The Complexity of Estimating Convergence Time

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Convergence diagnostics

- MCMC used in Bayesian inference, computational physics and chemistry, image processing, phylogeny ...

- Eventually the chain will converge to the desired target distribution.

- May or may not have bounds on the mixing time. Bounds may not be practical.

- How to tell whether the chain is close to converged?

- In practice many visual, statistical tests are used - convergence diagnostics.
Definitions

Probability measures $\mu$ and $\nu$ on finite $\Omega$. The \textbf{total variation distance} between $\mu$ and $\nu$ is

$$\|\mu - \nu\|_{tv} := \max_{A \subseteq \Omega} |\mu(A) - \nu(A)| = \frac{1}{2} \sum_{x \in \Omega} |\mu(x) - \nu(x)|$$

Markov chain $M$ on $\Omega$ with transition matrix $P$ and stationary distribution $\pi$.

$$d(t) := \max_{x, y \in \Omega} \|P^t(x, \cdot) - P^t(y, \cdot)\|_{tv}.$$ 

The $\varepsilon$-mixing time is

$$\tau(\varepsilon) := \inf\{t : d(t) \leq \varepsilon\}$$

The $\varepsilon$-mixing time started at $x$ is

$$\tau_x(\varepsilon) := \inf\{t : \|P^t(x, \cdot) - \pi\|_{tv} \leq \varepsilon\}$$
Traceplot

SAS/STAT(R) 9.22 User’s Guide - Assessing Markov Chain Convergence
### Statistical tests

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
<th>Interpretation of the Test</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gelman-Rubin</td>
<td>Uses parallel chains with dispersed initial values to test whether they all converge to the same target distribution. Failure could indicate the presence of a multi-mode posterior distribution (different chains converge to different local modes) or the need to run a longer chain (burn-in is yet to be completed).</td>
<td>One-sided test based on a variance ratio test statistic. Large $R_v$ values indicate rejection.</td>
</tr>
<tr>
<td>Geweke</td>
<td>Tests whether the mean estimates have converged by comparing means from the early and latter part of the Markov chain.</td>
<td>Two-sided test based on a $z$-score statistic. Large absolute $z$ values indicate rejection.</td>
</tr>
<tr>
<td>Heidelberger-Welch</td>
<td>Tests whether the Markov chain is a covariance (or weakly) stationary process. Failure could indicate that a longer Markov chain is needed.</td>
<td>One-sided test based on a Cramer-von Mises statistic. Small $p$-values indicate rejection.</td>
</tr>
<tr>
<td>Heidelberger-Welch (half-width test)</td>
<td>Reports whether the sample size is adequate to meet the required accuracy for the mean estimate. Failure could indicate that a longer Markov chain is needed.</td>
<td>If a relative half-width statistic is greater than a predetermined accuracy measure, this indicates rejection.</td>
</tr>
<tr>
<td>Raftery-Lewis</td>
<td>Evaluates the accuracy of the estimated (desired) percentiles by reporting the number of samples needed to reach the desired accuracy of the percentiles. Failure could indicate that a longer Markov chain is needed.</td>
<td>If the total samples needed are fewer than the Markov chain sample, this indicates rejection.</td>
</tr>
<tr>
<td>autocorrelation</td>
<td>Measures dependency among Markov chain samples.</td>
<td>High correlations between long lags indicate poor mixing.</td>
</tr>
<tr>
<td>effective sample size</td>
<td>Relates to autocorrelation; measures mixing of the Markov chain.</td>
<td>Large discrepancy between the effective sample size and the simulation sample size indicates poor mixing.</td>
</tr>
</tbody>
</table>

**[Cowles-Carlin '96]** Review of 13 diagnostics and scenarios where each can fail.
MC is a “rule” for determining next state.

Circuit $C : \{0,1\}^n \times \{0,1\}^m \rightarrow \{0,1\}^n$ specifies $P$ if

$$P(C(x,r) = y) = P(x,y)$$

Diagnostic algorithm $D$ decides if at time $t$:

- Chain within $1/4$ tv-distance of $\pi$: $\tau(1/4) \leq t$.
- Chain at least $1/4$ tv-distance from $\pi$: $\tau(1/4) > t$.

Exact distance at time $t$. 
Complexity theoretic framework for diagnostic algorithm

MC is a “rule” for determining next state.

Circuit $C : \{0, 1\}^n \times \{0, 1\}^m \rightarrow \{0, 1\}^n$ specifies $P$ if

$$\mathbb{P}(C(x, r) = y) = P(x, y)$$

Diagnostic algorithm $D$ decides at time $t$:

- mixed: Chain within $1/8$ in tv-distance of $\pi$: $\tau(1/8) \leq t$.
- not mixed: Chain at least $1/2$ in tv-distance from $\pi$: $\tau(1/2) > t$.

Allow a gap in approximation to tv-distance.
Complexity theoretic framework for diagnostic algorithm

MC is a “rule” for determining next state.

Circuit $C : \{0, 1\}^n \times \{0, 1\}^m \rightarrow \{0, 1\}^n$ specifies $P$ if

$$\mathbb{P}(C(x, r) = y) = P(x, y)$$

Diagnostic algorithm $D$ decides:

- mixed: At time $t$, chain within $1/8$ in tv-distance of $\pi$: $\tau(1/8) \leq t$.
- not mixed: At time $ct, c \geq 1$, chain at least $1/2$ in tv-distance from $\pi$: $\tau(1/2) > ct$.

Allow a gap in approximation to tv-distance as well as time.
**Diagnostic algorithm formulations**

**TestCon**\(_{c,\delta}\)  
**Input:** \(C\) specifies \(P\) on \(\Omega \subset \{0, 1\}^n\), \(x \in \Omega\), \(t \in \mathbb{N}\).  
**Promise:** \(P\) is ergodic.  
**YES:** \(\tau_x(1/4 - \delta) \leq t\).  
**NO:** \(\tau_x(1/4 + \delta) > ct\).

**PolyTestCon**\(_{c,\delta}\)  
**Input:** \((C, 1^t, 1^{t_{max}})\).  
**Promise:** \(P\) is ergodic and \(\tau(1/4) \leq t_{max}\).  
**YES:** \(\tau(1/4 - \delta) \leq t\).  
**NO:** \(\tau(1/4 + \delta) > ct\).

**PolyTestConInit**\(_{c,\delta}\)  
**Input:** \((C, x, 1^t, 1^{t_{max}})\).  
**Promise:** \(P\) is ergodic and \(\tau(1/4) \leq t_{max}\).  
**YES:** \(\tau_x(1/4 - \delta) \leq t\).  
**NO:** \(\tau_x(1/4 + \delta) > ct\).
Testing convergence in a general case

\[ \text{TestCon}_{c, \delta} \]

<table>
<thead>
<tr>
<th>Input:</th>
<th>( C ) specifies ( P ) on ( \Omega \subset {0, 1}^n ), ( x \in \Omega ), ( t \in \mathbb{N} ).</th>
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<tr>
<td>Promise:</td>
<td>( P ) is ergodic.</td>
</tr>
<tr>
<td>YES:</td>
<td>( \tau_x(1/4 - \delta) \leq t ).</td>
</tr>
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<td>NO:</td>
<td>( \tau_x(1/4 + \delta) &gt; ct ).</td>
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(PSPACE: set of all decision problems that can be solved by a Turing machine using space polynomial in the input.)

**Theorem 1 (B-Bogdanov-Mossel '11).** Let \( 1 \leq c \leq \exp\left(n^{O(1)}\right) \). Then,

- For \( \exp\left(-n^{O(1)}\right) < \delta \leq 1/4 \), \( \text{TestCon}_{c, \delta} \) is in PSPACE.
- For \( 0 \leq \delta < 1/4 \), \( \text{TestCon}_{c, \delta} \) is PSPACE-hard.
**TestCon**$_{c,\delta}$ is PSPACE-hard

Reduction from a PSPACE complete problem $A$ to **TestCon**$_{c,\delta}$.

Computation graph $G$ of Turing machine $T_A$ (reversible) MC on vertices of $G$

In the **YES** case, $s$ and $a$ are in the same component.
**TestCon**$_{c, \delta}$ is PSPACE-hard

Reduction from a PSPACE complete problem $A$ to **TestCon**$_{c, \delta}$.

In the **NO** case, $s$ and $a$ are not in the same component.

Note: $W$ must be chosen so that the reduction is polynomial in the input to $A$. 
**TestCon**

$\text{TestCon}_{c,\delta}$ is PSPACE-hard

Computation graph $G$ of Turing machine $T_A$

(reversible) MC on vertices of $G$

**YES case:** Each state of MC has const. degree $\leq D$.

$$\pi(x) = \frac{\sum_{y \sim x} w_{xy}}{\sum_{e \in E} w_e} \geq \frac{1}{D2^n}, \quad \Phi \geq \frac{W}{D2^n W} = \frac{1}{D2^n}$$

$$\tau(\epsilon) \leq \frac{2}{\Phi^2} \log \left( \frac{2}{\pi_{\text{min}} \epsilon} \right) \leq \frac{10D^3 2^{3n}}{\epsilon}.$$
**TestCon}_{c,\delta} is PSPACE-hard**

NO case: MCs $X_t$ started at $s$, $Y_t$ started at $a$.

$$d(t) \geq P(\forall t' \leq t, X_{t'} \notin cmp(a)) - P(\exists t' \leq t \text{ s.t. } Y_{t'} \in cmp(s)) \geq 1 - \frac{2t}{W}$$

So,

$$\tau(1/4 + \delta) \geq \tau(1/2) \geq \frac{W}{4}.$$  

Set $W = \frac{1000cD^32^{3n}}{1 - 4\delta}$, $t = \frac{10D^32^{3n}}{1 - 4\delta}$, $x = s$. 
Testing convergence with polynomial mixing bound

\[
\text{\textsc{PolyTestCon}}_{c,\delta}
\]

Input: \((C, 1^t, 1^{t_{\text{max}}})\).

Promise: \(P\) is ergodic and \(\tau(1/4) \leq t_{\text{max}}\).

Yes: \(\tau(1/4 - \delta) \leq t\).

No: \(\tau(1/4 + \delta) > ct\).

Theorem 2 (B-Bogdanov-Mossel '11).

- For \(0 \leq \delta < 1/4\), \(c < \frac{3/4-\delta}{2} \sqrt{t_{\text{max}}/t^2n^3}\), \textsc{PolyTestCon}_{c,\delta} is coNP-hard.

- For \(0 < \delta \leq 1/4\), \textsc{PolyTestCon}_{c,\delta} is in coAM.
co-NP hardness of $\text{POLYTestCon}_{c,\delta}$

By reduction from UNSAT. Input is $\Psi$ a CNF formula on $n$ variables.

$\text{POLYTestCon}_{c,\delta}$ instance $(C, 1^t, 1^{t_{\text{max}}})$:

\[ \tau \left( \frac{1}{4} - \delta \right) \leq C(\delta) n \log(n) \]

\[ \tau \left( \frac{1}{4} + \delta \right) > \frac{1}{2} n^{d-1} (3/4 - \delta) > cC(\delta) n \log(n) \]

By a lower bound on conductance, $t_{\text{max}} \leq 32 n^{2d+1}$.

Set $t = C(\delta) n \log(n)$. 
Testing convergence given polynomial mixing and initial state

<table>
<thead>
<tr>
<th>\text{POLYTestConInit}_{c,\delta}</th>
<th>\text{Input:} \quad (C, x, 1^t, 1^{t_{\text{max}}}).</th>
</tr>
</thead>
<tbody>
<tr>
<td>\text{Promise:} \quad P \text{ is ergodic and } \tau(1/4) \leq t_{\text{max}}.</td>
<td></td>
</tr>
<tr>
<td>\text{YES:} \quad \tau_x(1/4 - \delta) \leq t.</td>
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</tr>
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<td>\text{NO:} \quad \tau_x(1/4 + \delta) &gt; ct.</td>
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Theorem 3 (B-Bogdanov-Mossel ’11).

- For $0.11602 < \delta \leq 1/4$ and $c \geq 1$, \text{POLYTestConInit}_{c,\delta} \in \text{SZK}.$
- For $0 \leq \delta \leq 1/4$ and $c \leq \frac{2}{1+4\delta} t_{\text{max}}/t$, \text{PTCS}_{c,\delta}$ is \text{SZK}-hard.
- For $0 < \delta \leq 1/4$, \text{PTCS}_{c,\delta} \in \text{AM} \cap \text{coAM}.$

(SZK : Statistical Zero Knowledge)
Proof Systems

Proof system for a language $L \subset \{0, 1\}^n$ and a verification algorithm $V$ with

- Completeness: If $x \in L$, there is a proof $\pi$ so $V(x, \pi) = \text{accept}$.
- Soundness: If $x \notin L$, for all $\pi^*$, $V(x, \pi^*) = \text{reject}$.
- Efficiency: $V(x, \pi)$ runs in time polynomial in $|x|$.

NP is defined this way.

How much knowledge does one gain from verifying a proof?
Zero knowledge proofs


Interaction $(P, V)(x)$ between $P$ and $V$ with polynomial messages exchanged, and private coin tosses.

- Completeness: If $x \in L$, $V$ accepts in $(P, V)(x)$ w. p. $\geq 2/3$.
- Soundness: If $x \notin L$, for "any" $P^*$, $V$ accepts in $(P^*, V)(x)$ w.p. $\leq 1/3$.
- Efficiency: $V$ runs in time polynomial in $|x|$.

Zero knowledge: The verifier could have simulated the entire interaction.
“SZK”: Class of languages for which there is an interaction statistically indistinguishable from the simulator with ZK.

Canonical hard problem:

\[ \text{STATDIFF}_{s,c} \]

Input: Circuits \( C, C' : \{0, 1\}^n \rightarrow \{0, 1\}^n \) of dist. \( \mu_1, \mu_2 \) on \( \{0, 1\}^n \).

YES: \( \| \mu_1 - \mu_2 \|_{tv} \geq c \).

NO: \( \| \mu_1 - \mu_2 \|_{tv} < s \).

[Sahai-Vadhan '97] Let \( 0 \leq c, s \leq 1 \).

- For \( c^2 > s \), \( \text{STATDIFF}_{s,c} \) is in SZK.
- \( \text{STATDIFF}_{s,c} \) is SZK-hard.

SZK contains problems believed to be hard (e.g. GRAPHNONISO), but cannot contain \( NP \)-complete problems.
SZK-hardness for PolyTestConInit\(_{c,\delta}\)

By reduction from StatDiff\(_{s,c}\).

<table>
<thead>
<tr>
<th>StatDiff(_{s,c})</th>
<th>Input:</th>
<th>Circuits (C, C': {0, 1}^n \rightarrow {0, 1}^n) with (\mu_1, \mu_2) on ({0, 1}^n).</th>
</tr>
</thead>
<tbody>
<tr>
<td>YES:</td>
<td>(|\mu_1 - \mu_2|_{tv} \geq c).</td>
<td></td>
</tr>
<tr>
<td>NO:</td>
<td>(|\mu_1 - \mu_2|_{tv} &lt; s).</td>
<td></td>
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</table>

\((C, C')\): instance of StatDiff\(_{s,c}\) with \(c = 1, s = 1/4 - \delta\).

Construct an instance of PolyTestConInit\(_{c,\delta}\).

MC \((Y_t, Z_t)\) on \([M] \times \{0, 1\}^n\).

- Choose \(Z_{t+1}\):
  - If \(Y_t = 1\), choose \(Z_{t+1} \sim \mu_1\).
  - If \(Y_t = 2\), choose \(Z_{t+1} \sim \mu_2\).
  - Otherwise, set \(Z_{t+1} = Z_t\).

- Choose \(Y_{t+1}\) uniformly from \([M]\).

\[
\pi = U_{[M]} \times \frac{\mu_1 + \mu_2}{2}
\]
SZK-hardness for PolyTestConInit\(_{c,\delta}\)

Let \( x = (1, 0^n) \)

\[
\| P^t(x, \cdot) - \pi \|_{tv} = \frac{1}{2} \left( \frac{m - 2}{m} \right)^{t-1} \| \mu_1 - \mu_2 \|_{tv}
\]

**YES case:** For \( t \geq 1, M \geq 3 \)

\[
\| P^t(x, \cdot) - \pi \|_{tv} < \frac{1}{2} s < \frac{1}{4} - \delta
\]

**NO case:** If \( ct < \frac{M}{4} \ln \left( \frac{\frac{2}{1+4\delta}}{1} \right) \),

\[
\| P^t(x, \cdot) - \pi \|_{tv} \geq \frac{1}{2} \left( \frac{M - 2}{M} \right)^{ct-1} c > \frac{1}{4} + \delta
\]

In both cases \( \tau(1/4) \leq M \).

Set \( t_{max} = M, t = 1 \).
Conclusions

- Efficient algorithms are not believed to exist for PSPACE-complete, coNP-complete or SZK-complete problems.

- Diagnostic algorithms do not exist for large classes of MCMC algorithms, unless there are efficient algorithms for PSPACE or coNP or SZK.

- (Woodard) Hardness for diagnosing convergence from a given state when $\pi$ is known up to a global constant?

- Hardness for Gibbs samplers (conditional distribution of each variable can be sampled)?