

矩阵求导 Matrix cookbook

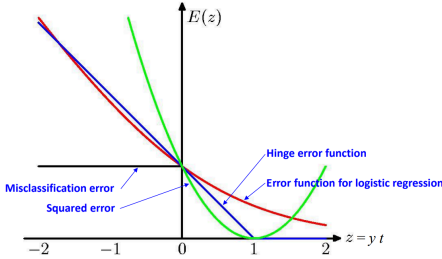
$\partial(X^T) = (\partial X)^T, \partial(X^{-1}) = -X^{-1}(\partial X)X^{-1}$

$\frac{\partial a^T X b}{\partial X} = ab^T, \frac{\partial (Xb+c)^T D(Xb+c)}{\partial X} = (D+D^T)(Xb+c)b^T, \frac{\partial \text{Tr}(AX^T B)}{\partial X} = BA$

$\frac{\partial \text{Tr}(AXBX^T C)}{\partial X} = A^T C^T X B^T + C A X B, \frac{\partial a^T X^{-1} b}{\partial X} = -X^{-T} a b^T X^{-T}$

误差函数 Error Function

Name	Equation	Application
MAE/L1 Loss	$\frac{1}{N} \sum y_i - \hat{y}_i $	/
MSE/L2 Loss	$\frac{1}{N} \sum (y_i - \hat{y}_i)^2$	Linear R
Cross-Entropy	$\sum y_i \ln(y_i) + (1 - y_i) \ln(1 - y_i)$	Logistic R/C
Hinge Loss	$\max(0, 1 - \hat{y}y)$	SVM
KL Divergence	$D_{\text{KL}}(p\ q) = -\sum_x p(x) \ln \frac{q(x)}{p(x)}$	EM
Neg Likelihood	$-\ln p$	Any



多元高斯分布 Multivariate Gaussian

$\mathcal{N}(x|\mu, \Sigma) = \frac{1}{(2\pi)^{\frac{D}{2}}} \frac{1}{|\Sigma|^{\frac{1}{2}}} \exp\left\{-\frac{1}{2}(x - \mu)^T \Sigma^{-1}(x - \mu)\right\}$

$\ln p(x|\mu, \sigma^2) = -\frac{1}{2\sigma^2} \sum_{n=1}^N (x_n - \mu)^2 - \frac{N}{2} \ln \sigma^2 - \frac{N}{2} \ln(2\pi)$

$\ln p(t|x, w, \beta) = -\frac{\beta}{2} \sum_{n=1}^N \{y(x_n, w) - t_n\}^2 + \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi)$

神经网络回归最大后验 Neural Networks Regression MAP

$E(w) = -\ln p(w|t) = \frac{\alpha}{2} w^T w + \frac{\beta}{2} \sum_{n=1}^N (y(x_n, w) - t_n)^2 + C$

$\nabla E(w) = \alpha w + \beta \sum_{n=1}^N (y_n - t_n) \nabla_w y(x, w)_n$

$A = \nabla \nabla E(w) = \alpha I + \beta H, H$: Hessian of Sum of Error function

$w_{\text{MAP}} \leftarrow w^{\text{new}} = w^{\text{old}} - A^{-1} \nabla E(w), q(w) = \mathcal{N}(w|w_{\text{MAP}}, A^{-1})$

$y(x, w) \simeq y(x, w_{\text{MAP}}) + g_{\text{MAP}}^T (w - w_{\text{MAP}})$

$p(t|x, w, \beta) = \mathcal{N}(t|y(x, w), \beta^{-1})$

$p(t|x, D, \alpha, \beta) = \mathcal{N}(t|y(x, w_{\text{MAP}}), g_{\text{MAP}}^T A^{-1} g_{\text{MAP}} + \beta^{-1})$

$g = \nabla_w y(x, w)$

神经网络分类最大后验 Neural Networks Classification MAP

$E(w) = \frac{\alpha}{2} w^T w - \sum_{n=1}^N (t_n \ln y_n + (1 - t_n) \ln(1 - y_n))$

$\nabla E(w) = \alpha w + \sum_{n=1}^N (y_n - t_n) g_n, A = \nabla \nabla E(w) = \alpha I + H$

$w_{\text{MAP}} \leftarrow w^{\text{new}} = w^{\text{old}} - A^{-1} \nabla E(w), q(w) = \mathcal{N}(w|w_{\text{MAP}}, A^{-1})$

$p(t|x, \mathcal{D}) \simeq p(t|x, w_{\text{MAP}}), y(x, w) \simeq y_{\text{MAP}}(x) + g^T (w - w_{\text{MAP}})$

最大边界分类器 Maximum Margin Classifier

Origin: $\text{argmax}_{w,b} \left\{ \frac{1}{\|w\|} \min_n [t_n (w^T \phi(x_n) + b)] \right\}$

Dual: $\text{argmin}_{w,b} \frac{1}{2} \|w\|^2$ subject to $t_n (w^T \phi(x_n) + b) \geq 1, n = 1 \dots N$

Lagrange: $L(w, b, a) = \frac{1}{2} \|w\|^2 - \sum_{n=1}^N a_n \{t_n (w^T \phi(x_n) + b) - 1\}$

Constraints: $a_n = 0$ or $a_n \neq 0 \cap t_n (w^T \phi(x_n) + b) = 1$

Let $\frac{\partial L}{\partial w} = \frac{\partial L}{\partial b} = 0, w = \sum_{n=1}^N a_n t_n \phi(x_n), \sum_{n=1}^N a_n t_n = 0$

Classifier: $y(x) = \sum_{n=1}^N a_n t_n k(x, x_n) + b, k(x, x_n) = \phi(x)^T \phi(x_n)$

quadratic: $\tilde{L}(a) = \sum_{n=1}^N a_n - \frac{1}{2} \sum_{n=1}^N \sum_{m=1}^N a_n a_m t_n t_m k(x_n, x_m), \sum_{n=1}^N a_n t_n = 0$

软边界分类器 Soft Margin Classifier

$t_n y(x_n) \geq 1 - \xi_n$. Minimize: $C \sum_{n=1}^N \xi_n + \frac{1}{2} \|w\|^2$.

$L(w, b, a) = \frac{1}{2} \|w\|^2 + C \sum_{n=1}^N \xi_n - \sum_{n=1}^N a_n \{t_n y(x_n) - 1 + \xi_n\} - \sum_{n=1}^N \mu_n \xi_n$

KKT conditions: $\mu_n \geq 0, \xi_n \geq 0, \mu_n \xi_n = 0$

$a_n \geq 0, t_n y(x_n) \geq 1 - \xi_n, a_n (t_n y(x_n) - 1 + \xi_n) = 0$

Let $\frac{\partial L}{\partial w} = \frac{\partial L}{\partial b} = \frac{\partial L}{\partial \xi_n} = 0,$

$w = \sum_{n=1}^N a_n t_n \phi(x_n), \sum_{n=1}^N a_n t_n = 0, a_n = C - \mu_n$

ν-支持向量机 ν-SVM

$\tilde{L}(a) = \sum_{n=1}^N a_n - \frac{1}{2} \sum_{n=1}^N \sum_{m=1}^N a_n a_m t_n t_m k(x_n, x_m), \sum_{n=1}^N a_n t_n = 0$

subject to $0 \leq a_n \leq \frac{1}{N}, \sum_{n=1}^N a_n t_n = 0, \sum_{n=1}^N a_n \geq \nu$

相关向量机 Relevance Vector Machine

$p(t|x, w, \beta) = \mathcal{N}(t|y(x), \beta^{-1}), y(x) = \sum_{n=1}^N w_n k(x, x_n) + b$

$p(t|X, w, \beta) = \prod_{n=1}^N p(t_n|x_n, w, \beta^{-1})$

$p(w|\alpha) = \prod_{n=1}^N \mathcal{N}(w_i|0, \alpha_i^{-1})$

K-均值聚类 K-means

$J = \sum_{n=1}^N \sum_{k=1}^K r_{nk} \|x_n - \mu_k\|^2, \mu_k = \frac{\sum_n r_{nk} x_n}{\sum_n r_{nk}}$

高斯混合模型 Gaussian Mixture Model

PDF: $p(x) = \sum_{k=1}^K \pi_k \mathcal{N}(x|\mu_k, \Sigma_k)$

E: responsibility $\gamma(z_{nk}) = \frac{\pi_k \mathcal{N}(x_n|\mu_k, \Sigma_k)}{\sum_j \pi_j \mathcal{N}(x_n|\mu_j, \Sigma_j)}$

M: $N_k = \sum_{n=1}^N \gamma(z_{nk})$

$\mu_k = \frac{1}{N_k} \sum_{n=1}^N \gamma(z_{nk}) x_n$

$\Sigma_k = \frac{1}{N_k} \sum_{n=1}^N \gamma(z_{nk}) (x_n - \mu_k)(x_n - \mu_k)^T$

$\pi_k = \frac{N_k}{N}$

log-likelihood: $\ln p(X|\mu, \Sigma, \pi) = \sum_{n=1}^N \ln \left\{ \sum_{k=1}^K \pi_k \mathcal{N}(x|\mu_k, \Sigma_k) \right\}$

伯努利混合模型 Mixtures of Bernoulli Distributions

$p(x|z, \mu) = \prod_{k=1}^K p(x|\mu_k)^{z_k}, p(z|\pi) = \prod_{k=1}^K \pi_k^{z_k}$

$\ln p(X|\mu, \pi) = \sum_{n=1}^N \ln \left\{ \sum_{k=1}^K \pi_k p(x_n|\mu_k) \right\}$

E: $\gamma(z_{nk}) = \mathbb{E}[z_{nk}] = \frac{\pi_k p(x_n|\mu_k)}{\sum_{j=1}^K \pi_j p(x_n|\mu_j)}$

M: $N_k = \sum_{n=1}^N \gamma(z_{nk}), \pi_k = \frac{N_k}{N}, \mu_k = \bar{x}_k = \frac{1}{N_k} \sum_{n=1}^N \gamma(z_{nk}) x_n$

通用 EM 算法 EM Algorithm in General

Difficult to optimize $p(X|\theta)$, easy to optimize $p(X, Z|\theta)$.

$\ln p(X|\theta) = \mathcal{L}(q, \theta) + \text{KL}(q\|p) = \sum_Z q(Z) \ln \frac{p(X, Z|\theta)}{q(Z)} - \sum_Z q(Z) \ln \frac{p(Z|X, \theta)}{q(Z)}$

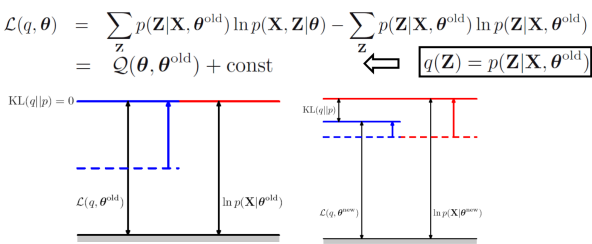
$\text{KL}(q\|p) \geq 0 \Rightarrow \mathcal{L}(q, \theta) \leq \ln p(X|\theta)$

E: Fix $\theta^{\text{old}}, \mathcal{L}(q, \theta^{\text{old}})$ maximized when $\text{KL}(q\|p) = 0, q(Z) = p(Z|X, \theta^{\text{old}})$

M: Fix $q(Z), \mathcal{L}(q, \theta^{\text{old}})$ maximized by updating θ making $\text{KL}(q\|p) > 0$

Q function: $Q(q, \theta^{\text{old}}) = \sum_Z p(Z|X, \theta^{\text{old}}) \ln p(X, Z|\theta)$

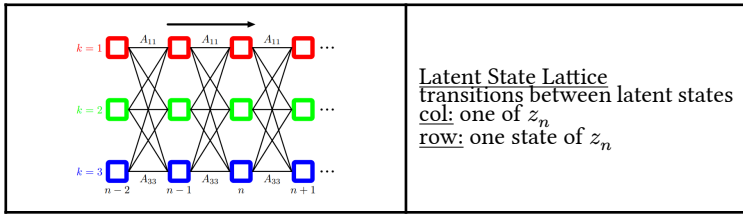
$\theta^{\text{new}} = \text{argmax}_{\theta} Q(q, \theta^{\text{old}})$



隐马尔可夫模型 Hidden Markov Model

PDF: $p(\{x_N\}, \{z_N\}) = p(z_1) \left[\prod_{n=2}^N p(z_n|z_{n-1}) \right] \prod_{n=1}^N p(x_n|z_n)$

$p(z_n = k|z_{n-1} = j) = A_{jk}, p(x_t|z_n = k) = \mathcal{N}(x_t|\mu_k, \Sigma_k), p(z_1 = k) = \pi_k$



E: forward: $\alpha(z_n) = p(x_{1...N}, z_n) = p(x_n | z_n) \sum_{z_{n-1}} \alpha(z_{n-1}) p(z_n | z_{n-1})$

back: $\beta(z_n) = p(x_{n+1...N} | z_n) = \sum_{z_{n+1}} \beta(z_{n+1}) p(x_{n+1} | z_{n+1}) p(z_{n+1} | z_n)$

$\gamma(z_{nk}) = \sum_z \gamma(z) z_{nk}$

$\xi(z_{n-1,j}, z_{nk}) = \sum_z \gamma(z) z_{n-1,j} z_{nk}$

$\gamma(z_n) = p(z_n | \mathbf{X}) = \frac{p(\mathbf{X} | z_n) p(z_n)}{p(\mathbf{X})} = \frac{\alpha(z_n) \beta(z_n)}{p(\mathbf{X})}, p(\mathbf{X}) = \sum_{z_n} \alpha(z_n) \beta(z_n)$

$x = \xi(z_{n-1}, z_n) = \frac{\alpha(z_{n-1}) p(x_n | z_{n-1}) p(z_n | z_{n-1}) \beta(z_n)}{p(\mathbf{X})}$

$p(\mathbf{X}) = \sum_{z_n} \alpha(z_n) \beta(z_n) = \sum_{z_N} \alpha(z_N)$

M: $Q(\theta, \theta^{\text{old}}) = \sum_Z p(Z | X, \theta^{\text{old}}) \ln p(X, Z | \theta) = \sum_{k=1}^K \gamma(z_{1k}) \ln \pi_k +$

$\sum_{n=2}^N \sum_{j=1}^K \sum_{k=1}^K \xi(z_{n-1,j}, z_{nk}) \ln A_{jk} + \sum_{n=2}^N \sum_{k=1}^K \gamma(z_{nk}) \ln p(x_n | \phi_k)$

$\pi_k = \frac{\gamma(z_{1k})}{\sum_{j=1}^K \gamma(z_{1j})}, A_{jk} = \frac{\sum_{n=2}^N \xi(z_{n-1,j}, z_{nk})}{\sum_{l=1}^K \sum_{n=2}^N \xi(z_{n-1,j}, z_{nl})}, \mu_k = \frac{\sum_{n=1}^N \gamma(z_{nk}) x_n}{\sum_{n=1}^N \gamma(z_{nk})}$

$\Sigma_k = \frac{\sum_{n=1}^N \gamma(z_{nk}) (x_n - \mu_k) (x_n - \mu_k)^T}{\sum_{n=1}^N \gamma(z_{nk})}$ or $B_{km} = \frac{\sum_{n=1}^N \gamma(z_{nk}) |x_n = m}{\sum_{l=1}^K \sum_{n=1}^N \gamma(z_{nl}) |x_n = m}$

Trans $\begin{bmatrix} .6 & .3 \\ .4 & .7 \end{bmatrix}$, Emit $\begin{bmatrix} .8 & .1 \\ .2 & .9 \end{bmatrix}$, $\pi = [.5, .5]$, $Z : \{\text{bull, bear}\}$, $X : \{\text{up, up, down}\}$

Evaluation: Sum-Product

$\alpha(z_1) = \begin{bmatrix} .8 \\ .1 \end{bmatrix} \circ \begin{bmatrix} .5 \\ .5 \end{bmatrix} = \begin{bmatrix} .4 \\ .05 \end{bmatrix}, \alpha(z_2) = \begin{bmatrix} .8 \\ .1 \end{bmatrix} \circ \begin{bmatrix} .6 \times .4 + .3 \times .05 \\ .4 \times .4 + .7 \times .05 \end{bmatrix} = \begin{bmatrix} .204 \\ .0195 \end{bmatrix}$

$\beta(z_3) = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \beta(z_2) = \begin{bmatrix} .2 \times .6 \times 1 + .9 \times .4 \times 1 \\ .2 \times .3 \times 1 + .9 \times .7 \times 1 \end{bmatrix} = \begin{bmatrix} .48 \\ .69 \end{bmatrix}, \beta(z_1) = \begin{bmatrix} .8 \times .6 \times .48 + .1 \times .4 \times .69 \\ .8 \times .3 \times .48 + .1 \times .7 \times .69 \end{bmatrix}$

Decoding: Max-Product

$\delta(z_1) = \begin{bmatrix} .8 \\ .1 \end{bmatrix} \circ \begin{bmatrix} .5 \\ .5 \end{bmatrix}, \delta(z_2) = \begin{bmatrix} .8 \\ .1 \end{bmatrix} \circ \begin{bmatrix} .4 \times .6 \\ .4 \times .4 \end{bmatrix}, \delta(z_3) = \begin{bmatrix} .2 \\ .9 \end{bmatrix} \circ \begin{bmatrix} .192 \times .6 \\ .192 \times .4 \end{bmatrix}$

Predict: $p(x_{N+1} | X) = \frac{1}{p(X)} \sum_{z_{N+1}} p(x_{N+1} | z_{N+1}) \sum_{z_N} p(z_{N+1} | z_N) \alpha(z_N)$

马尔可夫决策过程 Markov Decision Process

T-policy: $\pi_T(x) = \arg\max_u [r(x, u) + \int V_{T-1}(x') p(x' | u, x) dx']$

T-value: $V_T(x) = \gamma \max_u [r(x, u) + \int V_{T-1}(x') p(x' | u, x) dx']$

Value iteration: $\hat{V} \leftarrow \gamma \max_u [r(x, u) + \int \hat{V}_{T-1}(x') p(x' | u, x) dx']$

Policy: $R_T^\pi(x_t) = E \left[\sum_{\tau=1}^T \gamma^\tau r_{t+\tau} | u_{t+\tau} = \pi(z_{1:t+\tau-1} u_{1:t+\tau-1}) \right]$

Bellman equation: Optimize $v_*(s) = \max_{a \in \mathcal{A}} q_*(s, a)$

$v_\pi(s) = \sum_{a \in \mathcal{A}} \pi(s, a) q_\pi(s, a)$

$v_\pi(s) = E[r_{t+1} + \gamma v_\pi(S_{t+1}) | S_t = s]$

$q_\pi(s, a) = E[r_{t+1} + \gamma v_\pi(S_{t+1}, A_{t+1}) | S_t = s, A_t = a]$

$q_*(s, a) = r(s, a) + \gamma \sum_{s' \in \mathcal{S}} p(s' | s, a) v_*(s')$

常用分布 Distributions

Beta: $\text{Beta}(\mu | a, b) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \mu^{a-1} (1-\mu)^{b-1}$

Dirichlet: $\text{Dir}(\mu | \alpha) = \frac{\Gamma(\alpha_0)}{\Gamma(\alpha_1) \dots \Gamma(\alpha_K)} \prod_{k=1}^K \mu_k^{\alpha_k-1}, \alpha_0 = \sum_{k=1}^K \alpha_k$

Student-t: $\text{St}(x | \mu, \lambda, \nu) = \frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})} \left(\frac{\lambda}{\pi \nu} \right)^{\frac{1}{2}} \left(1 + \frac{\lambda(x-\mu)^2}{\nu} \right)^{-\frac{\nu+1}{2}}$

Gamma: $\Gamma(x) = \int_0^\infty t^{x-1} e^{-t} dt$

计算题 Numerical Calculation

1. Linear Regression for Least Square:

$y = ax + b$ and three points $\{(1, 0), (3, 3), (5, 4)\}$ using pseudo-inverse.

$$\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 3 & 1 \\ 5 & 1 \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ 3 \\ 4 \end{bmatrix} \Rightarrow \begin{bmatrix} 1 & 1 \\ 3 & 1 \\ 5 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 0 \\ 3 \\ 4 \end{bmatrix} \Rightarrow \begin{bmatrix} 1 & 3 & 5 \\ 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 3 & 1 \\ 5 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 1 & 3 & 5 \\ 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ 3 \\ 4 \end{bmatrix}$$

2. Maximum Margin Classifier:

$\mathcal{C}_1 = \{(1,2), (2,2)\}$ and $\mathcal{C}_2 = \{(4,4), (5,6)\}$ find support vectors and decision boundary function.

Support vectors are $\{(2,2), (4,4)\}$ (can be decided by checking whether deletion will change the boundary), the decision boundary is trivial.

3. Clustering:

$\{(1,2), (2,2), (4,4), (5,6)\}$ for 2-class clustering

Randomly pick 2 center $[(1.5, 2)$ and $(4.5, 5.5)$, for this problem to achieve 1 iteration convergence] then calculate distance of each data point to assign the class. Clac mean coordinate of data points as the new center of cluster.

Reinforcement Learning for MDP

1. What is the Bellman equation? How to solve the Bellman equation?

$v_\pi(s) = E[r_{t+1} + \gamma v_\pi(S_{t+1}) | S_t = s]$. Analytical sol: $\mathcal{V} = (I - \gamma \mathcal{P})^{-1} R$ using Guassian, can also be solved by dynamic programming, Monte-Carlo method, and temporal difference method.

What are the differences between policy iteration and value iteration? What are their advantages and disadvantages respectively?

- Policy iteration:** Policy evaluation + policy enhancement. (Attach equations to explain) Policy evaluation in the policy iteration uses the Bellman expectation equation to obtain the state value function of a policy, which is a dynamic planning process; while the value iteration directly uses the Bellman optimization equation for dynamic planning to obtain the final optimal state value.
- Value iteration:** (Attach equations to explain) Only one round of value updates in the policy evaluation, then do policy enhancements based directly on the updated values. Finally use T-policy (refer to MDP) to obtain the optimal policy.

Policy Iteration	Value Iteration
Complex algorithm	Simple algorithm
Cheaper to compute	Expensive to compute
Faster convergence	Slower convergence

3. What is the model-free reinforcement learning? How to achieve the model-free reinforcement learning? Please use specific examples to illustrate your points.

Methods that agent can only learn through data that comes from interacting with the environment is called model-free reinforcement learning (Sarsa and Q-learning).

Application: Complex environment like E-sport games.

4. What are the differences between on-line and off-line RL? What are their advantages and disadvantages respectively? Please use specific examples to illustrate your points.

Online RL: Learning from the data that sampled from the environment by the current policy, and once the policy is updated, the data points will be deprecated. (E.g. Sarsa, policy is greedy)

Offline RL: Use experience recall pool to store and reuse the historical samples (E.g. Q-learning). Offline RL can better make use of historical data and obtain lower complexity of sample, i.e. use smaller amount of data to achieve convergence.

复习课

$\ln p(X, Z | \theta) = \ln p(Z | X, \theta) + \ln p(X | \theta)$

EM:

$\ln p(x | \theta) = \ln(\sum p(x, z | \theta)), z: \text{latent}$

Jason inequivalence: $> = \sum_z p(z | x, \theta^{\text{old}}) \ln p(x, z | \theta) = Q(\theta, \theta^{\text{old}})$

$\theta^* = \arg\max Q(\theta, \theta^{\text{old}})$

KL divergence:

$\int q(z) \ln \frac{p(x, z | \theta)}{q(z)} dz - \int q(z) \ln \frac{p(z | x, \theta)}{q(z)} dz = \ln p(x | \theta)$

$\int q(z) \ln \frac{p(x, z | \theta)}{q(z)} dz = Q(\theta, \theta^{\text{old}}) + \text{const}$

non-convex EM, not converge to global maximum or may not converge

Policy iteration: $R_T^\pi(x_n) = \sum_{t=1}^T r(x_{n+t}, a_{n+t}), a_{n+t} = \pi(x_{n+t})$

Contributors (in no particular order)

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