Beyond Worst-Case Mixing Times for Markov Chains
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Convergence of MCMC

Definition (Total variation distance). Let $X$ and $Y$ be two random variables taking values in a set $\Omega$. The total variation distance between them is defined by
\[ d_{TV}(X, Y) = \sup_{A \subseteq \Omega} |P(X \in A) - P(Y \in A)|. \]

Definition (Absolute spectral gap). If $P \in \mathbb{R}^{d \times d}$ is the transition matrix of an irreducible, aperiodic, and reversible Markov chain, with eigenvalues
\[ 1 = \lambda_1 > \lambda_2 \geq \cdots \geq \lambda_d \geq -1, \]
the absolute spectral gap is defined by
\[ \gamma = 1 - \max_{j \neq 1} |\lambda_j|. \]

Theorem 1. If $(X_n)$ is an irreducible, aperiodic, and reversible Markov chain, and $\pi_n$ denotes the distribution of $X_n$, then
\[ d_{TV}(\pi_n, \pi) \leq \left( 1 - \frac{\gamma}{\sqrt{\min}} \right)^n \cdot d_{TV}(\pi_0, \pi). \]

Why is MCMC so hard?

Total variation is a worst-case measure of distance.

Theorem 2. If $X$ and $Y$ are random variables taking values in a set $\Omega$, the total variation distance between them satisfies
\[ d_{TV}(X, Y) = \sup_{f \in [0, 1]} |Ef(X) - Ef(Y)|. \]

Yet often we only care about very simple functions.

- Posterior mean corresponds to $f = x$.
- In a mixture model with cluster membership vector $z$, cluster co-membership probabilities correspond to $f = 1(z_i = z_j)$ for data indices $i \neq j$.

Function mixing

Instead, convergence with respect to individual functions.

Definition (Function variation distance). Let $X$ and $Y$ be two random variables taking values in a set $\Omega$ and let $f : \Omega \to [0, 1]$. The function variation distance with respect to $f$ is then defined by
\[ d_f(X, Y) = |Ef(X) - Ef(Y)|. \]

Definition (Function absolute spectral gap). Let $\eta_f$ be the (left) eigenvectors of the transition matrix $P$ and let $f : [d] \to [0, 1]$ be a function. Then the function absolute spectral gap is defined by
\[ \eta_f = 1 - \max_{j \neq 1} |\lambda_j|. \]

In words, it is the gap between $f$ and the largest absolute value of an eigenvalue whose eigenspace $f$ is not orthogonal to.

The function absolute spectral gap controls the rate of convergence in $d_f$.

Theorem 3. If $(X_n)$ is an irreducible, aperiodic, and reversible Markov chain with state space $[d]$, $\pi_n$ denotes the distribution of $X_n$, and $f : [d] \to [0, 1]$, then
\[ d_f(\pi_n, \pi) \leq \left( 1 - \frac{\eta_f}{\sqrt{\min}} \right)^n \cdot d_f(\pi_0, \pi). \]

Application: concentration of measure

Previous results give a single rate for all functions.

Theorem 4 (Uniform Hoeffding bound, Léon and Perron 2004). Let $(X_n)$ be an irreducible, aperiodic, and reversible Markov chain at equilibrium, and let $f : [d] \to [0, 1]$ be a function. If $\mu = E_\pi[f]$ is the equilibrium expectation of $f$, then
\[ P\left( \frac{1}{N} \sum_{i=1}^{N} f(X_i) - \mu \right) \geq \epsilon \leq 2 \exp\left( -\frac{\gamma_0}{2(\gamma_0^2 + \epsilon^2)} \epsilon^2 N \right), \]
where $\gamma_0 = \min(1 - \lambda_2, 1)$.

We prove adaptive rates.

Theorem 5 (Function-dependent Hoeffding bound). With notation as above,
\[ P\left( \frac{1}{N} \sum_{i=1}^{N} f(X_i) - \mu \right) \geq \epsilon \leq 2 \exp\left( -\frac{\gamma}{4\Lambda(\epsilon, \mu, \pi)} \epsilon^2 N \right), \]
where, letting $\nu = \min(\mu, 1 - \mu)$,
\[ \Lambda(\epsilon, \mu, \pi) = \log\left( \frac{4}{\nu \Lambda(2 \mu \nu)} \right). \]

Furthermore, this holds even if the chain is not at equilibrium.

Examples and simulations

Definition (Lazy random walk on $C_d$). The lazy random walk on the cycle graph with $2d$ vertices, $C_{2d}$, updates at each step according to the following rule:

- With probability $\frac{1}{2}$, stay at the current location.
- Otherwise, with probability $\frac{1}{2}$, move to the next node in clockwise order.
- Otherwise, move to the previous node in clockwise order.

We view the states in this Markov chain as indexed by integers in $\{0, \ldots, 2d - 1\}$. For this chain, we have
\[ \text{time until } d_{TV}(\pi_n, \pi) \leq \delta \text{ is on the order of } d^2 \log(1/\delta). \]

Example (Parity function). Let $f$ be the parity function defined by
\[ f(i) = \begin{cases} 1 & \text{if } i \text{ is odd}, \\ 0 & \text{otherwise}. \end{cases} \]

Since both neighbors of any vertex have the opposite of its parity, it is easy to see that
\[ E[f(X_i) | X_0 = i] = \frac{1}{2}, \]
so the function mixes in a single step.

Example (Trigonometric functions). For $0 < j < 2d$, the trigonometric functions
\[ g_j(i) = \frac{1 + \cos \left( \frac{2\pi i j}{2d} \right)}{2} \]
have
\[ \gamma_{g_j} = 1 - \cos \left( \frac{2\pi j}{2d} \right). \]

Therefore, when $j = d \pm e$ for some constant $e > 0$, the function absolute spectral gap is on the order of a constant, and the chain mixes with respect to $g_j$ in constant time.

Example (Random binary functions). Consider a random binary function obtained by sampling $f(i) \sim \text{Bern}(1/2)$ iid for each $i \in \{0, \ldots, 2d - 1\}$. With probability $\geq 1 - \frac{1}{\text{poly}(d)}$, we have that for any constant $0 < \delta < 1$,
\[ \text{time until } |E[f(X_i)] - \mu| \leq \delta \text{ is at most on the order of } d^3 \log^2 d. \]