Mathematical Foundations of Deep Neural Networks, M1407.001200
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Homework 10
Due 5pm, Wednesday, November 16, 2022

Problem 1: *Log-derivative trick for VAE.* Let $Z \in \mathbb{R}^k$ be a random variable. Let $q_\phi(z)$ be a probability density function for all $\phi \in \mathbb{R}^p$. Assume $q_\phi(z)$ is differentiable in ϕ for all fixed $z \in \mathbb{R}^k$. Let $h\colon \mathbb{R}^k \to \mathbb{R}$ satisfy $h(z) > 0$ for all $z \in \mathbb{R}^k$. Assume that the order of integration and differentiation can be swapped. Show

$$\nabla_\phi \mathbb{E}_{Z\sim q_\phi(z)}\left[\log\left(\frac{h(Z)}{q_\phi(Z)}\right)\right] = \mathbb{E}_{Z\sim q_\phi(z)}\left[(\nabla_\phi \log q_\phi(Z))\log\left(\frac{h(Z)}{q_\phi(Z)}\right)\right].$$

Hint. Since $q_\phi(z)$ is a probability density function,

$$\int \nabla_\phi q_\phi(z)\, dz = \nabla_\phi \int q_\phi(z)\, dz = \nabla_\phi 1 = 0.$$

Solution. Notice that

$$\begin{aligned}
\nabla_\phi \mathbb{E}_{Z\sim q_\phi(z)}\left[\log\left(\frac{h(Z)}{q_\phi(Z)}\right)\right] &= \nabla_\phi \int \log\left(\frac{h(Z)}{q_\phi(Z)}\right) q_\phi(z)\, dz \\
&= \nabla_\phi \left[\mathbb{E}_{Z\sim q_\phi(z)} \log\left(h(Z)\right) - \int \log\left(q_\phi(Z)\right) q_\phi(z)\, dz\right] \\
&= \nabla_\phi \left[\mathbb{E}_{Z\sim q_\phi(z)} \log\left(h(Z)\right)\right] - \nabla_\phi \int \log\left(q_\phi(Z)\right) q_\phi(z)\, dz \\
&= \nabla_\phi \left[\mathbb{E}_{Z\sim q_\phi(z)} \log\left(h(Z)\right)\right] - \int \left[1 + \log\left(q_\phi(Z)\right)\right] \nabla_\phi q_\phi(z)\, dz.
\end{aligned}$$

First, using the log-derivative trick,

$$\nabla_\phi \mathbb{E}_{Z\sim q_\phi(z)}\left[\log\left(h(Z)\right)\right] = \mathbb{E}_{Z\sim q_\phi(z)}\left[\log\left(h(Z)\right) \nabla_\phi q_\phi(z)\right].$$

Next, $q_\phi(z)$ is a probability density function,

$$\int \nabla_\phi q_\phi(z)\, dz = \nabla_\phi \int q_\phi(z)\, dz = \nabla_\phi 1 = 0.$$

Lastly,

$$\begin{aligned}
\int \log\left(q_\phi(Z)\right) \nabla_\phi q_\phi(z)\, dz &= \int \left[\log\left(q_\phi(Z)\right) \nabla_\phi \log(q_\phi(z))\right] q_\phi(z)\, dz \\
&= \mathbb{E}_{Z\sim q_\phi(z)}\left[\log\left(q_\phi(Z)\right) \nabla_\phi \log(q_\phi(z))\right]
\end{aligned}$$

Thus,

$$\begin{aligned}
\nabla_\phi \mathbb{E}_{Z\sim q_\phi(z)}\left[\log\left(\frac{h(Z)}{q_\phi(Z)}\right)\right] &= \mathbb{E}_{Z\sim q_\phi(z)}\left[\log\left(h(Z)\right) \nabla_\phi q_\phi(z)\right] - \mathbb{E}_{Z\sim q_\phi(z)}\left[\log\left(q_\phi(Z)\right) \nabla_\phi \log(q_\phi(z))\right] \\
&= \mathbb{E}_{Z\sim q_\phi(z)}\left[(\nabla_\phi \log q_\phi(Z))\log\left(\frac{h(Z)}{q_\phi(Z)}\right)\right].
\end{aligned}$$

■

Problem 2: *Projected gradient method.* Consider the optimization problem

$$\begin{array}{ll} \underset{x\in\mathbb{R}^n}{\text{minimize}} & f(x) \\ \text{subject to} & x \in C, \end{array}$$

where $C \subset \mathbb{R}^n$. Constrained optimization problems of this type can be solved with the *projected gradient method*

$$x^{k+1} = \Pi_C(x^k - \alpha\nabla f(x^k)),$$

where Π_C is the projection onto C. The projection of $y \in \mathbb{R}^n$ onto $C \subseteq \mathbb{R}^n$ is defined as the point in C that is closest to y:

$$\Pi_C(y) = \underset{x\in C}{\text{argmin}}\,\|x-y\|^2.$$

For the particular set

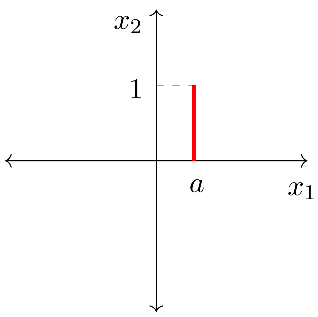
$$C = \{x \in \mathbb{R}^2 \,|\, x_1 = a,\, 0 \le x_2 \le 1\},$$

where $a \in \mathbb{R}$, show that

$$\Pi_C(y) = \begin{bmatrix} a \\ \min\{\max\{y_2, 0\}, 1\} \end{bmatrix},$$

where $y = (y_1, y_2)$.

Solution.



Note that $y \in \mathbb{R}^2$ should be projected on set C. Let $x = \begin{bmatrix} a \\ x_2 \end{bmatrix}$, and $y = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$. Then,

$$\Pi_C(y) = \underset{x\in C}{\text{argmin}}\,\|x-y\|^2 = \begin{bmatrix} a \\ \text{argmin}_{0\le x_2\le 1}(a-y_1)^2 + (x_2-y_2)^2 \end{bmatrix}.$$

If $y_2 \le 0$, $x_2 = 0$. If $0 \le y_2 \le 1$, $x_2 = y_2$. If $y_2 \ge 1$, $x_2 = 1$.
Therefore, $x_2 = \min\{\max\{y, 0\}, 1\}$, and $\Pi_C(y) = \begin{bmatrix} a \\ \min\{\max\{y_2, 0\}, 1\} \end{bmatrix}$. ■

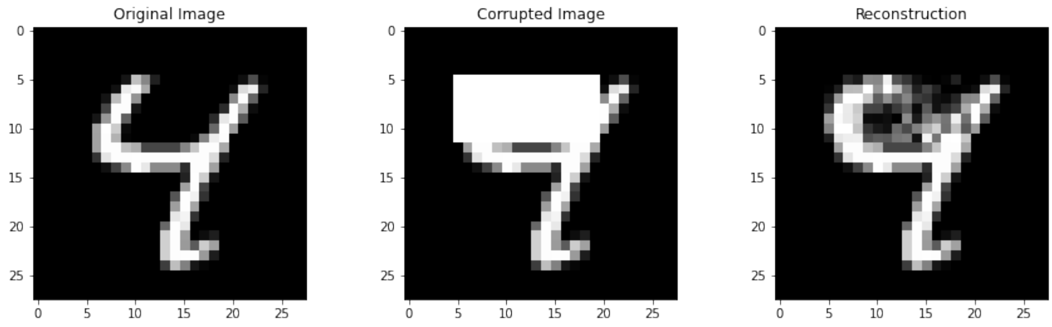


Figure 1: The original, corrupted, and inpainted MNIST image.

Problem 3: *Image inpainting with flow models.* Assume we have a trained flow model that we use to evaluate the likelihood function p. (Since we will not further train or update the flow model, we supress the network parameter θ and write p rather than p_θ.) The starter code `flow_inpainting.py` loads a NICE flow model pre-trained on the MNIST dataset saved in `nice.pt`. Let $X_{\text{true}} \in \mathbb{R}^{28\times 28}$ be an MNIST image with pixel intensities normalized to be in $[0,1]$. Let $M = \{0,1\}^{28\times 28}$ be a binary mask. We measure $M \odot X_{\text{true}}$, where $\odot$ denotes elementwise multiplication, and the goal is to inpaint the missing information $(1-M)\odot X_{\text{true}}$, where $1 - M \in \{0,1\}^{28\times 28}$ is the inverted mask. (See Figure 1.) Perform inpainting by solving the following constrained maximum likelihood estimation problem

$$\begin{array}{ll} \underset{X\in\mathbb{R}^{28\times 28}}{\text{minimize}} & -\log p(X) \\ \text{subject to} & M\odot X = M \odot X_{\text{true}} \\ & 0 \le X \le 1, \end{array}$$

where $0 \le X \le 1$ is enforced elementwise. Use the projected gradient method with learning rate 10^{-3} and 300 iterations.

Hint. Represent the optimization variable with

```
X = image.clone().requires_grad_(True)
```

while preserving `image`, the tensor containing the corrupted image. When manipulating `X` in the projection step, manipulate `X.data` rather than `X` itself so that the computation graph is not altered by the projection step. Use `clamp(...)` to enforce the $0 \le X \le 1$ constraint.

Remark. The optimization problem can be interpreted as finding the most likely reconstruction consistent with the measurements.

Remark. The NICE paper [2] obtains better inpainting results by using a learning rate scheduler (iteration-dependent stepsize) and adding noise to escape from local minima.

Solution. See `flow_inpainting_sol.py`.

Problem 4: *Ingredients of Glow [1].* Let

$$A = PL(U + \operatorname{diag}(s)) \in \mathbb{R}^{C\times C},$$

where $P \in \mathbb{R}^{C\times C}$ is a permutation matrix, $L \in \mathbb{R}^{C\times C}$ is a lower triangular matrix with unit diagonals, $U \in \mathbb{R}^{C\times C}$ is upper triangular with zero diagonals, and $s \in \mathbb{R}^C$. To clarify, $L_{ii} = 1$ for $i = 1,\dots,C$, $L_{ij} = 0$ for $1 \le i < j \le C$, and $U_{ij} = 0$ for $1 \le j \le i \le C$.

(a) Let $f_1(x) = Ax$. Show

$$\log\left|\frac{\partial f_1}{\partial x}\right| = \sum_{i=1}^{C} \log|s_i|.$$

(b) Given $h\colon \mathbb{R}^{a\times b\times c} \to \mathbb{R}^{a\times b\times c}$, define

$$\left|\frac{\partial h(X)}{\partial X}\right| = \left|\frac{\partial(h(X).\text{reshape}(abc))}{\partial(X.\text{reshape}(abc))}\right|,$$

i.e., we define the absolute value of the Jacobian determinant with the input and output tensors vectorized. Note that the reshape operation, which maps elements from the tensor in $\mathbb{R}^{a\times b\times c}$ to the elements of the vector in $\mathbb{R}^{abc}$, is not unique. Show that the definition of $\left|\frac{\partial h(X)}{\partial X}\right|$ does not depend on the specific choice of reshape.

(c) Let $f_2(X \mid P, L, U, s)$ be the 1×1 convolution from $\mathbb{R}^{C\times m\times n}$ to $\mathbb{R}^{C\times m\times n}$ with filter $w \in \mathbb{R}^{C\times C\times 1\times 1}$ defined as

$$w_{i,j,1,1} = A_{i,j}, \qquad \text{for } i = 1,\dots,C,\ j = 1,\dots,C.$$

So $X \in \mathbb{R}^{C\times m\times n}$ and $f_2(X \mid P, L, U, s) \in \mathbb{R}^{C\times m\times n}$. (Assume the batch size is 1.) Show

$$\log\left|\frac{\partial f_2(X \mid P, L, U, s)}{\partial X}\right| = mn\sum_{i=1}^{C} \log|s_i|.$$

(d) Consider the following coupling layer from $X \in \mathbb{R}^{2C\times m\times n}$ to $Z \in \mathbb{R}^{2C\times m\times n}$:

$$\begin{aligned} Z_{1:C,:,:} &= X_{1:C,:,:} \\ Z_{C+1:2C,:,:} &= f_2(X_{C+1:2C,:,:} | P, L(X_{1:C,:,:}), U(X_{1:C,:,:}), s(X_{1:C,:,:})), \end{aligned}$$

where P is a fixed permutation matrix, $L(\cdot)$ outputs lower triangular matrices with unit diagonals in $\mathbb{R}^{C\times C}$, $U(\cdot)$ outputs upper triangular matrices with zero diagonals in $\mathbb{R}^{C\times C}$, and $s(\cdot) \in \mathbb{R}^C$. Show

$$\log\left|\frac{\partial Z}{\partial X}\right| = mn\sum_{i=1}^{C} \log|s_i|.$$

Remark. Given any $A \in \mathbb{R}^{n\times n}$, a decomposition $A = PL(U + \operatorname{diag}(s))$ can be computed via the so-called PLU factorization, which performs steps analogous to Gaussian elimination.

Solution.

(a) First, derivative of linear transformation is the matrix multiplied with the input.Thus

$$\left|\frac{\partial f_1}{\partial x}\right| = |\det(A)|$$

Next, determinant can be split into its multiplicative factors.

$$|\det(A)| = |\det(P)\det(L)\det(U + \operatorname{diag}(s))|$$

Last, determinant value of triangular matrix is the product of its diagonal entries and absolute value of determinant is invariant under any permutation.

$$\begin{aligned}
&|\det(P)| = 1\\
&|\det(L)| = 1\\
&|\det(U + \operatorname{diag}(s))| = \Pi s_i
\end{aligned}$$

Combining all these results above, we get the desired conclusion.

(b) Reshape opereation can yield different values of determinant value of the derivative if the order of indices is changed. But the determinant of derivative is unique up to permutation, so the value of Jacobian determinant is unique since it takes ablsolute value.

(c) If we fix the second and third indices, notice that the 1×1 convolution is exactly the matrix multiplication map f_1 of (a).
Consider $(C \times m \times n) \times (C \times m \times n)$ Jacobian of block matrix

$$\left|\frac{\partial f_2(X \mid P, L, U, s)}{\partial X}\right| =$$

$$\begin{vmatrix}
\frac{\partial f_2(X_{:,1,1} \mid P,L,U,s)}{\partial X_{:,1,1}} & 0 & \cdots & & & & \\
0 & \frac{\partial f_2(X_{:,2,1} \mid P,L,U,s)}{\partial X_{:,2,1}} & 0 & \cdots & & & \\
\vdots & \vdots & \ddots & & & & \\
0 & 0 & 0 & \frac{\partial f_2(X_{:,C,1} \mid P,L,U,s)}{\partial X_{:,C,1}} & 0 & \cdots & \\
0 & 0 & 0 & 0 & \frac{\partial f_2(X_{:,1,2} \mid P,L,U,s)}{\partial X_{:,1,2}} & 0 & \cdots \\
\vdots & \vdots & \vdots & & & &
\end{vmatrix}$$

The Jacobian value of this block matrix all comes from the answer of (a). Since this block matrix has mn rows and mn columns, its value is

$$\left|\frac{\partial f_2(X \mid L, U, s)}{\partial X}\right| = \left(\prod_{i=1}^{C} |s_i|\right)^{mn}.$$

Taking logarithm on both sides of the equation, we get the result.

(d) It easily follows from (b) and the fact that

$$\begin{vmatrix} A & 0 \\ B & C \end{vmatrix} = \det(A)(C).$$

Indeed,

$$
\begin{aligned}
\left|\frac{\partial Z}{\partial X}\right| &= \left|\frac{\partial\left(Z_{1:C,:,:}, Z_{C:2C,:,:}\right)}{\partial\left(X_{1:C,:,:}, X_{C:2C,:,:}\right)}\right| \\
&= \left|\begin{matrix} I & 0 \\ \left|\frac{\partial f_2(X_{C:2C,:,:} \mid P, L, U, s)}{\partial X_{1:C,:,:}}\right| & \left|\frac{\partial f_2(X_{C:2C,:,:} \mid P, L, U, s)}{\partial X_{C:2C,:,:}}\right| \end{matrix}\right| \\
&= \det(I) \left|\frac{\partial f_2(X_{C:2C,:,:} \mid P, L, U, s)}{\partial X_{C:2C,:,:}}\right|.
\end{aligned}
$$

Hence

$$
\log\left|\frac{\partial Z}{\partial X}\right| = \log\left|\frac{\partial f_2(X_{C:2C,:,:} \mid P, L, U, s)}{\partial X_{C:2C,:,:}}\right| = mn\sum_{i=1}^{C}\log|s_i|.
$$

■

Problem 5: *Gambler's ruin.* You are a gambler at a casino with a starting balance of 100$. You will play a game in which you bet 1$ every game. With probability 18/37, you win and collect 2$ (so you make a 1$ profit). With probability 19/37, you lose and collect no money. You play until you reach a balance of 0$ or 200$ or until you play 600 games. Write a Monte Carlo simulation with importance sampling to estimate the probability that you leave the casino with 200$. Specifically, simulate playing up to 600 games until you reach the balance of 0$ or 200$ and repeat this $N = 3000$ times.

Hint. Regardless of the outcome, simulate $K = 600$ games. The outcomes of the games form a sequence of Bernoulli random variables with probability mass function

$$
f(X_1, \ldots, X_K) = \prod_{i=1}^{K} p^{X_i}(1-p)^{(1-X_i)}
$$

and $p = 18/37$. For the sampling distribution, also use a sequence of Bernoulli random variables with probability mass function

$$
g(Y_1, \ldots, Y_K) = \prod_{i=1}^{K} q^{Y_i}(1-q)^{(1-Y_i)}
$$

but with $q > p$. Try using $q = 0.55$.

Hint. The answer is approximately 2×10^{-6}. Submit Python code that produces this answer.

Solution. See `prob5.py`. ■

Problem 6: Solve

$$
\begin{array}{ll}
\underset{\mu,\sigma\in\mathbb{R}}{\text{minimize}} & \mathbb{E}_{X\sim\mathcal{N}(\mu,\sigma^2)}[X\sin(X)] + \frac{1}{2}(\mu-1)^2 + \sigma - \log\sigma \\
\text{subject to} & \sigma > 0
\end{array}
$$

using SGD combined with

(a) the log-derivative trick and

(b) the reparameterization trick.

Hint. Use the change of variables $\sigma = e^\tau$ to remove the constraint $\sigma > 0$.

Clarification. Implement SGD in Python and submit the code.

Solution. To remove the constraint, apply change of variables $\sigma = e^\tau$, then the equivalent problem is

$$\underset{\mu,\tau\in\mathbb{R}}{\text{minimize}} \quad \mathbb{E}_{X\sim\mathcal{N}(\mu,e^{2\tau})}[X\sin(X)] + e^\tau - \tau + \mu - 1.$$

(a) First, use the log-derivative. The log-pdf of $\mathcal{N}(\mu, e^{2\tau})$ is

$$\log f(x,\mu,e^{2\tau}) = -\frac{1}{2}\log(2\pi) - \tau - \frac{1}{2}\frac{(x-\mu)^2}{e^{2\tau}}.$$

The derivative of log-pdf of $\mathcal{N}(\mu, e^{2\tau})$ is

$$\begin{aligned}
\nabla_\mu \log f(x,\mu,e^{2\tau}) &= \frac{x-\mu}{e^{2\tau}} \\
\nabla_\tau \log f(x,\mu,e^{2\tau}) &= -1 + \frac{(x-\mu)^2}{e^{2\tau}}.
\end{aligned}$$

Thus, the gradient of the given problem is

$$\begin{aligned}
\nabla_\mu \left[\mathbb{E}_{X\sim\mathcal{N}(\mu,e^{2\tau})}[X\sin(X)] - \tau\right] &= \mathbb{E}_{X\sim\mathcal{N}(\mu,e^{2\tau})}\left[X\sin(X)\frac{X-\mu}{e^{2\tau}} + \mu - 1\right] \\
\nabla_\tau \left[\mathbb{E}_{X\sim\mathcal{N}(\mu,e^{2\tau})}[X\sin(X)] - \tau\right] &= \mathbb{E}_{X\sim\mathcal{N}(\mu,e^{2\tau})}\left[X\sin(X)\left(-1 + \frac{(X-\mu)^2}{e^{2\tau}}\right) + e^\tau - 1\right].
\end{aligned}$$

For the SGD, perform

$$\begin{aligned}
&X_1, X_2, ..., X_B \sim \mathcal{N}(\mu^k, e^{2\tau^k}) \\
&\mu^{k+1} = \mu^k - \alpha\frac{1}{B}\sum_{i=1}^{B}\left[X_i\sin(X_i)\frac{X_i-\mu^k}{e^{2\tau^k}} + \mu - 1\right] \\
&\tau^{k+1} = \tau^k - \alpha\frac{1}{B}\sum_{i=1}^{B}\left[X_i\sin(X_i)\left(-1 + \frac{(X_i-\mu^k)^2}{e^{2\tau^k}}\right) + e^\tau - 1\right].
\end{aligned}$$

(b) Now, for the reparameterization trick,

$$\mathbb{E}_{X\sim\mathcal{N}(\mu,e^{2\tau})}[X\sin(X)] = \mathbb{E}_{Z\sim\mathcal{N}(0,1)}[(e^\tau Z + \mu)\sin(e^\tau Z + \mu)]$$

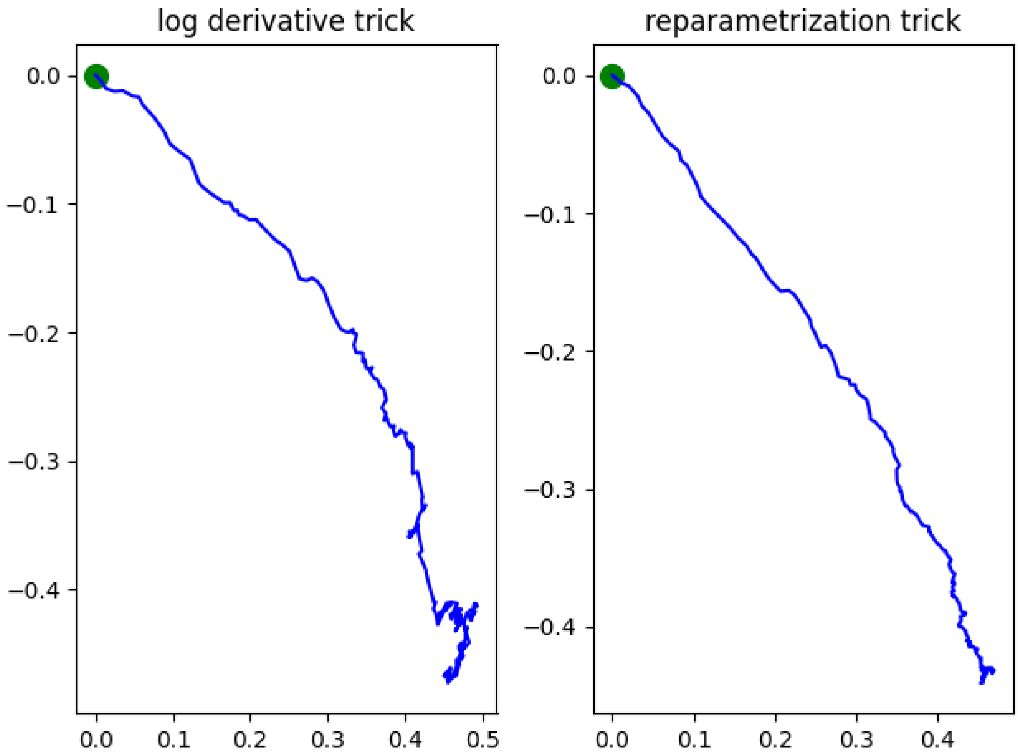
Thus, the gradient of the given problem is

$$\begin{aligned}
&\nabla_\mu\left[\mathbb{E}_{X\sim\mathcal{N}(\mu,e^{2\tau})}[X\sin(X)] + \sigma - \log\sigma + \frac{1}{2}(\mu-1)^2\right] \\
&\quad = \mathbb{E}_{Z\sim\mathcal{N}(0,1)}[(e^\tau Z + \mu)\cos(e^\tau Z + \mu) + \sin(e^\tau Z + \mu)] + \mu - 1 \\
&\nabla_\tau\left[\mathbb{E}_{X\sim\mathcal{N}(\mu,e^{2\tau})}[X\sin(X)] + \sigma - \log\sigma + \frac{1}{2}(\mu-1)^2\right] \\
&\quad = \mathbb{E}_{Z\sim\mathcal{N}(0,1)}\left[e^\tau Z\left\{\sin(e^\tau Z + \mu) + (e^\tau Z + \mu)\cos(e^\tau Z + \mu)\right\}\right] + e^\tau - 1.
\end{aligned}$$

For the SGD, perform

$$
\begin{aligned}
&Z_1, Z_2, ..., Z_B \sim \mathcal{N}(0,1) \\
&\mu^{k+1} = \mu^k - \alpha \frac{1}{B} \sum_{i=1}^{B} \left[(e^{\tau^k} Z_i + \mu^k) \cos(e^{\tau^k} Z_i + \mu^k) + \sin(e^{\tau^k} Z_i + \mu^k) + \mu^k - 1 \right] \\
&\tau^{k+1} = \tau^k - \alpha \frac{1}{B} \sum_{i=1}^{B} \left[e^{\tau^k} Z_i \left\{ \sin(e^{\tau^k} Z_i + \mu^k) + (e^{\tau^k} Z_i + \mu^k) \cos(e^{\tau^k} Z_i + \mu^k) \right\} + e^{\tau^k} - 1 \right]
\end{aligned}
$$

The implementation of SGD by python is done in the prob6.py file. Following figure is the path by (μ, τ) using log-derivative trick and reparameterization trick.



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References

[1] D. P. Kingma and P. Dhariwal, Glow: Generative flow with invertible 1x1 convolutions, *NeurIPS*, 2018.

[2] L. Dinh, D. Krueger, and Y. Bengio, NICE: Non-linear independent components estimation, *ICLR Workshop*, 2015.