

Variational Gaussian Copula Inference

Supplementary Material

Shaobo Han

Xuejun Liao

David B. Dunson[†]

Lawrence Carin

Department of ECE, Department of Statistical Science[†], Duke University, Durham, NC 27708, USA

A: KL Additive Decomposition

Letting the variational proposal in Sklar's representation be $q_{VC}(\mathbf{x}) = c(\mathbf{u}) \prod_{j=1}^p f_j(x_j)$, and the true posterior be $p(\mathbf{x}|\mathbf{y}) = c^*(\mathbf{v}) \prod_j f_j^*(x_j)$, where $\mathbf{u} = F(\mathbf{x}) = [F_1(x_1), \dots, F_p(x_p)]$, $\mathbf{v} = F^*(\mathbf{x}) = [F_1^*(x_1), \dots, F_p^*(x_p)]$. The KL divergence decomposes into additive terms,

$$\begin{aligned} \text{KL}\{q(\mathbf{x})||p(\mathbf{x}|\mathbf{y})\} &= \int q(\mathbf{x}) \left(\log \frac{q(\mathbf{x})}{p(\mathbf{x}|\mathbf{y})} \right) d\mathbf{x} \\ &= \int c[F(\mathbf{x})] \prod_j f_j(x_j) \left(\log \frac{c[F(\mathbf{x})] \prod_j f_j(x_j)}{c^*[F^*(\mathbf{x})] \prod_j f_j^*(x_j)} \right) d\mathbf{x} \\ &= \int c[F(\mathbf{x})] \left(\log \frac{c[F(\mathbf{x})]}{c^*[F^*(\mathbf{x})]} \right) \prod_j dF_j(x_j) \\ &\quad + \int c[F(\mathbf{x})] \prod_j f_j(x_j) \left(\log \frac{\prod_j f_j(x_j)}{\prod_j f_j^*(x_j)} \right) \prod_j dx_j. \end{aligned} \quad (1)$$

The first term in (1)

$$\begin{aligned} &\int c[F(\mathbf{x})] \left(\log \frac{c[F(\mathbf{x})]}{c^*[F^*(\mathbf{x})]} \right) \prod_j dF_j(x_j) \\ &= \int c(\mathbf{u}) \left(\log \frac{c(\mathbf{u})}{c^*(F^{-1}(\mathbf{u}))} \right) d\mathbf{u} \\ &= \text{KL}\{c(\mathbf{u})||c^*[F^*(F^{-1}(\mathbf{u}))]\}, \end{aligned}$$

The second term in (1)

$$\begin{aligned} &\int c[F(\mathbf{x})] \prod_j f_j(x_j) \left(\log \frac{\prod_j f_j(x_j)}{\prod_j f_j^*(x_j)} \right) \prod_j dx_j \\ &= \sum_j \int c[F(\mathbf{x})] \prod_j f_j(x_j) \left(\log \frac{f_j(x_j)}{f_j^*(x_j)} \right) \prod_j dx_j \\ &= \sum_j \int f_j(x_j) \left(\log \frac{f_j(x_j)}{f_j^*(x_j)} \right) dx_j \quad (\text{Marginal Closed Property}) \\ &= \sum_j \text{KL}\{f_j(x_j)||f_j^*(x_j)\}, \end{aligned}$$

Therefore

$$\begin{aligned} \text{KL}\{q(\mathbf{x})||p(\mathbf{x}|\mathbf{y})\} &= \text{KL}\{c[F(\mathbf{x})]||c^*[F^*(\mathbf{x})]\} \\ &\quad + \sum_j \text{KL}\{f_j(x_j)||f_j^*(x_j)\} \end{aligned} \quad (2)$$

B: Model-Specific Derivations

B1: Skew Normal Distribution

1. $\ln p(x) \propto \ln \phi(x) + \ln \Phi(\alpha x)$ and $\partial \ln p(x)/\partial x = -x + \alpha \phi(\alpha x)/\Phi(\alpha x)$, α is the shape parameter
2. $\Psi(x)$ is predefined as CDF of $\mathcal{N}(0, 1)$

B2: Student's t Distribution

1. $\ln p(x) \propto -(\nu + 1)/2 \ln(1 + x^2/\nu)$ and $\partial \ln p(x)/\partial x = -(\nu + 1)x/(\nu + x^2)$, $\nu > 0$ is the degrees of freedom
2. $\Psi(x)$ is predefined as CDF of $\mathcal{N}(0, 1)$

B3: Gamma Distribution

1. $\ln p(x) \propto (\alpha - 1) \ln x - \beta x$ and $\partial \ln p(x)/\partial x = (\alpha - 1)/x - \beta$, α is the shape parameter, β is the rate parameter
2. $\Psi(x)$ is predefined as CDF of $\text{Exp}(1)$

B4: Beta Distribution

1. $\ln p(x) \propto (a - 1) \ln x + (b - 1) \ln(1 - x)$ and $\partial \ln p(x)/\partial x = (a - 1)/x - (b - 1)/(1 - x)$, both $a, b > 0$
2. $\Psi(x)$ is predefined as CDF of $\text{Beta}(2, 2)$

B5: Bivariate Log-Normal

1. $\ln p(x_1, x_2) \propto -\ln x_1 - \ln x_2 - \zeta/2$ and

$$\begin{aligned}\frac{\partial \ln f(x_1, x_2)}{\partial x_1} &= -\frac{1}{x_1} - \frac{\alpha_1(x_1) - \rho\alpha_2(x_2)}{(1-\rho^2)x_1\sigma_1} \\ \frac{\partial \ln f(x_1, x_2)}{\partial x_2} &= -\frac{1}{x_2} - \frac{\alpha_2(x_2) - \rho\alpha_1(x_1)}{(1-\rho^2)x_2\sigma_2}\end{aligned}$$

2. $\Psi(x)$ is predefined as CDF of $\text{Exp}(1)$

C. Derivations in Horseshoe Shrinkage

The equivalent hierarchical model is

$$y|\tau \sim \mathcal{N}(0, \tau), \quad \tau|\gamma \sim \text{InvGa}(0.5, \gamma), \quad \gamma \sim \text{Ga}(0.5, 1)$$

C1: Gibbs Sampler

The full conditional posterior distributions are

$$p(\tau|y, \gamma) = \text{InvGa}\left(1, y^2/2 + \gamma\right), \quad p(\gamma|\tau) = \text{Ga}\left(1, \tau^{-1} + 1\right)$$

C2: Mean-field Variational Bayes

The ELBO under MFVB is

$$\begin{aligned}\mathcal{L}_{\text{MFVB}}[q_{\text{VB}}(\tau, \gamma)] &= \mathbb{E}_{q(\tau)q(\gamma)}[\ln p(y, \tau, \gamma)] \\ &\quad + H_1[q(\tau; \alpha_1, \beta_1)] + H_2[q(\gamma; \alpha_2, \beta_2)]\end{aligned}$$

where

$$\begin{aligned}\mathbb{E}_{q(\tau)q(\gamma)}[\ln p(y, \tau, \gamma)] &= -0.5 \ln(2\pi) - 2 \ln \Gamma(0.5) - 2 \langle \ln \tau \rangle \\ &\quad - y^2 \langle \tau^{-1} \rangle / 2 - \langle \gamma \rangle \langle \tau^{-1} \rangle - \langle \gamma \rangle \\ H_1[q(\tau; \alpha_1, \beta_1)] &= \alpha_1 + \ln \beta_1 + \ln [\Gamma(\alpha_1)] - (1 + \alpha_1)\psi(\alpha_1) \\ H_2[q(\gamma; \alpha_2, \beta_2)] &= \alpha_2 - \ln \beta_2 + \ln [\Gamma(\alpha_2)] + (1 - \alpha_2)\psi(\alpha_2)\end{aligned}$$

The variational distribution

$$\begin{aligned}q(\tau) &= \mathcal{IG}(\tau; \alpha_1, \beta_1) = \mathcal{IG}(\tau; 1, y^2/2 + \langle \gamma \rangle), \\ q(\gamma) &= \mathcal{G}(\gamma; \alpha_2, \beta_2) = \mathcal{G}(\gamma; 1, \langle \tau^{-1} \rangle + 1)\end{aligned}$$

where

$$\begin{aligned}\langle \ln \tau \rangle &= \ln \beta_1 - \psi(\alpha_1) = \ln (y^2/2 + \langle \gamma \rangle) - \psi(1), \\ \langle \tau^{-1} \rangle &= \frac{\alpha_1}{\beta_1} = \frac{1}{(y^2/2 + \langle \gamma \rangle)}, \quad \langle \gamma \rangle = \frac{\alpha_2}{\beta_2} = \frac{1}{\langle \tau^{-1} \rangle + 1}\end{aligned}$$

C3: Deterministic VGC-LN

Denoting $\mathbf{x} = (x_1, x_2) = (\tau, \gamma)$, we construct a variational Gaussian copula proposal with (1) a bivariate Gaussian copula, and (2) fixed-form margin for both $x_1 = \tau \in (0, \infty)$ and $x_2 = \gamma \in (0, \infty)$; we employ $f_j(x_j; \mu_j, \sigma_{jj}^2) = \mathcal{LN}(x_j; \mu_j, \sigma_{jj}^2), x_j = h_j(\tilde{z}_j) = \exp(\tilde{z}_j) = g(z_j) = \exp(\sigma_{jj}z_j + \mu_j)$, $j = 1, 2$. The ELBO of VGC-LN is

$$\begin{aligned}\mathcal{L}_{\text{VGC}}(\boldsymbol{\mu}, \mathbf{C}) &= c_1 - \mu_1 + \mu_2 - \frac{y^2 \exp\left(-\mu_1 + \frac{C_{11}^2}{2}\right)}{2} \\ &\quad - \ell_0 - \exp\left(\mu_2 + \frac{C_{21}^2 + C_{22}^2}{2}\right) + \ln |\mathbf{C}| \\ \ell_0 &= \exp\left((\mu_2 - \mu_1) + \frac{C_{11}^2 - 2C_{11}C_{21} + C_{21}^2 + C_{22}^2}{2}\right)\end{aligned}$$

where $c_0 = -0.5 \ln(2\pi) - 2 \ln \Gamma(0.5)$, $c_1 = c_0 + \ln(2\pi e)$.

The gradients are

$$\begin{aligned}\frac{\partial \mathcal{L}_{\text{VGC}}(\boldsymbol{\mu}, \mathbf{C})}{\partial \mu_1} &= -1 + \frac{y^2}{2} \exp\left(\frac{C_{11}^2}{2} - \mu_1\right) + \ell_0 \\ \frac{\partial \mathcal{L}_{\text{VGC}}(\boldsymbol{\mu}, \mathbf{C})}{\partial \mu_2} &= 1 - \ell_0 - \exp\left(\mu_2 + \frac{C_{21}^2 + C_{22}^2}{2}\right) \\ \frac{\partial \mathcal{L}_{\text{VGC}}(\boldsymbol{\mu}, \mathbf{C})}{\partial C_{11}} &= -\frac{y^2}{2} C_{11} \exp\left(\frac{C_{11}^2}{2} - \mu_1\right) - (C_{11} - C_{21})\ell_0 + \frac{1}{C_{11}} \\ \frac{\partial \mathcal{L}_{\text{VGC}}(\boldsymbol{\mu}, \mathbf{C})}{\partial C_{21}} &= (C_{11} - C_{21})\ell_0 - C_{21} \exp\left(\mu_2 + \frac{C_{21}^2 + C_{22}^2}{2}\right) \\ \frac{\partial \mathcal{L}_{\text{VGC}}(\boldsymbol{\mu}, \mathbf{C})}{\partial C_{22}} &= -C_{22}\ell_0 - C_{22} \exp\left(\mu_2 + \frac{C_{21}^2 + C_{22}^2}{2}\right) + \frac{1}{C_{22}}\end{aligned}$$

C4: Stochastic VGC-LN

The stochastic part of the ELBO is,

$$\ell_s(\tilde{\mathbf{z}}) = c_0 + \tilde{z}_2 - \tilde{z}_1 - \frac{y^2 \exp(-\tilde{z}_1)}{2} - \exp(\tilde{z}_2 - \tilde{z}_1) - \exp(\tilde{z}_2)$$

and

$$\begin{aligned}\nabla_{\tilde{z}_1} \ell_s(\tilde{\mathbf{z}}) &= -1 + \frac{y^2 \exp(-\tilde{z}_1)}{2} + \exp(\tilde{z}_2 - \tilde{z}_1) \\ \nabla_{\tilde{z}_2} \ell_s(\tilde{\mathbf{z}}) &= 1 - \exp(\tilde{z}_2 - \tilde{z}_1) - \exp(\tilde{z}_2)\end{aligned}$$

C5: Stochastic VGC-BP

1. $\ln p(y, x_1, x_2) = c_0 - 2 \ln x_1 - y^2/(2x_1) - x_2/x_1 - x_2$,

$$\partial \ln p(y, x_1, x_2)/\partial x_1 = -2/x_1 + y^2/(2x_1^2) + x_2/x_1^2,$$

$$\partial \ln p(y, x_1, x_2)/\partial x_2 = -1/x_1 - 1$$

2. $\Psi(x)$ is predefined as CDF of $\text{Exp}(0.01)$.

D. Derivations in Poisson Log Linear Regression

For $i = 1, \dots, n$, the hierarchical model is

$$y_i \sim \text{Poisson}(\mu_i), \quad \log(\mu_i) = \beta_0 + \beta_1 x_i + \beta_2 x_i^2, \\ \beta_0 \sim N(0, \tau), \quad \beta_1 \sim N(0, \tau), \quad \beta_2 \sim N(0, \tau), \quad \tau \sim \text{Ga}(1, 1)$$

The log likelihood and prior,

$$\ln p(\mathbf{y}, \boldsymbol{\beta}, \tau) = \sum_{i=1}^n \ln p(y_i | \boldsymbol{\beta}) + \ln \mathcal{N}(\beta_0; 0, \tau) + \ln \mathcal{N}(\beta_1; 0, \tau) \\ + \ln \mathcal{N}(\beta_2; 0, \tau) + \ln \text{Ga}(\tau; 1, 1)$$

where $\ln p(y_i | \boldsymbol{\beta}) = y_i \ln \mu_i - \mu_i - \ln y_i!$, and $\mu_i = \exp(\beta_0 + \beta_1 x_i + \beta_2 x_i^2)$.

The derivatives are

$$\frac{\partial \ln p(\mathbf{y}, \boldsymbol{\beta}, \tau)}{\partial \beta_0} = \left[\sum_{i=1}^n (y_i - \mu_i) \right] - \tau^{-1} \beta_0$$

$$\frac{\partial \ln p(\mathbf{y}, \boldsymbol{\beta}, \tau)}{\partial \beta_1} = \left[\sum_{i=1}^n x_i (y_i - \mu_i) \right] - \tau^{-1} \beta_1$$

$$\frac{\partial \ln p(\mathbf{y}, \boldsymbol{\beta}, \tau)}{\partial \beta_2} = \left[\sum_{i=1}^n x_i^2 (y_i - \mu_i) \right] - \tau^{-1} \beta_2$$

$$\frac{\partial \ln p(\mathbf{y}, \boldsymbol{\beta}, \tau)}{\partial \tau} = -\frac{3}{2\tau} + \frac{\beta_0^2 + \beta_1^2 + \beta_2^2}{2\tau^2} + \frac{a_0 - 1}{\tau} - b_0$$