u_{p+1}^{(3)}) > -\frac{\left(\frac{2\omega}{\sqrt{2\pi}\gamma} \exp(-\frac{1}{2})R\right)}{\nu_{p+1} \exp(-\log(\sigma))} \\ \infty & \text{otherwise} \end{cases}\end{aligned}$$

$$u_{p+1}^{(1)}, u_{p+1}^{(2)}, u_{p+1}^{(3)} \sim Unif(0, 1).$$

*Proof.* Sampling stopping times according to the computational bounds in Lemma 2 requires, for the regression coefficients,  $j = 1, \dots, p$ , following the procedure outlined in Corollary 1 with

$$\begin{aligned}a_j &:= \frac{|\beta_j - \mu_0|}{s_0^2} + \frac{2w \frac{1}{n} \sum_{i=1}^n |x_{ij}|}{\sqrt{2\pi}\gamma} \exp\left(-\frac{1}{2}\right) \\ b_j &:= \frac{1}{s_0^2}\end{aligned}$$

For the residual variance with  $\theta_{p+1} = \log(\sigma)$  we write

$$\hat{\Lambda}_{p+1}(\theta + \nu \cdot t, \nu) = \Lambda_{p+1}^{(1)}(\theta + \nu \cdot t, \nu) + \Lambda_{p+1}^{(2)}(\theta + \nu \cdot t, \nu) + \Lambda_{p+1}^{(3)}(\theta + \nu \cdot t, \nu)$$

with  $\Lambda_{p+1}^{(1)}(\theta + \nu \cdot t, \nu) = a_0$  and  $\Lambda_{p+1}^{(2)}(\theta + \nu \cdot t, \nu) = 2b_0 \exp(-2(\log(\sigma) + \nu_{p+1}t))$  and  $\Lambda_{p+1}^{(3)}(\theta + \nu \cdot t, \nu) := \frac{2\omega}{\sqrt{2\pi}\sigma^2} \exp(-\frac{1}{2}) \exp(\log(\sigma) + \nu_{p+1}t)R$ , allows us to sample stopping times  $\tau_{p+1}$  from a Poisson process with rate  $\int_0^t \Lambda_{p+1}(\theta + \nu \cdot s, \nu) ds$  via Poisson superposition, first sampling  $\tau_{p+1}^{(l)}$  according to a Poisson process with rate  $\int_0^t \Lambda_{p+1}^{(l)}(\theta + \nu \cdot s, \nu) ds$ ,  $l = 1, \dots, 3$  and setting  $\tau_{p+1} = \min\{\tau_{p+1}^{(1)}, \tau_{p+1}^{(2)}, \tau_{p+1}^{(3)}\}$ .

Sampling  $\tau_{p+1}^{(1)}$  requires evaluating

$$\int_0^t \Lambda_{p+1}^{(1)}(\theta + \nu \cdot s, \nu) ds = \int_0^t a_0 ds = a_0 t$$

which by Cinlar's Algorithm (Cinlar, 1975) (Algorithm 1) means that for  $u^{(1)} \sim Unif(0, 1)$

$$\tau_{p+1}^{(1)} := \inf \{t : a_0 t \geq s\} = \frac{-\log(u^{(1)})}{a_0}$$

Sampling  $\tau_{p+1}^{(2)}$  requires evaluating

$$\begin{aligned} \int_0^t \Lambda_{p+1}^{(2)}(\theta + \nu \cdot s, \nu) ds &= \int_0^t 2b_0 \exp(-2(\log(\sigma) + \nu_{p+1}s)) ds \\ &= 2b_0 \left[ -\frac{1}{2\nu_{p+1}} \exp(-2(\log(\sigma) + \nu_{p+1}s)) \right]_0^t \\ &= \frac{b_0}{\nu_{p+1}} [\exp(-2\log(\sigma)) - \exp(-2(\log(\sigma) + \nu_{p+1}t))] \end{aligned}$$

which by Cinlar's Algorithm (Cinlar, 1975) (Algorithm 1) means that for  $u^{(2)} \sim Unif(0, 1)$

$$\begin{aligned} \tau_{p+1}^{(2)} &:= \inf \left\{ t : \frac{b_0}{\nu_{p+1}} [\exp(-2\log(\sigma)) - \exp(-2(\log(\sigma) + \nu_{p+1}t))] \geq -\log(u^{(2)}) \right\} \\ &= \inf \left\{ t : [1 - \exp(-2\nu_{p+1}t)] \geq \frac{-\log(u^{(2)})\nu_{p+1} \exp(2\log(\sigma))}{b_0} \right\} \\ &= -\frac{1}{2\nu_{p+1}} \log \left( 1 + \frac{\log(u^{(2)})\nu_{p+1} \exp(2\log(\sigma))}{b_0} \right) \end{aligned}$$

for  $-\log(u^{(2)}) < \frac{b_0}{\nu_{p+1} \exp(2\log(\sigma))}$  or else  $\tau_{p+1}^{(2)} = \infty$ .

Lastly, sampling  $\tau_{p+1}^{(3)}$  requires evaluating

$$\begin{aligned} \int_0^t \Lambda_{p+1}^{(3)}(\theta + \nu \cdot s, \nu) ds &= \int_0^t \exp(\log(\sigma) + \nu_{p+1}s) \left( \frac{2\omega}{\sqrt{2\pi\gamma}} \exp\left(-\frac{1}{2}\right) R \right) ds \\ &= \frac{1}{\nu_{p+1}} \left( \frac{2\omega}{\sqrt{2\pi\gamma}} \exp\left(-\frac{1}{2}\right) R \right) [\exp(\log(\sigma) + \nu_{p+1}s)]_0^t \\ &= \frac{1}{\nu_{p+1}} \left( \frac{2\omega}{\sqrt{2\pi\gamma}} \exp\left(-\frac{1}{2}\right) R \right) [\exp(\log(\sigma) + \nu_{p+1}t) - \exp(\log(\sigma))] \end{aligned}$$

which by Cinlar's Algorithm (Cinlar, 1975) (Algorithm 1) means that for  $u^{(3)} \sim \text{Unif}(0, 1)$

$$\begin{aligned} \tau_{p+1}^{(3)} &:= \inf \left\{ t : \frac{1}{\nu_{p+1}} \left( \frac{2\omega}{\sqrt{2\pi\gamma}} \exp\left(-\frac{1}{2}\right) R \right) [\exp(\log(\sigma) + \nu_{p+1}t) - \exp(\log(\sigma))] \geq -\log(u^{(3)}) \right\} \\ &= \inf \left\{ t : [\exp(\nu_{p+1}t) - 1] \geq \frac{-\log(u^{(3)})\nu_{p+1} \exp(-\log(\sigma))}{\left( \frac{2\omega}{\sqrt{2\pi\gamma}} \exp\left(-\frac{1}{2}\right) R \right)} \right\} \\ &= \frac{1}{\nu_{p+1}} \log \left( 1 - \frac{\log(u^{(3)})\nu_{p+1} \exp(-\log(\sigma))}{\left( \frac{2\omega}{\sqrt{2\pi\gamma}} \exp\left(-\frac{1}{2}\right) R \right)} \right) \end{aligned}$$

for  $-\log(u^{(3)}) > -\frac{\left( \frac{2\omega}{\sqrt{2\pi\gamma}} \exp\left(-\frac{1}{2}\right) R \right)}{\nu_{p+1} \exp(-\log(\sigma))}$  or else  $\tau_{p+1}^{(3)} = \infty$ . □

## 2.3 Robustified copula with the MMD

Here we provide implementation details for Section 5.1 of the paper.

We propose a Bayesian extension of Alquier and Gerber (2024) that uses the zig-zag to sample from the MMD-Bayes posterior for copula parameter  $\rho$ . We place a beta prior with hyperparameter  $a_0 = 1$  and  $b_0 = 1$  on  $\frac{\rho+1}{2} \in [0, 1]$  and reparametrise  $\rho \mapsto \theta$  with  $\rho(\theta) = \frac{2}{1+\exp(-\theta)} - 1$  so that the zig-zag can sample from the implied posterior of  $\theta \in \mathbb{R}$ . Lemma 3 provides computational bounds for this example and Corollary 3 shows how sampling from these is implemented.

**Lemma 3** (Computational Bounds for MMD-Bayes for Gaussian Copula model). *Consider the MMD-Bayes posterior for a bivariate Gaussian copula model with  $\text{Beta}(a_0, b_0)$  prior on*

$\frac{\rho+1}{2}$  where  $\rho$  is the unknown correlation. We reparametrise  $\rho \mapsto \theta$  with  $\rho(\theta) = \frac{2}{1+\exp(-\theta)} - 1$  so that the zig-zag can sample from  $\theta \in \mathbb{R}^1$ . The zig-zag switching rates are given by

$$\begin{aligned} \hat{\lambda}(\theta, \nu) := & \max \left( 0, \nu b_0 - \nu(a_0 + b_0) \frac{\exp(-\theta)}{(1 + \exp(-\theta))} \right. \\ & \left\{ -\frac{2w\nu}{mn} \sum_{i=1}^n \sum_{k=1}^b \frac{(\Phi^{-1}(\hat{u}_{2i}) - G_{\theta}^{(2)}(v_k))}{2\pi\gamma^2} \right. \\ & \exp \left( -\frac{(\Phi^{-1}(\hat{u}_{1i}) - v_{k1})^2 + (\Phi^{-1}(\hat{u}_{2i}) - (\rho(\theta)v_{k1} + \sqrt{1 - \rho(\theta)^2}v_{k2}))^2}{2\gamma} \right) \left( v_{k1} - \frac{\rho(\theta)}{\sqrt{1 - \rho(\theta)^2}}v_{k2} \right) \\ & - \frac{\nu w}{m(m-1)} \sum_{k=1}^b \sum_{k' \neq k}^m \frac{((\rho(\theta)v_{k1} + \sqrt{1 - \rho(\theta)^2}v_{k2}) - (\rho(\theta)v_{k'1} + \sqrt{1 - \rho(\theta)^2}v_{k'2}))}{2\pi\gamma^2} \\ & \exp \left( -\frac{(v_{k1} - v_{k'1})^2 + ((\rho(\theta)v_{k1} + \sqrt{1 - \rho(\theta)^2}v_{k2}) - (\rho(\theta)v_{k'1} + \sqrt{1 - \rho(\theta)^2}v_{k'2}))^2}{2\gamma} \right) \\ & \cdot \left( \left( v_{k1} - \frac{\rho(\theta)}{\sqrt{1 - \rho(\theta)^2}}v_{k2} \right) - \left( v_{k'1} - \frac{\rho(\theta)}{\sqrt{1 - \rho(\theta)^2}}v_{k'2} \right) \right) \left. \right\} \frac{2 \exp(-\theta)}{(1 + \exp(-\theta))^2} \end{aligned}$$

where  $v_1, \dots, v_m \sim p_v$  with  $p_v(v) = \mathcal{N}(v_1; 0, 1)\mathcal{N}(v_2; 0, 1)$ .

Computational bounds are given by

$$\hat{\Lambda}_j(\theta + \nu \cdot t, \nu) = \max\{a_0, b_0\} + \frac{4\omega}{(2\pi\gamma)^{3/2}} R \exp \left( -\frac{1}{2} \right) \left( 2 + \exp \left( -\frac{1}{2}\theta - \frac{1}{2}\nu \cdot t \right) \right)$$

where  $R$  is an assumed upper bound on  $|v|$  for  $v \sim \mathcal{N}(0, 1)$ .

The bounds in Lemma 3 are slightly different from those in Corollary 4 of the main paper. While Corollary 4 proves that an upper bound exists, obtaining those bounds requires solving an intractable optimisation. Lemma 3 is therefore an approximation of Corollary 4. Although  $v$  has unbounded support Corollary 4 guarantees that as long as we take  $R$  big enough this will in fact be an upper bound, i.e. looser than the bounds in Corollary 4. We find however setting  $R = 3$  provides a bound that is never exceeded. We keep track of the maximum value of  $\hat{\lambda}(\theta + \nu \cdot t, \nu)/\Lambda(\theta + \nu \cdot t, \nu)$  throughout the sampling and check that this is always less than 1.



*Proof.* Firstly, we can indirectly sample  $u_{1:b} \sim p_\theta(u)$  where  $p_\theta(u)$  is the density of a bivariate Gaussian copula with parameter  $\rho$  by first  $v_{1:b}$  with  $v_k = \{v_{k1}, v_{k2}\} \sim p_v$  and  $p_v(v) = \mathcal{N}(v_1; 0, 1)\mathcal{N}(v_2; 0, 1)$  and setting  $u_k = \{v_{k1}, v_{k2}\} = \{G_\theta^{(1)}(v_k), G_\theta^{(2)}(v_k)\} = F(v_k; \theta)$  with

$$\begin{aligned} G_{\theta,1}(v_k) &= \Phi(v_1) \\ G_{\theta,2}(v_k) &= \Phi(\rho v_1 + \sqrt{1 - \rho^2} v_2). \end{aligned}$$

As a result, for the MMD-Bayes posterior

$$\begin{aligned} \Psi_n(\theta) &:= -\log \pi(\theta) + w \mathbf{L}_n^{\mathcal{K}_\gamma}(\theta) \\ &= b_0 \theta + (a_0 + b_0) \log(1 + \exp(-\theta)) \\ &\quad - \frac{\omega}{n} \sum_{i=1}^n 2\mathbb{E}_{v \sim p_0(\cdot)} [\mathcal{K}_\gamma(\hat{u}_i, G_\theta(v))] + \omega \mathbb{E}_{v, v' \sim p_0(\cdot)} [\mathcal{K}_\gamma(G_\theta(v), G_\theta(v'))] \\ &= b_0 \theta + (a_0 + b_0) \log(1 + \exp(-\theta)) \\ &\quad - \frac{\omega}{n} \sum_{i=1}^n 2\mathbb{E}_{v \sim p(\cdot)} \left[ \frac{1}{2\pi\gamma} \exp \left( \frac{(\Phi^{-1}(\hat{u}_{i1}) - \Phi^{-1}(G_{\theta,1}(v)))^2 + (\Phi^{-1}(\hat{u}_{i2}) - \Phi^{-1}(G_{\theta,2}(v)))^2}{2\gamma} \right) \right] \\ &\quad + \omega \mathbb{E}_{v, v' \sim p(\cdot)} \left[ \frac{1}{2\pi\gamma} \exp \left( \frac{(\Phi^{-1}(G_{\theta,1}(v)) - \Phi^{-1}(G_{\theta,1}(v')))^2 + (\Phi^{-1}(G_{\theta,2}(v)) - \Phi^{-1}(G_{\theta,2}(v')))^2}{2\gamma} \right) \right] \\ &= b_0 \theta + (a_0 + b_0) \log(1 + \exp(-\theta)) \\ &\quad - \frac{\omega}{n} \sum_{i=1}^n 2\mathbb{E}_{v \sim p(\cdot)} \left[ \frac{1}{2\pi\gamma} \exp \left( \frac{(\Phi^{-1}(\hat{u}_{i1}) - v_1)^2 + (\Phi^{-1}(\hat{u}_{i2}) - v_2)^2}{2\gamma} \right) \right] \\ &\quad + \omega \mathbb{E}_{v, v' \sim p(\cdot)} \left[ \frac{1}{2\pi\gamma} \exp \left( \frac{(\Phi^{-1}(v_1 - v'_1))^2 + (v_2 - v'_2)^2}{2\gamma} \right) \right] \end{aligned}$$

The zig-zag requires the evaluation of

$$\hat{\lambda}(\theta, \nu) = \max \left( 0, \nu \left( -\frac{\partial}{\partial \theta} \log(\pi(\theta)) + \omega \varphi_{b,n}(\theta) \right) \right)$$

and bounding of  $\hat{\lambda}(\mu + \nu \cdot t, \nu)$ , where

$$\begin{aligned}
\varphi_{b,n}(\theta) &= -\frac{1}{n} \sum_{i=1}^n 2 \frac{1}{b} \sum_{k=1}^b \frac{1}{2\pi\gamma^2} \exp \left( -\frac{(\Phi^{-1}(\hat{u}_{1i}) - v_{k1})^2 + (\Phi^{-1}(\hat{u}_{2i}) - (\rho(\theta)v_{k1} + \sqrt{1 - \rho(\theta)^2}v_{k2}))^2}{2\gamma} \right) \\
&\quad \cdot \left\{ (\Phi^{-1}(\hat{u}_{1i}) - v_{k1}) \frac{\partial}{\partial \theta} v_{k1} + (\Phi^{-1}(\hat{u}_{2i}) - (\rho(\theta)v_{k1} + \sqrt{1 - \rho(\theta)^2}v_{k2})) \frac{\partial}{\partial \theta} (\rho(\theta)v_{k1} + \sqrt{1 - \rho(\theta)^2}v_{k2}) \right\} \\
&\quad + \frac{1}{m(m-1)} \sum_{k=1}^b \sum_{k' \neq k}^m -\frac{1}{2\pi\gamma^2} \exp \left( -\frac{(v_{k1} - v_{k'1})^2 + ((\rho(\theta)v_{k1} + \sqrt{1 - \rho(\theta)^2}v_{k2}) - (\rho(\theta)v_{k'1} + \sqrt{1 - \rho(\theta)^2}v_{k'2}))^2}{2\gamma} \right) \\
&\quad \cdot \left\{ (v_{k1} - v_{k'1}) \left( \frac{\partial}{\partial \theta} v_{k1} - \frac{\partial}{\partial \theta} v_{k'1} \right) \right. \\
&\quad \left. + ((\rho(\theta)v_{k1} + \sqrt{1 - \rho(\theta)^2}v_{k2}) - (\rho(\theta)v_{k'1} + \sqrt{1 - \rho(\theta)^2}v_{k'2})) \left( \frac{\partial}{\partial \theta} (\rho(\theta)v_{k1} + \sqrt{1 - \rho(\theta)^2}v_{k2}) - \frac{\partial}{\partial \theta} (\rho(\theta)v_{k'1} + \sqrt{1 - \rho(\theta)^2}v_{k'2}) \right) \right\} \\
&= -\frac{1}{n} \sum_{i=1}^n 2 \frac{1}{b} \sum_{k=1}^b \frac{1}{2\pi\gamma^2} \exp \left( -\frac{(\Phi^{-1}(\hat{u}_{1i}) - v_{k1})^2 + (\Phi^{-1}(\hat{u}_{2i}) - (\rho(\theta)v_{k1} + \sqrt{1 - \rho(\theta)^2}v_{k2}))^2}{2\gamma} \right) \\
&\quad \cdot \left\{ (\Phi^{-1}(\hat{u}_{2i}) - (\rho(\theta)v_{k1} + \sqrt{1 - \rho(\theta)^2}v_{k2})) \right\} \left( v_{k1} - \frac{\rho(\theta)}{\sqrt{1 - \rho(\theta)^2}} v_{k2} \right) \frac{2 \exp(-\theta)}{(1 + \exp(-\theta))^2} \\
&\quad - \frac{1}{m(m-1)} \frac{\omega}{n} \sum_{k=1}^b \sum_{k' \neq k}^m \frac{1}{2\pi\gamma^2} \exp \left( -\frac{(v_{k1} - v_{k'1})^2 + ((\rho(\theta)v_{k1} + \sqrt{1 - \rho(\theta)^2}v_{k2}) - (\rho(\theta)v_{k'1} + \sqrt{1 - \rho(\theta)^2}v_{k'2}))^2}{2\gamma} \right) \\
&\quad \cdot ((\rho(\theta)v_{k1} + \sqrt{1 - \rho(\theta)^2}v_{k2}) - (\rho(\theta)v_{k'1} + \sqrt{1 - \rho(\theta)^2}v_{k'2})) \\
&\quad \cdot \left( \left( v_{k1} - \frac{\rho(\theta)}{\sqrt{1 - \rho(\theta)^2}} v_{k2} \right) - \left( v_{k'1} - \frac{\rho(\theta)}{\sqrt{1 - \rho(\theta)^2}} v_{k'2} \right) \right) \frac{2 \exp(-\theta)}{(1 + \exp(-\theta))^2}
\end{aligned}$$

with  $v_1, \dots, v_b \sim p_v$ . This uses the fact that

$$\begin{aligned}
\rho(\theta) &= \frac{2}{1 + \exp(-\theta)} - 1 \\
\partial \rho(\theta) &= \frac{2 \exp(-\theta)}{(1 + \exp(-\theta))^2}
\end{aligned}$$

While Corollary 4 of the main paper proves that a finite bound on this exists, the bounds derived in Corollary 4 are intractable to use in practice. Instead, we use the fact

that

$$\begin{aligned} \left| \frac{(y - y')}{\sqrt{2\pi\gamma^{3/2}}} \exp\left(-\frac{(y - y')^2}{2\gamma}\right) \right| &\leq \frac{1}{\sqrt{2\pi\gamma}} \exp\left(-\frac{1}{2}\right) \\ \left| \frac{1}{\sqrt{2\pi\gamma}} \exp\left(-\frac{(y - y')^2}{2\gamma}\right) \right| &\leq \frac{1}{\sqrt{2\pi\gamma}} \end{aligned}$$

for any value of  $y$  or  $y'$ , and

$$\left| \left( v_1 - \frac{\rho(\theta)}{\sqrt{1 - \rho(\theta)^2}} v_2 \right) \frac{2 \exp(-\theta)}{(1 + \exp(-\theta))^2} \right| \leq \frac{2}{\sqrt{2\pi}} v_1 + \frac{1}{\sqrt{2\pi}} v_2$$

for all  $v, \theta \in \Theta$ , and use the following *approximate* bound

$$\begin{aligned} \hat{\lambda}(\theta + \nu \cdot t, \nu) &:= \max \left( 0, \nu \left( -\frac{\partial}{\partial \theta} \log(\pi(\theta + \nu \cdot t)) + \omega \varphi_{b,n}(\theta + \nu \cdot t) \right) \right) \\ &\leq \max\{a_0, b_0\} + \frac{12\omega}{(2\pi\gamma)^{3/2}} R \exp\left(-\frac{1}{2}\right) \\ &= \Lambda(\theta + \nu \cdot t, \nu) \end{aligned}$$

where  $R$  is an assumed upper bound on  $|v|$  for  $v \sim \mathcal{N}(0, 1)$ . □

**Corollary 3.** *Sampling stopping times according to the computational bound in Lemma 3 is achieved by setting*

$$\tau^* = \frac{-\log(u)}{a}$$

with  $a = \max\{a_0, b_0\} + \frac{12\omega}{(2\pi\gamma)^{3/2}} R \exp\left(-\frac{1}{2}\right)$  and  $u \sim U[0, 1]$ .

*Proof.* Sampling  $\tau^*$  requires evaluating

$$\int_0^t \hat{\Lambda}(\theta + \nu \cdot s, \nu) ds = \int_0^t a ds = at$$

where  $a = \max\{a_0, b_0\} + \frac{12\omega}{(2\pi\gamma)^{3/2}} R \exp\left(-\frac{1}{2}\right)$ , which by Cinlar's Algorithm (Cinlar, 1975) (Algorithm 1) means that for  $u^{(1)} \sim \text{Unif}(0, 1)$

$$\tau^* := \inf \{t : at \geq s\} = \frac{-\log(u)}{a}.$$

□

## 2.4 Robustified Poisson regression with the $\beta$ -Divergence

Here we provide implementation details for Section 5.2.2 of the paper.

In Poisson regression the mass function of count data  $y$ , conditional on predictor variables  $x$  is given by  $p_\theta(y; x) = e^{yx^\top \theta} e^{-e^{x^\top \theta}} / y!$ . The  $\beta$ D-loss for such a model involves the infinite sum  $\sum_{u=0}^{\infty} p_\theta(u; x)^{\beta+1}$  which for  $\beta > 0$  is not available in closed form. We therefore use the zig-zag to sample from the  $\beta$ D-Bayes posterior for  $\theta$ . We place Gaussian priors with mean  $\mu_0 = 0$  and variance  $s_0^2 = 1$  on each  $\theta_j$ ,  $j = 1, \dots, d$ . Lemma 4 provides computational bounds for this example and Corollary 4 shows how sampling from these is implemented.

**Lemma 4** (Computational Bounds for  $\beta$ D-Bayes for Poisson regression model ). *Consider the  $\beta$ D-Bayes posterior for a Poisson regression model with  $\mathcal{N}(\mu_0, s_0^2)$  priors on unknown regression coefficients  $\theta = \{\theta_1, \dots, \theta_d\}$ . The zig-zag switching rates are given by*

$$\hat{\lambda}_j(\theta, \nu) := \max \left( 0, \nu_j \frac{\theta_j - \mu_0}{s_0^2} + \nu_j \frac{\omega(\beta + 1)}{n} \sum_{i=1}^n \left\{ \frac{1}{b} \sum_{k=1}^b p_\theta(u_{ik}; x_i)^\beta (u_{ik} - e^{x_i^\top(\theta)}) x_{ij} \right. \right. \\ \left. \left. - p_\theta(y_i; x_i)^\beta \left( y_i - e^{x_i^\top(\theta + \nu \cdot t)} \right) x_{ij} \right\} \right),$$

$j = 1, \dots, d$  where  $u_{i1}, \dots, u_{ik} \sim p_\theta(\cdot; x_i)$   $i = 1, \dots, n$  with  $p_\theta(y; x) = \frac{e^{yx^\top \theta} e^{-e^{x^\top \theta}}}{y!}$ .

Computational bounds are given by

$$\begin{aligned}\hat{\Lambda}_j(\theta + \nu \cdot t, \nu) &:= \left( \frac{|\theta_j - \mu_0|}{s_0^2} + \frac{\omega(\beta + 1)}{n} \sum_{i=1}^n |x_{ij}| \left( y_i + \frac{1}{\beta} \right) \right) + \frac{1}{s_0^2} t \\ &\quad + e^{\max_{i=1, \dots, n} \{\sum_{j=1}^p |x_{ij}|\} t} \frac{\omega(\beta + 1)^2}{n\beta} \sum_{i=1}^n |x_{ij}| e^{x_i^\top \theta}.\end{aligned}$$

*Proof.* As the  $\beta$ D-loss requires evaluation of models density, in any case, we *directly* sample from the poison regression model in order to estimate  $\mathsf{L}_n^\beta(\theta)$ .

As a result, for the  $\beta$ D-Bayes posterior

$$\begin{aligned}\Psi_n(\theta) &:= - \sum_{j=1}^p \log \pi(\theta_j) + w \mathsf{L}_n^\beta(\theta) \\ &= - \sum_{j=1}^p \log \pi(\theta_j) + \frac{\omega}{n} \sum_{i=1}^n \left\{ \mathbb{E}_{u \sim p_\theta(\cdot; x_i)} [p_\theta(u; x_i)^\beta] - \frac{\beta + 1}{\beta} p_\theta(y_i; x_i)^\beta \right\}\end{aligned}$$

The zig-zag requires the evaluation of

$$\hat{\lambda}_j(\theta, \nu) := \max \left( 0, \nu_j \left( - \frac{\partial}{\partial \theta_j} \log(\pi(\theta)) + \omega [\varphi_{b,n}(\theta + \nu \cdot t)]_j \right) \right),$$

and bounding of  $\hat{\lambda}_j(\theta + \nu \cdot t, \nu)$  for  $j = 1, \dots, p$ . The log-derivative trick provides that

$$\begin{aligned}[\varphi_{b,n}(\theta)]_j &:= \frac{(\beta + 1)}{n} \sum_{i=1}^n \left\{ \frac{1}{b} \sum_{k=1}^b p_{\theta + \nu \cdot t}(u_{ik}; x_i)^\beta \nabla_{\theta_j} \log p_{\theta + \nu \cdot t}(u_{ik}; x_i) \right. \\ &\quad \left. - p_{\theta + \nu \cdot t}(y_i; x_i)^{\beta-1} \nabla_{\theta_j} p_{\theta + \nu \cdot t}(y_i; x_i) \right\}\end{aligned}$$

for  $u_i = \{u_{i1}, \dots, u_{ib}\}$  with  $u_{ik} \sim p_\theta(\cdot; x_i)$ ,  $i = 1, \dots, n$ ,  $k = 1, \dots, b$ . Next, we can use that

$$\begin{aligned}\nabla_{\theta_j} p_\theta(y; x) &= (y - e^{x^\top \theta}) x_j p_\theta(y; x) \\ \nabla_{\theta_j} \log p_\theta(y; x) &= (y - e^{x^\top \theta}) x_j\end{aligned}$$

to rewrite

$$\begin{aligned}\varphi_{b,n}(\theta) &= \frac{(\beta + 1)}{n} \sum_{i=1}^n \left\{ \frac{1}{b} \sum_{k=1}^b p_{\theta+\nu \cdot t}(u_{ik}; x_i)^\beta (u_{ik} - e^{x_i^\top (\theta)}) x_{ij} \right. \\ &\quad \left. - p_{\theta+\nu \cdot t}(y_i; x_i)^\beta (y_i - e^{x_i^\top (\theta)}) x_{ij} \right\}\end{aligned}$$

Then, using the fact that  $p_{\theta+\nu \cdot t}(u_{ik}; x_i)^\beta u_{ik} < \frac{\exp(x_i^\top \theta) + 1}{\beta}$  and that  $p$  is a probability mass function, so  $p_\theta(\cdot, x) \leq 1$ , and only has support on the positive integers, we can write

$$\begin{aligned}\nu_j[\varphi_{b,n}(\theta + \nu \cdot t)]_j &\leq \frac{(\beta + 1)}{n} \sum_{i=1}^n |x_{ij}| \left( \frac{\exp(x_i^\top (\theta + \nu \cdot t)) + 1}{\beta} \right. \\ &\quad \left. + e^{x_i^\top (\theta + \nu \cdot t)} + y_i \right) \\ &\leq \frac{(\beta + 1)}{n} \sum_{i=1}^n |x_{ij}| \left( y_i + \frac{1}{\beta} \right) + \frac{(\beta + 1)}{n} \sum_{i=1}^n |x_{ij}| \frac{\beta + 1}{\beta} e^{x_i^\top \theta} e^{x_i^\top \nu \cdot t} \\ &\leq \frac{(\beta + 1)}{n} \sum_{i=1}^n |x_{ij}| \left( y_i + \frac{1}{\beta} \right) + e^{\max_{i=1, \dots, n} \{\sum_{j=1}^p |x_{ij}|\} t} \frac{(\beta + 1)^2}{\beta} \frac{1}{n} \sum_{i=1}^n |x_{ij}| e^{x_i^\top \theta}.\end{aligned}$$

and therefore

$$\begin{aligned}\hat{\lambda}_{m,j}(\theta + \nu \cdot t, \nu) &:= \max \left( 0, \nu_j \left( -\frac{\partial}{\partial \theta_j} \log(\pi(\theta + \nu \cdot t)) + \omega[\varphi_{m,n}(\theta + \nu \cdot t)]_j \right) \right) \\ &\leq \left( \frac{|\theta_j - \mu_0|}{s_0^2} + \frac{\omega(\beta + 1)}{n} \sum_{i=1}^n |x_{ij}| \left( y_i + \frac{1}{\beta} \right) \right) + \frac{1}{s_0^2} t + e^{\max_{i=1, \dots, n} \{\sum_{j=1}^p |x_{ij}|\} t} \frac{(\beta + 1)^2}{\beta} \frac{\omega}{n} \sum_{i=1}^n |x_{ij}| e^{x_i^\top \theta} \\ &= \hat{\Lambda}_j(\theta + \nu \cdot t, \nu).\end{aligned}$$

□

**Corollary 4.** *Sampling stopping times according to the computational bound in Lemma 4 is achieved for  $j = 1, \dots, d$  by setting*

$$\tau_j^* = \min\{\tau_j^{(1)}, \tau_j^{(2)}\}$$

with

$$\begin{aligned}\tau_j^{(1)} &= \frac{\sqrt{a_j^2 - 2 \log(u_j^{(1)}) b_j} - a_j}{b_j} \\ \tau_j^{(2)} &= \frac{1}{\max_{i=1, \dots, n} \{\sum_{j=1}^p |x_{ij}|\}} \log \left( 1 - \log(u_j^{(2)}) \frac{\max_{i=1, \dots, n} \{\sum_{j=1}^p |x_{ij}|\}}{\frac{(\beta+1)^2}{\beta} \frac{\omega}{n} \sum_{i=1}^n |x_{ij}| e^{x_i^\top \theta}} \right) \\ a_j &= \left( \frac{|\theta_j - \mu_0|}{s_0^2} + \frac{\omega(\beta+1)}{n} \sum_{i=1}^n |x_{ij}| \left( y_i + \frac{1}{\beta} \right) \right) \\ b_j &= \frac{1}{s_0^2}.\end{aligned}$$

with  $u_j^{(1)}, u_j^{(2)} \sim \text{Unif}(0, 1)$ .

*Proof.* Writing

$$\hat{\Lambda}_j(\theta + \nu \cdot t, \nu) = \Lambda_j^{(1)}(\theta + \nu \cdot t, \nu) + \Lambda_j^{(2)}(\theta + \nu \cdot t, \nu)$$

with  $\Lambda_j^{(1)}(\theta + \nu \cdot t, \nu) = \left( \frac{|\theta_j - \mu_0|}{s_0^2} + \frac{\omega(\beta+1)}{n} \sum_{i=1}^n |x_{ij}| \left( y_i + \frac{1}{\beta} \right) \right) + \frac{1}{s_0^2} t$  and  $\Lambda_j^{(2)}(\theta + \nu \cdot t, \nu) = e^{\max_{i=1, \dots, n} \{\sum_{j=1}^p |x_{ij}|\} t \frac{(\beta+1)^2}{\beta} \frac{\omega}{n} \sum_{i=1}^n |x_{ij}| e^{x_i^\top \theta}}$ , allows us to sample stopping times  $\tau_j$  from a Poisson process with rate  $\int_0^t \hat{\Lambda}_j(\theta + \nu \cdot s, \nu) ds$  as required by Lemma 4 via Poisson superposition, first sampling  $\tau_j^{(l)}$  according to a Poisson process with rate  $\int_0^t \Lambda_j^{(l)}(\theta + \nu \cdot s, \nu) ds$ ,  $l = 1, \dots, 2$  and setting  $\tau_j = \min\{\tau_j^{(1)}, \tau_j^{(2)}\}$ .

Sampling  $\tau_j^{(1)}$  for  $j = 1, \dots, d$  can be done following the procedure outlined in Corollary

1 with

$$a_j := \left( \frac{\theta_j - \mu_0}{s_0^2} + \frac{\omega(\beta + 1)}{n} \sum_{i=1}^n |x_{ij}| \left( y_i + \frac{1}{\beta} \right) \right)$$

$$b_j := \frac{1}{s_0^2}.$$

Sampling  $\tau_j^{(2)}$  requires evaluating

$$\begin{aligned} \int_0^t \Lambda_{p+1}^{(2)}(s; \theta, \nu) ds &= \int_0^t e^{\max_{i=1, \dots, n} \{\sum_{j=1}^p |x_{ij}|\} s} \frac{(\beta + 1)^2 \omega}{\beta} \frac{1}{n} \sum_{i=1}^n |x_{ij}| e^{x_i^\top \theta} ds \\ &= \frac{(\beta + 1)^2 \omega}{\beta} \frac{1}{n} \sum_{i=1}^n |x_{ij}| e^{x_i^\top \theta} \left[ \frac{e^{\max_{i=1, \dots, n} \{\sum_{j=1}^p |x_{ij}|\} s}}{\max_{i=1, \dots, n} \{\sum_{j=1}^p |x_{ij}|\}} \right]_0^t \\ &= \frac{(\beta + 1)^2 \omega}{\beta} \frac{1}{n \max_{i=1, \dots, n} \{\sum_{j=1}^p |x_{ij}|\}} \left[ e^{\max_{i=1, \dots, n} \{\sum_{j=1}^p |x_{ij}|\} t} - 1 \right] \end{aligned}$$

and therefore the stopping times can be simulated following Cinlar's Algorithm ([Cinlar, 1975](#)) (Algorithm 1) by sampling  $u_j^{(2)} \sim Unif(0, 1)$  and solving

$$\begin{aligned} \tau_j^{(2)} &:= \inf \left\{ t : \frac{(\beta + 1)^2 \omega}{\beta} \frac{\sum_{i=1}^n |x_{ij}| e^{x_i^\top \theta}}{n \max_{i=1, \dots, n} \{\sum_{j=1}^p |x_{ij}|\}} \left[ e^{\max_{i=1, \dots, n} \{\sum_{j=1}^p |x_{ij}|\} t} - 1 \right] \geq -\log(u_j^{(2)}) \right\} \\ &= \inf \left\{ t : \left[ e^{\max_{i=1, \dots, n} \{\sum_{j=1}^p |x_{ij}|\} t} - 1 \right] \geq -\log(u_j^{(2)}) \frac{\max_{i=1, \dots, n} \{\sum_{j=1}^p |x_{ij}|\}}{\frac{(\beta+1)^2 \omega}{\beta} \frac{1}{n} \sum_{i=1}^n |x_{ij}| e^{x_i^\top \theta}} \right\} \\ &= \frac{1}{\max_{i=1, \dots, n} \{\sum_{j=1}^p |x_{ij}|\}} \log \left( 1 - \log(u_j^{(2)}) \frac{\max_{i=1, \dots, n} \{\sum_{j=1}^p |x_{ij}|\}}{\frac{(\beta+1)^2 \omega}{\beta} \frac{1}{n} \sum_{i=1}^n |x_{ij}| e^{x_i^\top \theta}} \right). \end{aligned}$$

□

## References

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Cinlar, E. (1975). *Introduction to stochastic processes*. Englewood Cliffs, NJ: Prentice-Hall.

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