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Bayesian inverse modeling and source location of an unintended ^{131}I release in Europe in the fall of 2011

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1 Variational Bayes inference of LS-APC model

The LS-APC model (Tichý et al., 2016) is formulated as (see details in the main paper)

$$p(\mathbf{y}|\mathbf{x},\omega) = \mathcal{N}\left(M\mathbf{x}, \omega^{-1}I_p\right), \tag{1}$$
$$p(\omega) = \mathcal{G}\left(\vartheta_0, \rho_0\right), \tag{2}$$
$$p(x_{j+1}|x_j, l_j, \upsilon_j) = t\mathcal{N}\left(-l_j x_j, \upsilon_{j+1}^{-1}, [0,\infty]\right), \text{ for } j = 1, \ldots, n-1, \tag{3}$$
$$p(\upsilon_j) = \mathcal{G}\left(\alpha_0, \beta_0\right), \text{ for } j = 1, \ldots, n, \tag{4}$$
$$p(l_j|\psi_j) = \mathcal{N}\left(-1, \psi_j^{-1}\right), \text{ for } j = 1, \ldots, n-1, \tag{5}$$
$$p(\psi_j) = \mathcal{G}\left(\zeta_0, \eta_0\right), \text{ for } j = 1, \ldots, n-1, \tag{6}$$

where symbol $\mathcal{N}$ denotes (multivariate) Gaussian distribution, $\mathcal{G}$ denotes gamma distribution, $t\mathcal{N}$ denotes truncated Gaussian distribution with given interval, and I_p denotes identity matrix of the given size.

1.1 Estimation of model parameters

Since the analytical estimation of the parameters of the model (1)–(6) is not tractable, we employ the Variational Bayes (VB) method (Šmídl and Quinn, 2006). Here, posterior distributions satisfy conditional independence which uniquely determine their forms as

$$\tilde{p}(\omega|\mathbf{y}) = \mathcal{G}\left(\vartheta, \rho\right), \tag{7}$$
$$\tilde{p}(\mathbf{x}|\mathbf{y}) = t\mathcal{N}\left(\mu_{\mathbf{x}}, \Sigma_{\mathbf{x}}\right), \tag{8}$$
$$\tilde{p}(\upsilon_j|\mathbf{y}) = \mathcal{G}\left(\alpha_j, \beta_j\right), \ \forall j = 1, \ldots, n, \tag{9}$$
$$\tilde{p}(l_j|\mathbf{y}) = \mathcal{N}\left(\mu_{l_j}, \Sigma_{l_j}\right), \ \forall j = 1, \ldots, n-1, \tag{10}$$
$$\tilde{p}(\psi_j|\mathbf{y}) = \mathcal{G}\left(\zeta_j, \eta_j\right), \ \forall j = 1, \ldots, n-1, \tag{11}$$

with shaping parameters $\vartheta, \rho, \mu_{\mathbf{x}}, \Sigma_{\mathbf{x}}, \alpha_j, \beta_j, \mu_{l_j}, \Sigma_{l_j}, \zeta_j, \eta_j$. These are derived as

$$\vartheta = \vartheta_0 + \frac{p}{2}, \qquad \rho = \rho_0 + \frac{1}{2}\mathrm{tr}\left(\left\langle \mathbf{x}\mathbf{x}^T \right\rangle M^T M\right) - \frac{1}{2}2\mathbf{y}^T M \langle \mathbf{x} \rangle + \frac{1}{2}\mathbf{y}^T\mathbf{y}, \tag{12}$$
$$\Sigma_{\mathbf{x}} = \left(\langle\omega\rangle M^T M + \left\langle L \Upsilon L^T \right\rangle\right)^{-1}, \qquad \mu_{\mathbf{x}} = \Sigma_{\mathbf{x}}\left(\langle\omega\rangle M^T \mathbf{y}\right), \tag{13}$$
$$\alpha = \alpha_0 + \frac{1}{2}\mathbf{1}_{n,1}, \qquad \beta = \beta_0 + \frac{1}{2}\mathrm{diag}\left(\left\langle L^T \mathbf{x}\mathbf{x}^T L \right\rangle\right), \tag{14}$$
$$\Sigma_{l_j} = \left(\langle\upsilon_j\rangle\left\langle x_{j+1}^2\right\rangle + \langle\psi_j\rangle\right)^{-1}, \qquad \mu_{l_j} = \Sigma_{l_j}\left(-\langle\upsilon_j\rangle\langle x_j x_{j+1}\rangle - \langle\psi_j\rangle\right), \tag{15}$$
$$\zeta_j = \zeta_0 + \frac{1}{2}, \qquad \eta_j = \eta_0 + \frac{1}{2}\left\langle (l_j+1)^2 \right\rangle, \ j = 1, \ldots, n-1, \tag{16}$$

where symbol $\langle \mathbf{x} \rangle$ denotes the moment with respect to the distribution on the variable in the argument, the matrix L is composed from $l_1, \ldots, l_{n-1}$ as $L = \begin{pmatrix} 1 & 0 & 0 & 0 \\ l_1 & 1 & 0 & 0 \\ 0 & \ddots & 1 & 0 \\ 0 & 0 & l_{n-1} & 1 \end{pmatrix}$, and Υ is diagonal matrix with $\upsilon_1, \ldots, \upsilon_n$ on its diagonal. While the moments of Gaussian and Gamma distributions are standard, relatively non-standard moments of truncated Gaussian distribution are computed according to appendix in the main paper.

Reference implementation is available from http://www.utia.cz/linear_inversion_methods.

1.2 Model selection

The model selection property, the term $\mathcal{L}_{M_k}$ need to be evaluated,

$$\mathcal{L}_{M_k} = \mathrm{E}\left[\ln p(\mathbf{y},\mathbf{x},\Upsilon,L,\psi_1,\ldots,\psi_{n-1},\omega,M_k)\right] - \mathrm{E}\left[\ln \tilde{p}(\omega)\right] - \mathrm{E}\left[\ln \tilde{p}(\mathbf{x})\right] - \mathrm{E}\left[\ln \tilde{p}(\Upsilon)\right] - \mathrm{E}\left[\ln \tilde{p}(L)\right] - \mathrm{E}\left[\ln \tilde{p}(\psi_1,\ldots,\psi_{n-1})\right], \tag{17}$$

where E[] denotes expected value . The terms of (17) computed using shaping parameters and moments from Sec. 1.1 are follow:

$$\begin{aligned}
&\mathrm{E}\left[\ln p(\mathbf{y},\mathbf{x},\Upsilon,L,\psi_1,\ldots,\psi_{n-1},\omega,M_k)\right] = \\
&-\frac{p}{2}\ln(2\pi) + \frac{p}{2}\langle \ln\omega\rangle - \frac{1}{2}\langle\omega\rangle\left(\mathrm{tr}\left(\langle \mathbf{x}\mathbf{x}^T\rangle M_k^T M_k\right) - 2\mathbf{y}^T M_k \langle\mathbf{x}\rangle + \mathbf{y}^T\mathbf{y}\right) + \\
&-\ln\Gamma(\vartheta_0) + \vartheta_0\ln\rho_0 + (\vartheta_0 - 1)\langle\ln\omega\rangle - \rho_0\langle\omega\rangle + \\
&+ n\ln\sqrt{2} + \sum_{j=1}^{n}\left(-\frac{\langle x_j^2\rangle}{2\langle L\Upsilon L^T\rangle_{j,j}^{-1}} - \ln\sqrt{\pi\langle L\Upsilon L^T\rangle_{j,j}^{-1}}\right) + \\
&- n\ln\Gamma(\alpha_0) + n\alpha_0\ln\beta_0 + \sum_{j=1}^{n}\left((\alpha_0 - 1)\langle\ln\upsilon_j\rangle - \beta_0\langle\upsilon_j\rangle\right) + \\
&- \frac{n-1}{2}\ln(2\pi) + \sum_{j=1}^{n-1}\left(\frac{1}{2}\langle\ln\psi_j\rangle - \frac{1}{2}\left(\langle l_j^2\rangle\langle\psi_j\rangle + 2\langle\psi_j\rangle\langle l_j\rangle + \langle\psi_j\rangle\right)\right) + \\
&\qquad - (n-1)\ln\Gamma(\zeta_0) + (n-1)\zeta_0\ln\eta_0 + \sum_{j=1}^{n-1}\left((\zeta_0 - 1)\langle\ln\psi_j\rangle - \eta_0\langle\psi_j\rangle\right).
\end{aligned} \tag{18}$$

$$\mathrm{E}\left[\ln\tilde{p}(\omega)\right] = -\ln\Gamma(\vartheta) + \vartheta\ln\rho + (\vartheta - 1)\langle\ln\omega\rangle - \rho\langle\omega\rangle, \tag{19}$$

$$\mathrm{E}\left[\ln\tilde{p}(\mathbf{x})\right] = n\ln\sqrt{2} + \sum_{j=1}^{n}\left(-\frac{1}{2\left(\Sigma_{\mathbf{x}}\right)_{j,j}}\left(\langle x_j\rangle - \left(\mu_{\mathbf{x}}\right)_j\right)^2 - \ln\sqrt{\left(\Sigma_{\mathbf{x}}\right)_{j,j}\pi} - \ln\left(1 - \mathrm{erf}\left(\frac{-\left(\mu_{\mathbf{x}}\right)_j}{\sqrt{2\left(\Sigma_{\mathbf{x}}\right)_{j,j}}}\right)\right)\right), \tag{20}$$

$$\mathrm{E}\left[\ln\tilde{p}(\Upsilon)\right] = -\sum_{j=1}^{n}\ln\Gamma(\alpha_j) + \sum_{j=1}^{n}\alpha_j\ln\beta_j + \sum_{j=1}^{n}(\alpha_j - 1)\langle\ln\upsilon_j\rangle - \sum_{j=1}^{n}\beta_j\langle\upsilon_j\rangle, \tag{21}$$

$$\mathrm{E}\left[\ln\tilde{p}(L)\right] = -\frac{n-1}{2}\ln(2\pi) - \sum_{j=1}^{n-1}\frac{1}{2}\ln\Sigma_{l_j} - \frac{1}{2}\sum_{j=1}^{n-1}\left(\left(\langle l_j\rangle - \mu_{l_j}\right)^T\Sigma_{l_j}^{-1}\left(\langle l_j\rangle - \mu_{l_j}\right)\right), \tag{22}$$

$$\mathrm{E}\left[\ln\tilde{p}(\psi_1,\ldots,\psi_{n-1})\right] = \sum_{j=1}^{n-1}\left(-\ln\Gamma(\zeta_j) + \zeta_j\ln\eta_j + (\zeta_j - 1)\langle\ln\psi_j\rangle - \eta_j\langle\psi_j\rangle\right), \tag{23}$$

where $\Gamma(z)$ is gamma function defined as $\Gamma(z) = \int_0^\infty x^{z-1}\exp(-x)\mathrm{d}x$ and $\mathrm{erf}(z)$ is error function defined as $\mathrm{erf}(z) = \frac{2}{\sqrt{\pi}}\int_0^z\exp(-x^2)\mathrm{d}x$.

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