Advanced Markov Modeling 2015

Lecture 6: Illustrations and Examples / 1

Monte Carlo simulation of lasers
(A work with J. Arnaud and L. Chusseau, IES)

F. Philippe    A. Jean-Marie

LIRMM

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Outline

Lasers

Some theoretic points
  Einstein’s prescription
  Boltzmann’s distribution

Modelization
  Quick introduction
  Lasers as Markov chains

Simulation

Goals
Basics
  Algorithm
  Implementation

Practical issues
Some solutions
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A birth-death process

Planck  
Energy exchanges between matter (particles) and light (wave, frequency $\omega$): only by integer multiples of energy quantum $\delta = \hbar \omega$

Emission (absorption) of a photon corresponds to a particle going down (up) between two energy levels $\varepsilon, \varepsilon + \delta$. 
A birth-death process

**Planck** Energy exchanges between matter (particles) and light (wave, frequency $\omega$): only by integer multiples of energy quantum $\delta = \hbar \omega$

Emission (absorption) of a photon corresponds to a particle going down (up) between two energy levels $\varepsilon$, $\varepsilon + \delta$.

**Einstein** Time evolution of the photon number $m(t)$ is a birth-death process, jump probabilities in interval $[t, t + dt]$:

$$\pi(m \to m - 1) \propto n_{\delta \uparrow} m,$$
$$\pi(m \to m + 1) \propto n_{\delta \downarrow} (m + 1).$$

At time $t$: $n_{\delta \uparrow}(t)$ is the number of particles that may jump from a level $\varepsilon$ to level $\varepsilon + \delta$. 
Thermal bath

Canonical ensemble: System in contact with a (large) heat bath, temperature $T$, define $q = e^{-k_B/T} \in (0, 1)$. Energy exchanges only (not particles).

**Boltzmann** The probability for the system to have energy $U$ at equilibrium is $\propto q^U$. 
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Which simple Markov chains have this kind of stationary distributions? Example: one particle, equidistant energy levels $\varepsilon_n = n\varepsilon$. (geometric distribution, constant-rate birth-death)

$$
\pi(\varepsilon_n \rightarrow \varepsilon_{n-1}) \propto p,
$$

$$
\pi(\varepsilon_n \rightarrow \varepsilon_{n+1}) \propto pq^\varepsilon.
$$
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How it works

Atomic laser: 4-level atoms, mirrors

- Pumping: population inversion
- Disexcitation
- Lasing levels (1,2):
  - Stimulated absorption / emission

\[
P_{\pi}(m \rightarrow m-1) \propto n_1 m \\
P_{\pi}(m \rightarrow m+1) \propto n_2 (m+1)
\]
How it works

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Disexcitation

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Stimulated absorption / emission

Coherent emission (absorption by sink)
Semi-conductor lasers

Electrons, two bands of energy levels, 0-1 electron by level

valence band

energy gap

conduction band

(lasing levels)
Semi-conductor lasers

Electrons, two bands of energy levels, 0-1 electron by level

(valence band) — energy gap — (conduction band)

stimulated absorption

stimulated emission

pumping

(lasing levels)

Other/further moves:

upward and downward thermalization

(Auger effect, coherent pumping, spontaneous emission, ...)
States and events

\( n \) electrons, \( n \) energy levels in each band

A state: a repartition of the \( n \) electrons among the \( 2n \) levels, and the number \( m \) of photons in the optical cavity.
States and events

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Events: electronic pumping, thermalization (up and down) → bands
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optronic stimulated emission, stimulated absorption → interaction bands / cavity
**States and events**

$n$ electrons, $n$ energy levels in each band

**A state:** a repartition of the $n$ electrons among the $2n$ levels, and the number $m$ of photons in the optical cavity.

**Events:**

- **Electronic** pumping,
  thermalization (up and down)
  → **bands**

- **Optronic** stimulated emission,
  stimulated absorption
  → **interaction bands / cavity**

- **Photonic** coherent emission
  → **cavity**
Processes

Homogeneous Poisson processes
pumping (quiet), thermalization
Processes

Homogeneous Poisson processes
pumping (quiet), thermalization

Cox processes
stimulated emission/absorption, laser emission
Processes

Homogeneous Poisson processes
  pumping (quiet), thermalization

Cox processes
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(+ periodic events if regular pumping)
Processes

Homogeneous Poisson processes
  pumping (quiet), thermalization

Cox processes
  stimulated emission/absorption,
  laser emission

(\textit{+ periodic events if regular pumping})

Superposition of similar processes
  upward thermalization, 
  downward thermalization
## Rates

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<th>Variables and parameters</th>
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<td>$m/\tau$</td>
<td>$m(t)$ number of photons in the cavity, $\tau$ their mean lifetime.</td>
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<td>Thermalization</td>
<td>$pN_\downarrow$ or $pqN_\uparrow$</td>
<td>$p$ lattice coupling, $N_\downarrow$ electrons may move a level down. $q$ temperature (Boltzmann) $N_\uparrow$ electrons may move a level up.</td>
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<td>Thermalization downwards</td>
<td>$pN_{\downarrow}$</td>
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<td>Thermalization upwards</td>
<td>$pqN_{\uparrow}$</td>
<td>$q$ temperature (Boltzmann)</td>
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<td>Pumping</td>
<td>$J$</td>
<td>(Poissonian pump)</td>
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Laser Noise

Thermal light: \[ \pi(m) \propto q^{m\delta} \]

Generating function: \[ \phi(z) = \frac{1-q^\delta}{1-zq^\delta}. \]

Mean, variance: \[ \langle m \rangle = \frac{q^\delta}{1-q^\delta}, \quad V_m = \frac{q^\delta}{(1-q^\delta)^2} = \langle m \rangle + \langle m \rangle^2. \]

Laser light: poissonian

Is it possibly sub-poissonian? Under which conditions?

Thermique

Laser

Laser ‘Quiet’
Statistics of the number of photons in the cavity (stationary)
Fano factor $\mathcal{F}$: variance/mean (1 for Poisson variables)
Laser noise

Intensity of the laser: stationnary process $Q$, let $\Delta Q = Q - \langle Q \rangle$.

Spectral density $S(\Omega) = \frac{1}{\langle Q \rangle} S_\Delta Q(\Omega)$, $\mathcal{F} = \int S(\Omega) d\Omega$.

Frequencies $\Omega$ for which $S(\Omega) < 1$?
Levels occupancies
Spectral hole burning at lasing levels
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Algorithm

Simulation of 1 trajectory of the CTMC  \hspace{1cm} (MC?)
Known as dynamic MC, kinetic MC, Doob-Gillespie, etc… \hspace{1cm} (MC?)

Method
At time $t_k$:
- simulate the waiting time $\tau$ before next event
- choose the event according to rates
- $t_{k+1} = t_k + \tau$
Implementation

Initialization \( (t = 0) \)

Any state, e.g., all electrons in VB, no photon in the cavity.

Loop \( (\text{while } t < T) \)

- random number \( r = U(0, 1) \) for the waiting time:
  \[ \tau = -\ln r \Lambda, \quad \Lambda = \sum_{i\geq 1} \lambda_i, \]

- random number \( r' = U(0, 1) \) for the next event:
  \[ \text{index} = \min\{i : \sum_{j=1}^{i} \lambda_j \geq r' \Lambda\}, \]

- update rates and state,

- perform other statistical computations:
  occupancies, histogram, spectral density. \( (t = t + \tau) \)
Typical values

800 energy levels in each band, 800 electrons
Simulation duration $T = 100–10^5$

Rates:

|                          | $J$                  | $J = 100–500$
|--------------------------|----------------------|-------------------
| Pumping                 | $J$                  | $J = 100–500$
| Absorption (sink)       | $m/\tau$             | $\tau = 2$
| Emission                | $m + 1$ or 0         | $<m> = \tau J$
| Absorption              | $m$ or 0             |                   
| Thermalization          | $pN_\downarrow$      | $p = 50000$
|                          | $pqN_\uparrow$       | $q = 0.9$

0.5 $10^{12}$ events for 6 $10^6$ useful points

\[ \Lambda = \sum_{i \geq 1} \lambda_i \]

\[ pN_\downarrow \quad \text{other rates...} \quad pqN_\uparrow \]
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Pseudorandom generators

Rather large choice. How to choose?

- **period?** number of events to be generated?
  (e.g., $0.5 \times 10^{12}$ events)
- **speed?** is it critical?
- **biases?** which randomness is desirable?

See GSL, Dieharder, ...
Stationnarity

- How do we know?
  In many cases, it must be checked *a posteriori*...
- Ergodicity assumptions (time averages / ensemble averages)
- Predictible averages?
  Population (balance) equations at equilibrium?
- Which one to choose? (most frequent? fastest to compute?)
**Spectral density approximation**

Direct computation? Fourier transform of autocorrelation?
Not incremental.
Estimation by periodogram (duration $T$, $K$ points $\Omega_k = \frac{2k\pi}{T}$).

$$S(\Omega) \approx S_T(\Omega) = \frac{1}{T} \left| \sum_{n=1}^{N} e^{-i\Omega t_n} \right|^2$$

Correct approximation?
Spectral density approximation

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Estimation by periodogram (duration $T$, $K$ points $\Omega_k = \frac{2k\pi}{T}$).

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Correct approximation?
In average, and for large $T$!
Variance is independent of $T$...
Spectral density approximation

Bartlett: average $N$ parts of a unique simulation of duration $NT$. Here for $N = 10$:

A little better...
For one curve, more than a week...
Searching for optimal parameters

Efficient thermalization \((p = 50000)\), 800 levels in each band
Variable pumping rate:

For each point, nearly a week...
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Technical track : Distributing simulations

Condor server
Computers of the UFR rooms (300-600), evening and weekend

Method

- initialisation (stationary state)
- 1 initial occupancies computation
- $k$ small mixing runs, average duration $T/100$
- $k$ simulation runs, duration $T$
- 1 final occupancies computation
Improvements

Variance of periodogram
Improvements

Fano factor vs runs

error bars: from 0.3 (10 runs) to 0.03 (1000 runs)
Theoretical track : Getting rid of thermalization?

Rare events: pumping, photon emission/absorption, photon escape.
→ their rates depend on the occupation of few levels only

Between two rare events, only thermalization occurs — so, the number of electrons in each band is left unchanged
Theoretical track: Getting rid of thermalization?

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Consider thermalization processes in a band of $B$ levels, with $N$ electrons inside.

- Can we compute a random state after $K$ steps? ($K \approx 10^5$)
- Better: Can we compute the occupancy of a given level?
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- Can we compute a random state after $K$ steps? ($K \approx 10^5$)
- Better: Can we compute the occupancy of a given level?
- Even better: May we consider that $K = \infty$?
  → simple N-recursive formula for the occupancy of a given level!