

Exercise 1 (Monte Carlo for Gaussians)

1. Let's prove that $E[\phi(X)] = E[\phi(X + \theta) \exp(\frac{-1}{2}\theta^T \theta - \theta^T X)]$.

$$\begin{aligned} E[\phi(X + \theta) \exp(\frac{-1}{2}\theta^T \theta - \theta^T X)] &= \int_{\mathbb{R}^d} \phi(x + \theta) \exp(\frac{-1}{2}\theta^T \theta - \theta^T X) \pi(x) dx_1 \dots dx_d = \\ &= \int_{\mathbb{R}^d} \phi(x + \theta) \exp\left(\frac{-1}{2}\theta^T \theta - \theta^T X\right) \exp(-x^T x/2) \frac{1}{(\sqrt{2\pi})^d} dx_1 \dots dx_d = \\ &= \int_{\mathbb{R}^d} \phi(x + \theta) \exp\left(\frac{-1}{2}(x - \theta)^T (x - \theta)\right) \frac{1}{(\sqrt{2\pi})^d} dx_1 \dots dx_d \end{aligned}$$

Finally, making $x - \theta = y$,

$$\int_{\mathbb{R}^d} \phi(y) \exp\left(\frac{-1}{2}(y)^T (y)\right) \frac{1}{(\sqrt{2\pi})^d} dx_1 \dots dx_d = E[\phi(Y)]$$

□

2. Let's show that

$$\sigma^2(\theta) = E\left[\phi^2(X) \exp\left(\frac{-1}{2}X^T X + \frac{1}{2}(X - \theta)^T (X - \theta)\right)\right] - (E[\phi(X)])^2$$

Note that, using the result in the previous item we have:

$$\begin{aligned} \sigma^2(\theta) &= V\left[\phi(X + \theta) \exp\left(\frac{-1}{2}\theta^T \theta - \theta^T X\right)\right] = \\ &= E\left[\left(\phi(X + \theta) \exp\left(\frac{-1}{2}\theta^T \theta - \theta^T X\right)\right)^2\right] - E\left[\phi(X + \theta) \exp\left(\frac{-1}{2}\theta^T \theta - \theta^T X\right)\right]^2 = \\ &= E\left[\left(\phi(X + \theta) \exp\left(\frac{-1}{2}\theta^T \theta - \theta^T X\right)\right)^2\right] - E[\phi(X)]^2 \end{aligned}$$

Now, let's rearrange the first term in the variance.

$$\sigma^2(\theta) = \int_{\mathbb{R}^d} \phi(x + \theta)^2 \exp(-\theta^T \theta - 2\theta^T X) \exp(-x^T x/2) \frac{1}{(\sqrt{2\pi})^d} dx_1 \dots dx_d =$$

Make $X + \theta = Y$, then:

$$\begin{aligned}
& \int_{\mathbb{R}^d} \phi(y)^2 \exp(-\theta^T \theta - 2\theta^T(y - \theta)) \exp(-(y - \theta)^T(y - \theta)/2) \frac{1}{(\sqrt{2\pi})^d} dx_1 \dots dx_d = \\
& = \int_{\mathbb{R}^d} \phi(y)^2 \exp\left(\frac{1}{2}(y - \theta)^T(y - \theta) - \frac{y^T y}{2}\right) \exp\left(\frac{-y^T y}{2}\right) \frac{1}{(\sqrt{2\pi})^d} dx_1 \dots dx_d = \\
& = E\left[\phi^2(X) \exp\left(\frac{-1}{2}X^T X + \frac{1}{2}(X - \theta)^T(X - \theta)\right)\right]
\end{aligned}$$

Therefore,

$$\sigma^2(\theta) = E\left[\phi^2(X) \exp\left(\frac{-1}{2}X^T X + \frac{1}{2}(X - \theta)^T(X - \theta)\right)\right] - (E[\phi(X)])^2$$

□

3. Let's calculate $\nabla^2 \sigma^2(\theta) = H(\theta)$.

$$\begin{aligned}
\frac{\partial \sigma^2(\theta)}{\partial \theta_i} &= \frac{E[\phi(X)^2 \exp(\frac{-X^T X + (X - \theta)^T(X - \theta)}{2})]}{\partial \theta_i} = \\
&= \int_{\chi} \phi(x)^2 \exp(-x^T x) \frac{\partial}{\partial \theta_i} \exp\left(\frac{(x - \theta)^T(x - \theta)}{2}\right) \frac{1}{(\sqrt{2\pi})^d} dx = \\
&= \int_{\chi} \phi(x)^2 \exp(-x^T x) (\theta_i - x_i) \exp\left(\frac{(x - \theta)^T(x - \theta)}{2}\right) \frac{1}{(\sqrt{2\pi})^d} dx
\end{aligned}$$

We calculated the gradient, let's now calculate the second derivative. First the diagonal.

$$\begin{aligned}
& \frac{\partial}{\partial \theta_i} \int_{\chi} \phi(x)^2 \exp(-x^T x) (\theta_i - x_i) \exp\left(\frac{(x - \theta)^T(x - \theta)}{2}\right) \frac{1}{(\sqrt{2\pi})^d} dx = \\
& = E[\phi(X)^2] + \int_{\chi} \phi(x)^2 \exp(-x^T x) \exp\left(\frac{(x - \theta)^T(x - \theta)}{2}\right) (x_i - \theta_i)(x_i - \theta_i) \frac{1}{(\sqrt{2\pi})^d} dx
\end{aligned}$$

Now the rest:

$$\begin{aligned}
& \frac{\partial}{\partial \theta_j} \int_{\chi} \phi(x)^2 \exp(-x^T x) (\theta_i - x_i) \exp\left(\frac{(x - \theta)^T(x - \theta)}{2}\right) \frac{1}{(\sqrt{2\pi})^d} dx = \\
& = \int_{\chi} \phi(x)^2 \exp(-x^T x) \exp\left(\frac{(x - \theta)^T(x - \theta)}{2}\right) (x_i - \theta_i)(x_j - \theta_j) \frac{1}{(\sqrt{2\pi})^d} dx
\end{aligned}$$

□

4. We already know that the Hessian is positive definite. Hence, we only need to show that the derivative is equal to zero at θ^* .

$$\begin{aligned}
 \nabla \sigma^2(\theta) &= \int_{\mathcal{X}} \phi(x)^2 \exp(-x^T x) (\theta - x) \exp\left(\frac{-(x - \theta)^T (x - \theta)}{2}\right) \frac{1}{(\sqrt{2\pi})^d} dx = \\
 &= \int_{\mathcal{X}} \phi(x)^2 \exp(-x^T x) (\theta - x) \exp\left(\frac{-(x - \theta)^T (x - \theta)}{2}\right) \frac{1}{(\sqrt{2\pi})^d} dx = \\
 &= \int_{\mathcal{X}} \phi(x)^2 (\theta - x) \exp\left(\frac{-x^T x}{2} - \theta^T x + \frac{-\theta^T \theta}{2}\right) \frac{1}{(\sqrt{2\pi})^d} dx = \\
 &= \int_{\mathcal{X}} \phi(x)^2 (\theta - x) \exp(-\theta^T x) \exp(-x^T x/2) \frac{\exp(\theta^T \theta/2)}{(\sqrt{2\pi})^d} dx = 0
 \end{aligned}$$

Finally, since the last term doesn't depend on X , we can eliminate it, obtaining:

$$E[\phi(X)^2 (\theta - X) \exp(-\theta^T X)] = 0$$

□

5. Couldn't solve.

Exercise 2 (Metropolis-Hastings)

1. First, generate $Y \sim q(X_t, \cdot)$. With probability equal to $\alpha(x, y)$, make $X_{t+1} = Y$, and with probability $1 - \sum_{z \in \mathbb{Z}} \alpha(x, z)q(x, z)$ make $X_{t+1} = X_t$. Then, repeat the process.
2. We want to show that $\pi(x)T(x, y) = \pi(y)T(y, x)$. For $y = x$, this is trivial. Now, assume $y \neq x$. Therefore:

$$\begin{aligned}\pi(x)T(x, y) &= \pi(x)\alpha(x, y)q(x, y) = \pi(x)\frac{\gamma(x, y)}{\pi(x)q(x, y)} = \gamma(y, x) = \\ &= \pi(y)\frac{\gamma(y, x)q(y, x)}{\pi(y)q(y, x)} = \pi(y)T(y, x)\end{aligned}$$

□

3. Using Metropolis-Hastings, one has:

$$\alpha = \min \left\{ 1, \frac{\pi(x^*)q(x_{t-1} | x^*)}{\pi(x_{t-1})q(x^* | x_{t-1})} \right\}$$

So, $\alpha(x, y) = \frac{\gamma(x, y)}{\pi(x)q(x, y)}$, for $x = x_{t-1}, x^* = y, q(x, y) = q(x^* | x_{t-1})$.

Make:

$$\begin{aligned}\gamma(x, y) &= \max \{ \pi(y)q(y, x), \pi(x)q(x, y) \} \\ &\quad \therefore \\ \alpha(x, y) &= \frac{\max \{ \pi(y)q(y, x), \pi(x)q(x, y) \}}{\pi(x)q(x, y)} = \\ &= \min \left\{ 1, \frac{\pi(y)q(y, x)}{\pi(x)q(x, y)} \right\}\end{aligned}$$

□

4. First, let's rewrite the estimate as a function of Y . Note that $Y^{(k)} = X^{(\tau_k)}$, hence:

$$\frac{1}{\tau_k - 1} \sum_{t=1}^{\tau_k-1} \phi(X^{(t)}) = \frac{1}{k - 1} \sum_{t=1}^{k-1} \phi(Y^{(t)})$$

Now, let's prove it has the transition desired transition kernel.

$$K(x, y) = P(Y^{(k)} = y | Y^{(k-1)} = x) = P(X^{(\tau_k)} = y | X^{(\tau_k-1)} = x)$$

The event $X^{(\tau_k)} = y | X^{(\tau_k-1)} = x$ is equivalent to selecting y starting from x and then accepting y , hence $q(x, y) \cdot \alpha(x, y) = P(X^{(\tau_k)} = y | X^{(\tau_k-1)} = x)$.

Therefore, $P(Y^{(k)} = y | Y^{(k-1)} = x) = \frac{q(x, y)\alpha(x, y)}{\sum_{z \in \mathbb{Z}} \alpha(x, z)q(x, z)}$.

□

5. Let's show that $\tilde{\pi}(x)K(x, y) = \tilde{\pi}(y)K(y, x)$.

$$\frac{\pi(x)m(x)}{\sum_{z \in \mathbb{Z}} \pi(z)m(z)} \cdot \frac{q(x, y)\alpha(x, y)}{\sum_{z \in \mathbb{Z}} \alpha(x, z)q(x, z)} = \frac{\pi(x)q(x, y)\alpha(x, y)}{\sum_{z \in \mathbb{Z}} \pi(z)m(z)}$$

Note that $\alpha(x, y) = \frac{\gamma(x, y)}{\pi(x)q(x, y)} = \frac{\gamma(y, x)}{\pi(x)q(x, y)}$. Therefore:

$$\frac{\pi(x)q(x, y)\gamma(x, y)}{\alpha(x, z)q(x, z) \sum_{z \in \mathbb{Z}} \pi(z)m(z)} = \frac{\gamma(y, x)}{\sum_{z \in \mathbb{Z}} \pi(z)m(z)} = \frac{\alpha(y, x)\pi(y)q(y, x)}{\sum_{z \in \mathbb{Z}} \pi(z)m(z)} = \tilde{\pi}(y)K(y, x)$$

□

6. Couldn't solve.

Exercise 3 (Metropolis-Hastings)

1. Let's show that $\int_{\mathcal{X}} \pi(x)(\alpha(x)q(y)(1 - \alpha(x)))\delta_x(y)dx = \pi(y)$. Note that, $\pi(x) = \frac{q(x)}{\alpha(x)Z_{\pi}}$, hence:

$$\begin{aligned}\int_{\mathcal{X}} \pi(x)(\alpha(x)q(y)(1 - \alpha(x)))\delta_x(y)dx &= \int_{\mathcal{X}} \frac{q(x)}{\alpha(x)Z_{\pi}}(\alpha(x)q(y)(1 - \alpha(x)))\delta_x(y)dx = \\ &= \int_{\mathcal{X}} \frac{q(x)}{\alpha(x)Z_{\pi}}\alpha(x)q(y)dx + \pi(y)(1 - \alpha(y)) = \frac{q(y)}{Z_{\pi}} \int_{\mathcal{X}} q(x)dx + \pi(y)(1 - \alpha(y)) = \\ &= \pi(y)\alpha(y) + \pi(y)(1 - \alpha(y)) = \pi(y)\end{aligned}$$

□

2. Couldn't solve.

Exercise 4 (Gibbs Sampler)

1.

$$\pi(x | y) = \frac{\pi(x, y)}{\pi(y)} \propto \frac{\exp((x-1)^2(y-2)^2)/2}{(y-2)^{-1}} \sim N(1, (y-2)^{-2})$$

Now, follow the same procedure to for $\pi(y | x)$, hence:

$$\pi(y | x) \sim N(2, (x-1)^{-2})$$

□

2. The sampler doesn't make sense, because:

$$\begin{aligned} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \pi(x, y) dx dy &\propto \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp((x-1)^2(y-2)^2)/2 dx dy = \\ &= \int_{-\infty}^{\infty} \sqrt{2\pi}((y-2)^{-2})^{\frac{1}{2}} dy = \infty \end{aligned}$$

□

Exercise 5 (Gibbs Sampler)

1.

$$\begin{aligned}
p(Z_i = z \mid \theta_1, \theta_2) &= p(X_i + Y_i = z \mid \theta_1, \theta_2) = \sum_{y=0}^z p(X_i + Y_i = z \mid Y_i = y, \theta_1, \theta_2) p(Y_i = y \mid \theta_2) = \\
&= \sum_{y=0}^z p(X_i = z - y \mid \theta_1) p(Y_i = y \mid \theta_2) = \sum_{y=0}^z \binom{m_i}{z-y} \theta_1^{z-y} (1-\theta_1)^{m_i-(z-y)} \binom{n_i}{y} \theta_2^y (1-\theta_2)^{n_i-y} \therefore \\
p(Z_1, \dots, Z_T \mid \theta_1, \theta_2) &= \prod_{i=1}^T \left(\sum_{y_i=0}^{z_i} \binom{m_i}{z_i - y_i} \theta_1^{z_i - y_i} (1 - \theta_1)^{m_i - (z_i - y_i)} \binom{n_i}{y_i} \theta_2^{y_i} (1 - \theta_2)^{n_i - y_i} \right)
\end{aligned}$$

□

2. To sample from $p(\theta_1, \theta_2 \mid Z_1, \dots, Z_T)$ we will use auxiliary variables $X_{1:T}, Y_{1:T}$.

$$\begin{aligned}
p(\theta_1 \mid \theta_2, X_{1:T}, Y_{1:T}, Z_{1:T}) &\propto \pi(\theta_1 \mid \theta_2, Y_{1:T}) p(X_{1:T} \mid \theta_1, \theta_2, Y_{1:T}) \propto \\
&\propto \pi(\theta_1) p(X_{1:T} \mid \theta_1) \propto \theta_1^{\sum x_i} (1 - \theta_1)^{\sum m_i - x_i} \therefore
\end{aligned}$$

$$\theta_1 \mid X_{1:T} \sim \text{Beta} \left(1 + \sum_{i=1}^T x_i, 1 + \sum_{i=1}^T m_i - x_i \right)$$

Similarly to θ_2 :

$$\theta_2 \mid Y_{1:T} \sim \text{Beta} \left(1 + \sum_{i=1}^T y_i, 1 + \sum_{i=1}^T n_i - y_i \right)$$

Finally,

$$p(X_{1:T}, Y_{1:T} \mid \theta_1, \theta_2, Z_{1:T}) \propto \prod_{i=1}^T \binom{m_i}{x_i} \theta_1^{x_i} (1 - \theta_1)^{m_i - x_i} \binom{n_i}{y_i} \theta_2^{y_i} (1 - \theta_2)^{n_i - y_i} \mathbb{I}_{\{x_i + y_i = z_i\}}$$

Note that we can now use a Gibbs sampler by first sampling $\theta_1^{(0)}$ and $\theta_2^{(0)}$ from independent $U_{[0,1]}$. Secondly, we can sample $X^{(0)}$ and $Y^{(0)}$ from $p(X_{1:T}, Y_{1:T} \mid \theta_1^{(0)}, \theta_2^{(0)}, Z_{1:T})$, since the distribution found is discrete with finite support, hence, we can calculate the probability for each possible value of $X^{(0)}$ and $Y^{(0)}$. With the values for the auxiliary variables, we sample $\theta_1^{(1)}$ and $\theta_2^{(1)}$ from their posteriors, which is possible since they are Beta distributions. Again we sample X, Y using the updated θ_1, θ_2 and repeat the process. □

Simulation question (Normal mixture model - Gibbs sampling)

1.

$$\begin{aligned}
 P(X_i = x_i \mid p, \mu, \sigma^2) &= \sum_{z_i=1}^k P(X_i = x_i \mid Z_i = z_i, p, \mu, \sigma^2) P(Z_i = z_i \mid p, \mu, \sigma^2) = \\
 &= \sum_{z_i=1}^k \varphi(x_i; \mu_{z_i}, \sigma_{z_i}^2) p_{z_i}
 \end{aligned}$$

□

2.

$$\begin{aligned}
 P(Z_i = z_i \mid X_i, p, \mu, \sigma^2) &\propto P(X_i \mid Z_i, p, \mu, \sigma^2) P(Z_i \mid p, \mu, \sigma^2) \propto \\
 \varphi(x_i; \mu_{z_i}, \sigma_{z_i}^2) p_{z_i} &\propto \frac{\exp\left(\frac{-(x_i - \mu_{z_i})^2}{2\sigma_{z_i}^2}\right)}{\sqrt{2\pi\sigma_{z_i}^2}} p_{z_i}
 \end{aligned}$$

The above distribution is discrete with finite support, hence, one can calculate the value for each z_i and then normalize by the sum, obtaining a probability mass function from which values can be sampled. □

3.

$$P(p \mid X, Z, \mu, \sigma^2) \propto P(X, Z \mid \mu, \sigma^2, p) P(p \mid \mu, \sigma^2) \propto P(X \mid Z, \mu, \sigma^2, p) P(Z \mid \mu, \sigma^2, p) \pi(p)$$

Note that $P(X \mid Z, \mu, \sigma^2, p) \propto \prod_{i=1}^N \phi(x_i; \mu_i, \sigma_i^2)$ is not a function p , so it can be thrown as a constant. Also, $P(Z \mid \mu, \sigma^2, p) = P(Z \mid p)$ therefore:

$$P(p \mid X, Z, \mu, \sigma^2) \propto \pi(p) \prod_{i=1}^N p_{z_i} \propto \prod_{j=1}^K p_j^{\gamma_j - 1} \prod_{i=1}^N p_{z_i}$$

Let $n_j = \sum_{i=1}^N z_i \mathbb{I}_{z_i=j}$, so n_j is the number of times the j -th Gaussian has being picked. Finally:

$$\begin{aligned}
 P(p \mid X, Z, \mu, \sigma^2) &\propto \prod_{j=1}^K p_j^{\gamma_j - 1 + n_j} \\
 p \mid X, Z, \mu, \sigma^2 &\sim \text{Dirichlet}
 \end{aligned}$$

Since the distribution is a Dirichlet, it is known how to sample from it. □

4.

$$\begin{aligned}
P(\mu \mid X, Z, p, \sigma^2) &\propto P(X, Z \mid \mu, p, \sigma^2) P(\mu \mid p, \sigma^2) \propto \\
&P(X \mid Z, \mu, p, \sigma^2) P(Z \mid \mu, p, \sigma^2) \pi(\mu) \propto \\
&\left(\prod_{j=1}^N \exp \left(\frac{-(x_j - \mu_{z_j})^2 p_{z_j}}{2\sigma_{z_j}^2} \right) \right) \prod_{k=1}^K \exp \left(\frac{-(\mu_k - m)^2}{2\tau^2} \right) \propto \\
&\prod_{k=1}^K p_k^{n_k} \exp \left(\frac{-\sum_{i=1}^{n_k} (x_i^{(k)} - \mu_k)^2}{2\sigma_k^2} - \frac{(\mu_k - m)^2}{2\tau^2} \right) \\
&\quad \vdots
\end{aligned}$$

$$P(\mu_k \mid X, Z, p, \sigma^2) \propto \exp \left(\frac{-\sum_{i=1}^{n_k} (x_i^{(k)} - \mu_k)^2}{2\sigma_k^2} - \frac{(\mu_k - m)^2}{2\tau^2} \right)$$

First, note that $x_i^{(k)}$ is the i -th value from X such that $z = k$, in other words, it is the i -th sampled value that came from the k -th Gaussian distribution.

Note that the above equation is the same as updating each Normal prior distribution $\mu_k \sim N(m, \tau^2)$ and $X^{(k)} \mid \mu_k \sim N(\mu_k, \sigma_k^2)$ with σ_k^2 known. Therefore, let \bar{x}_k be the sample average, then:

$$\mu_j \mid X, Z, p, \sigma^2 \sim N \left(\frac{n_k \sigma_k^{-2} \bar{x}_k + \tau^{-2} m}{\tau^{-2} + n_k \sigma_k^{-2}}, [n_k \sigma_k^{-2} + \tau^{-2}]^{-1} \right)$$

□

5.

$$\begin{aligned}
P(\sigma_k^2 \mid X, Z, p, \mu) &\propto P(X \mid Z, p, \mu, \sigma_k^2) P(Z \mid p) \pi(\sigma_k^2) \propto \\
&\frac{p_k^{n_k} \exp \left(\frac{-\sum_{i=1}^{n_k} (x_i - \mu_k)^2}{2\sigma_k^2} \right)}{\sigma_k^{n_k}} \sigma_k^{-\alpha-1} \exp(-\beta \sigma_k^{-2}) \propto \\
&\exp \left(\left[\frac{-\sum_{i=1}^{n_k} (x_i - \mu_k)^2}{2} - \beta \right] \sigma_k^{-2} \right) \sigma_k^{-\alpha-1-\frac{n_k}{2}} \sim \text{Inverse Gamma} \left(\alpha + \frac{n_k}{2}, \beta + \frac{\sum_{i=1}^{n_k} (x_i - \mu_k)^2}{2} \right)
\end{aligned}$$

To sample from the Inverse Gamma, just sample Y from a Gamma with these parameters and then do Y^{-1} . □

6. To sample (y_1, \dots, y_N) from a mixture model, use $p = (p_1, \dots, p_k)$ to sample $Z = (z_1, \dots, z_k)$. Then, sample each y_i from $N(\mu_{z_i}, \sigma_{z_i}^2)$.

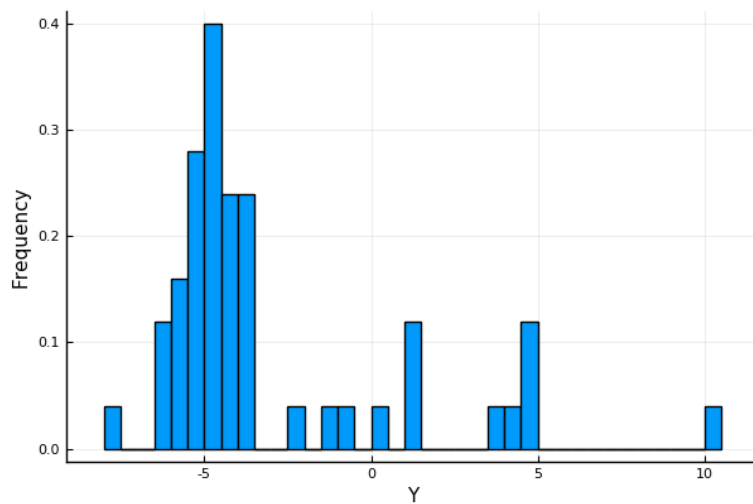


Figure 1: Histogram for 30 samples from Gaussian Mixture model with $\mu = (-5, 0, 5)$, $\sigma^2 = (1, 2, 3)$, $p = (0.5, 0.2, 0.3)$.