Optimization and Simulation

Markov Chain Monte Carlo Methods

Michel Bierlaire

Transport and Mobility Laboratory
School of Architecture, Civil and Environmental Engineering
Ecole Polytechnique Fédérale de Lausanne

Outline

The knapsack problem

- Patricia prepares a hike in the mountain.
- She has a knapsack with capacity W kg.
- She considers carrying a list of n items.
- Each item has a utility u_i and a weight w_i.
- What items should she take to maximize the total utility, while fitting in the knapsack?

Knapsack problem

Simulation

- Let $\mathcal{X}$ be the set of all possible configurations (2^n).
- Define a probability distribution:

$$P(x) = \frac{e^{U(x)}}{\sum_{y \in \mathcal{X}} e^{U(y)}}$$

- Question: how to draw from this discrete random variable?

Bayesian inference

Choice model

- Consider a commuter n.
- Possible modes: $\mathcal{C}_n = \{car, bus, bike\}$.
- Utility

$$U_{in} = V_{in}(time, cost, weather, \ldots; \beta) + \varepsilon_{in}$$

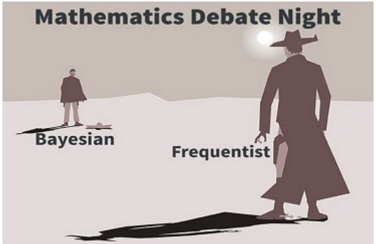
- Choice model:

$$P_n(i) = \Pr(U_{in} \geqslant U_{jn}, j \in \mathcal{C}_n).$$

- If ε_{in} is EV distributed, we have the logit model:

$$P_n(i; x, \beta) = \frac{e^{V_{in}(x;\beta)}}{\sum_{j \in \mathcal{C}_n} e^{V_{jn}(x;\beta)}}.$$

Bayesian inference



Inference

- Data: $Y = (i_n, x_n)_{n=1}^{N}$.
- Inference: estimate the true value of β.
- Likelihood:

$$L(Y|\beta) = \prod_{n=1}^{N} P_n(i_n; x_n, \beta).$$

- Frequentist inference: maximum likelihood estimation.
- Bayesian inference.

Bayesian inference

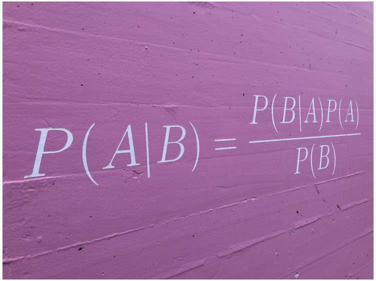
Bayesian concepts

- Likelihood:

$$L(Y|\beta) = \prod_{n=1}^{N} P_n(i_n; x_n, \beta).$$

- Prior: $f(\beta)$.
- Posterior:

$$f(\beta|Y) = \frac{L(Y|\beta)f(\beta)}{L(Y)} = \frac{L(Y|\beta)f(\beta)}{\int L(Y|\beta)f(\beta)d\beta}.$$



Bayesian inference

Prior: $N(\mu, \Sigma)$

$$f(\beta) = (2\pi)^{-\frac{K}{2}} \det(\Sigma)^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\beta-\mu)^T \Sigma^{-1} (\beta-\mu)\right)$$

Posterior for logit

$$f(\beta|Y) = \frac{f(\beta) \prod_{n=1}^{N} \frac{e^{V_{i_n n}(x_n;\beta)}}{\sum_{j \in \mathcal{C}_n} e^{V_{jn}(x_n;\beta)}}}{\int_{\gamma} f(\gamma) \prod_{n=1}^{N} \frac{e^{V_{i_n n}(x_n;\gamma)}}{\sum_{j \in \mathcal{C}_n} e^{V_{jn}(x_n;\gamma)}}}.$$

Prediction

Plug-in prediction

$$\bar{\beta} = \int \beta f(\beta|Y) d\beta.$$

Ignores parameter uncertainty.

Prediction

Posterior predictive

- Future unobserved data: Y_f

$$f(Y_f|Y) = \int_\beta f(Y_f, \beta|Y)d\beta = \int_\beta f(Y_f|\beta, Y)f(\beta|Y)d\beta.$$

- Assumption for prediction: Y and Y_f are independent, cond. on β:

$$f(Y_f|Y) = \int_\beta f(Y_f|\beta)f(\beta|Y)d\beta.$$

Average of the likelihood on Y_f over the posterior of β.

Bayesian inference

Difficulties

- Complicated integrals.
- Critical to draw from the posterior.
- Must rely on simulation.
- But how do we draw from such complex distributions?

Outline

Markov chains

Stochastic process

X_t, $t = 0, 1, \ldots,$, collection of r.v. with same support, or state space $\{1, \ldots, i, \ldots, J\}$.

Markov process: (short memory)

$$\Pr(X_t = i | X_0, \ldots, X_{t-1}) = \Pr(X_t = i | X_{t-1})$$

Homogeneous Markov process

$$\Pr(X_t = j | X_{t-1} = i) = \Pr(X_{t+k} = j | X_{t-1+k} = i) = P_{ij} \;\; \forall t \geqslant 1, k \geqslant 0.$$

Markov chains

Stationary distribution

Unique solution of the system:

$$\pi_j = \sum_{i=1}^{J} P_{ij}\pi_i, \forall j = 1, \ldots, J,$$

$$\sum_{j=1}^{J} \pi_j = 1.$$

Markov chains

We assume...

- Homogeneous: transition probabilities do not depend on time,

$$\Pr(X_{t+1} = j \mid X_t = i) = P_{ij}.$$

- Irreducible: every state can be reached from any other state in a finite number of steps with positive probability.
- Aperiodic: the chain does not get trapped in deterministic cycles (returns to a state can occur at irregular times).
- Time reversible:

$$\pi_i P_{ij} = \pi_j P_{ji}, \qquad i \neq j.$$

Simulation with Markov chains

Procedure

- We want to simulate a r.v. X with pmf

$$\Pr(X = j) = p_j.$$

- We generate a Markov process with stationary probability p_j (how?)
- We simulate the evolution of the process.

$$p_j = \pi_j = \lim_{t\to\infty} \Pr(X_t = j) \quad j = 1, \ldots, J.$$

Example

- A machine can be in 4 states with respect to wear
  - perfect condition,
  - partially damaged,
  - seriously damaged,
  - completely useless.
- The degradation process can be modeled by an irreducible aperiodic homogeneous Markov process, with the following transition matrix:

$$P = \begin{pmatrix} 0.95 & 0.04 & 0.01 & 0.0 \\ 0.0 & 0.90 & 0.05 & 0.05 \\ 0.0 & 0.0 & 0.80 & 0.20 \\ 1.0 & 0.0 & 0.0 & 0.0 \end{pmatrix}$$

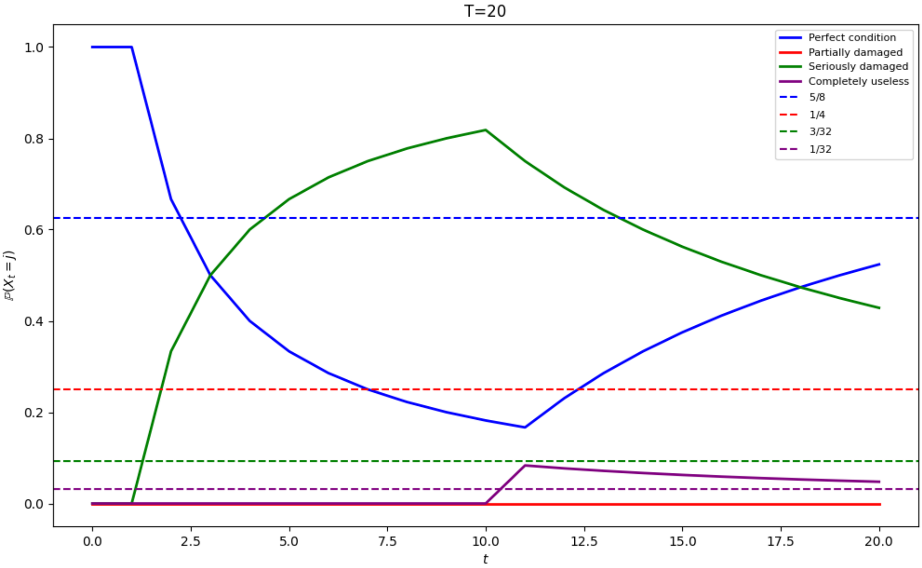
Example

Stationary distribution: $\left(\frac{5}{8}, \frac{1}{4}, \frac{3}{32}, \frac{1}{32}\right)$

$$\left(\frac{5}{8}, \frac{1}{4}, \frac{3}{32}, \frac{1}{32}\right) \begin{pmatrix} 0.95 & 0.04 & 0.01 & 0.0 \\ 0.0 & 0.90 & 0.05 & 0.05 \\ 0.0 & 0.0 & 0.80 & 0.20 \\ 1.0 & 0.0 & 0.0 & 0.0 \end{pmatrix} = \left(\frac{5}{8}, \frac{1}{4}, \frac{3}{32}, \frac{1}{32}\right)$$

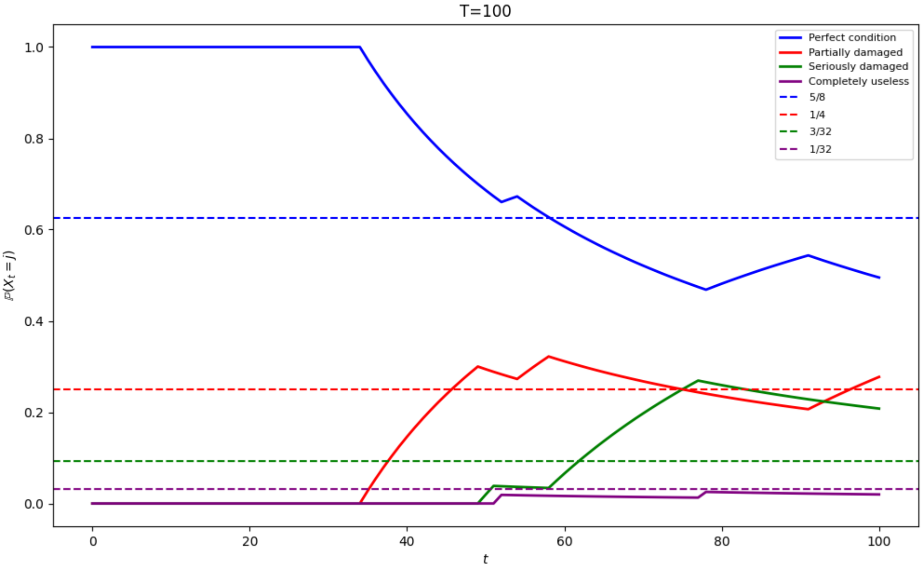
- Machine in perfect condition 5 days out of 8, in average.
- Repair occurs in average every 32 days

Example: $T = 20$

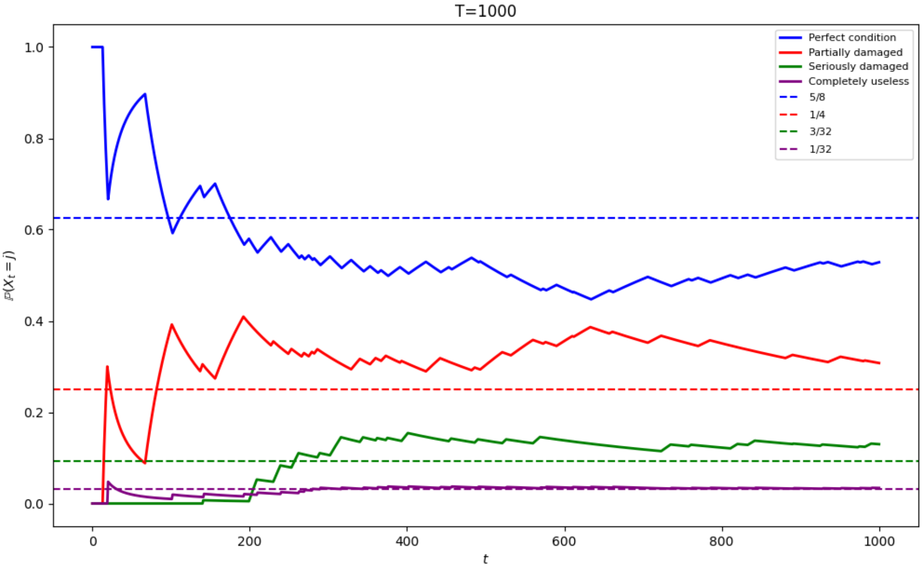


T=20
Perfect condition
Partially damaged
Seriously damaged
Completely useless
5/8
1/4
3/32
1/32
1.0
0.8
0.6
0.4
0.2
0.0
$\mathbb{P}(X_t = j)$
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
t

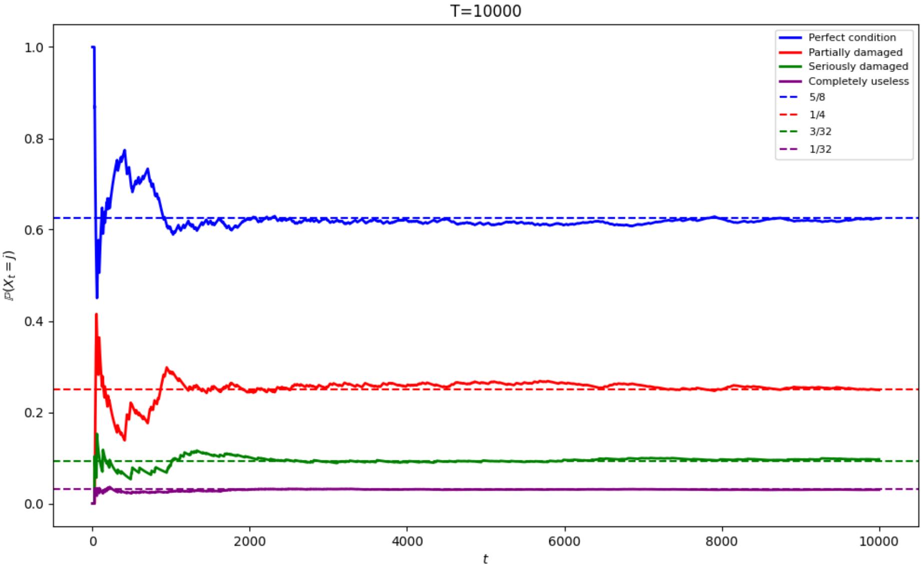
Example: $T = 100$



Example: $T = 1000$



Example: $T = 10000$



Simulation

Assume that we are interested in simulating

$$E[f(X)] = \sum_{j=1}^{J} f(j)p_j.$$

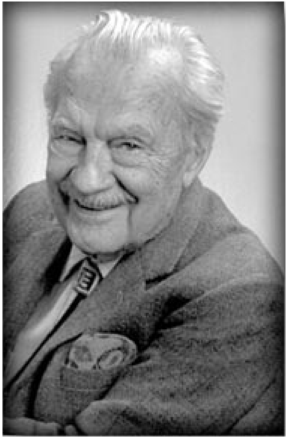
Property of Markov chain: ergodicity

$$E[f(X)] = \lim_{T\to\infty} \frac{1}{T} \sum_{t=1}^{T} f(X_t).$$

Drop early states (see above example)

$$E[f(X)] \approx \frac{1}{T} \sum_{t=1+k}^{T+k} f(X_t).$$

Metropolis-Hastings



Nicholas Metropolis
1915 – 1999

Wilfred Keith Hastings
1930 – 2016

Metropolis-Hastings

Context

- Let b_j, $j = 1, \ldots, J$ be positive numbers.
- Let $B = \sum_j b_j$. If J is huge, B cannot be computed.
- Let $\pi_j = b_j / B$.
- We want to simulate a r.v. with pmf π_j.

Explore the set

- Consider a Markov process on $\{1, \ldots, J\}$ with transition probability Q.
- Designed to explore the space $\{1, \ldots, J\}$ efficiently
- Not too fast (and miss important points to sample)
- Not too slowly (and take forever to reach important points)

Metropolis-Hastings

Define another Markov process

- Based on the exact same states $\{1, \ldots, J\}$ as the previous ones
- Assume the process is in state i, that is $X_t = i$.
- Simulate the (candidate) next state j according to Q.
- Define

$$X_{t+1} = \begin{cases} j & \text{with probability } \alpha_{ij} \\ i & \text{with probability } 1 - \alpha_{ij} \end{cases}$$

Metropolis-Hastings

Transition probability P

$$
\begin{array}{lcll}
P_{ij} & = & Q_{ij}\alpha_{ij} & \text{if } i \neq j \\
P_{ii} & = & Q_{ii}\alpha_{ii} + \sum_{\ell \neq i} Q_{i\ell}(1 - \alpha_{i\ell}) & \text{otherwise}
\end{array}
$$

Must verify the property

$$
\begin{array}{rcl}
1 = \sum_j P_{ij} & = & P_{ii} + \sum_{j \neq i} P_{ij} \\
& = & Q_{ii}\alpha_{ii} + \sum_{\ell \neq i} Q_{i\ell}(1 - \alpha_{i\ell}) + \sum_{j \neq i} Q_{ij}\alpha_{ij} \\
& = & Q_{ii}\alpha_{ii} + \sum_{\ell \neq i} Q_{i\ell} - \sum_{\ell \neq i} Q_{i\ell}\alpha_{i\ell} + \sum_{j \neq i} Q_{ij}\alpha_{ij} \\
& = & Q_{ii}\alpha_{ii} + \sum_{\ell \neq i} Q_{i\ell}
\end{array}
$$

As $\sum_j Q_{ij} = 1$, we have $\alpha_{ii} = 1$.

Metropolis-Hastings

Time reversibility

$$\pi_i P_{ij} = \pi_j P_{ji}, \quad i \neq j$$

that is

$$\pi_i Q_{ij} \alpha_{ij} = \pi_j Q_{ji} \alpha_{ji}, \quad i \neq j$$

It is satisfied if

$$\alpha_{ij} = \frac{\pi_j Q_{ji}}{\pi_i Q_{ij}} \text{ and } \alpha_{ji} = 1$$

or

$$\frac{\pi_i Q_{ij}}{\pi_j Q_{ji}} = \alpha_{ji} \text{ and } \alpha_{ij} = 1$$

Metropolis-Hastings

As α_{ij} is a probability

$$\alpha_{ij} = \min\left(\frac{\pi_j Q_{ji}}{\pi_i Q_{ij}}, 1\right)$$

Simplification

Remember: $\pi_j = b_j / B$. Therefore

$$\alpha_{ij} = \min\left(\frac{b_j B Q_{ji}}{b_i B Q_{ij}}, 1\right) = \min\left(\frac{b_j Q_{ji}}{b_i Q_{ij}}, 1\right)$$

The normalization constant B does not play a role in the computation of α_{ij}.

Metropolis-Hastings

In summary

- Given Q and b_j
- defining α as above
- creates a Markov process characterized by P
- with stationary distribution π.

Metropolis-Hastings

Algorithm

1. Choose a Markov process characterized by Q.
2. Initialize the chain with a state i: $t = 0$, $X_0 = i$.
3. Simulate the (candidate) next state j based on Q.
4. Let r be a draw from $U[0,1[$.
5. Compare r with $\alpha_{ij} = \min\left(\frac{b_j Q_{ji}}{b_i Q_{ij}}, 1\right)$. If
$$r < \alpha_{ij}$$
then $X_{t+1} = j$, else $X_{t+1} = i$.
6. Increase t by one.
7. Go to step 3.

Metropolis-Hastings

Implementation note

Preferable to work in the log-space

$$\ln r < \ln \alpha_{ij}$$

where

$$\ln \alpha_{ij} = \min(\ln b_j + \ln Q_{ji} - \ln b_i - \ln Q_{ij}, 0).$$

It is equivalent to the condition

$$\ln r < \ln b_j + \ln Q_{ji} - \ln b_i - \ln Q_{ij}.$$

Simple example

$$
\begin{aligned}
b &= (20, 8, 3, 1) \\
\pi &= \left(\frac{5}{8}, \frac{1}{4}, \frac{3}{32}, \frac{1}{32}\right)
\end{aligned}
$$

$$
Q = \begin{pmatrix}
\frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\
\frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\
\frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\
\frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4}
\end{pmatrix}
$$

Run MH for 10000 iterations. Collect statistics after 1000.

- Accept: [2488, 1532, 801, 283]
- Reject: [0, 952, 1705, 2239]
- Simulated: [0.627, 0.250, 0.095, 0.028]
- Target: [0.625, 0.250, 0.09375, 0.03125]

Outline

Metropolis–Hastings: discrete vs continuous

Discrete state space

- Finite set of states $\{1, \ldots, J\}$.
- Target distribution:
$$\pi_j = \frac{b_j}{\sum_{\ell=1}^{J} b_\ell}.$$
- Transition probabilities: matrix P_{ij}.
- Stationarity:
$$\pi_j = \sum_{i=1}^{J} \pi_i P_{ij}.$$
- If the chain is irreducible, the stationary distribution is unique.

Metropolis–Hastings: continuous state space

Continuous state space

- State space: $\beta \in \mathbb{R}^K$.
- Target density:
$$\pi(\beta) = \frac{b(\beta)}{\int b(\gamma)\, d\gamma},$$
where the normalizing constant is unknown.
- Transitions are described by a proposal density
$$q(\beta' \mid \beta).$$
- Stationarity is expressed by an integral equation:
$$\pi(\beta') = \int \pi(\beta)\, p(\beta' \mid \beta)\, d\beta.$$

Metropolis–Hastings in continuous spaces

Algorithm

From the current state β:

1. Draw a candidate $\beta' \sim q(\cdot \mid \beta)$.
2. Accept β' with probability

$$\alpha(\beta, \beta') = \min\left(\frac{b(\beta')\, q(\beta \mid \beta')}{b(\beta)\, q(\beta' \mid \beta)}, 1\right).$$

Key property

The normalizing constant of $\pi(\beta)$ cancels out. Only the unnormalized density $b(\beta)$ is needed.

Bayesian inference

Prior: $N(\mu, \Sigma)$

$$f(\beta) = (2\pi)^{-\frac{K}{2}} \det(\Sigma)^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\beta-\mu)^T\Sigma^{-1}(\beta-\mu)\right)$$

We need to draw from

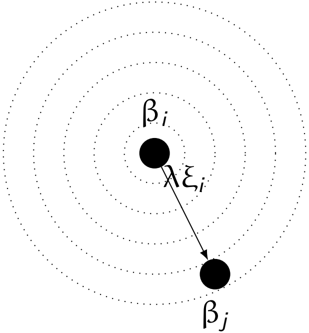
$$\begin{aligned}
f(\beta|Y) &= \frac{f(\beta)\prod_{n=1}^{N}\frac{e^{V_{i_n n}(x_n;\beta)}}{\sum_{j\in\mathcal{C}_n} e^{V_{jn}(x_n;\beta)}}}{\int_\gamma f(\gamma)\prod_{n=1}^{N}\frac{e^{V_{i_n n}(x_n;\gamma)}}{\sum_{j\in\mathcal{C}_n} e^{V_{jn}(x_n;\gamma)}}} \\
&\propto f(\beta)\prod_{n=1}^{N}\frac{e^{V_{i_n n}(x_n;\beta)}}{\sum_{j\in\mathcal{C}_n} e^{V_{jn}(x_n;\beta)}} \\
&\propto f(\beta)L(Y|\beta).
\end{aligned}$$

Markov chain Q: continuous case

Random walk

- Current state: $\beta_i \in \mathbb{R}^K$.
- Draw $\xi_i \in \mathbb{R}^K$ from $N(0, I)$.
- Next state: $\beta_j = \beta_i + \lambda\xi_i$.

$$Q_{ij} = Q_{ji} = \phi(\xi_i)$$
$$= \phi\left(\frac{\beta_j - \beta_i}{\lambda}\right).$$



Markov chain Q: continuous case

Reject criterion of MH

$$\begin{aligned}
\alpha_{ij} &= \min\left(\frac{b_j Q_{ji}}{b_i Q_{ij}}, 1\right) \\
&= \min\left(\frac{b_j}{b_i}, 1\right) \\
&= \min\left(\frac{f(\beta_j) L(Y|\beta_j)}{f(\beta_i) L(Y|\beta_i)}, 1\right)
\end{aligned}$$

- Ratio of posteriors.
- In the log-space, difference of log of posteriors.

Case study

Swissmetro

- a revolutionary mag-lev underground system in Switzerland,
- 500 km/h.

swissmetro.ch

Transportation mode choice

1. Train
2. Swissmetro
3. Car

The model

Variables

- Travel time: TRAIN_TT, SM_TT, CAR_TT.
- Travel cost: TRAIN_CO, SM_CO, CAR_CO.
- Yearly subscription: GA.

Utility functions

- ASC_TRAIN + B_TIME * TRAIN_TT + B_COST * TRAIN_CO * (GA == 0).
- B_TIME * SM_TT + B_COST * SM_CO * (GA == 0).
- ASC_CAR + B_TIME * CAR_TT + B_COST * CAR_CO.

Four unknown parameters.

Data

Stated preferences

- Collected in March 1998.
- 750 respondents.
- 6768 choice data.

Python code

```
def logPosteriorDensity(beta, loglike):
    prior = np.array([0, 0, 0, 0])
    variance = 100
    lognorm = lognormpdf(beta - prior)
    return loglike + lognorm / variance
```

Code for `lognormpdf` in the Appendix.

Python code

```
beta = np.array([0, 0, 0, 0])
loglike = biogeme.calculateLikelihood(beta)
logPosterior = logPosteriorDensity(beta, loglike)

T = 100000
draws = []
for total in range(T):
    ksi = np.random.normal(size=len(beta))
    next = beta + stepRandomWalk * ksi
    nextLoglike = biogeme.calculateLikelihood(next)
    logPosteriorNext = logPosteriorDensity(next, nextLoglike)

    diff = logPosteriorNext - logPosterior
    r = np.random.uniform()
    if np.log(r) <= diff:
        beta = next
        logPosterior = logPosteriorNext
    draws += [beta]
```

Tuning random-walk MH: acceptance vs mixing

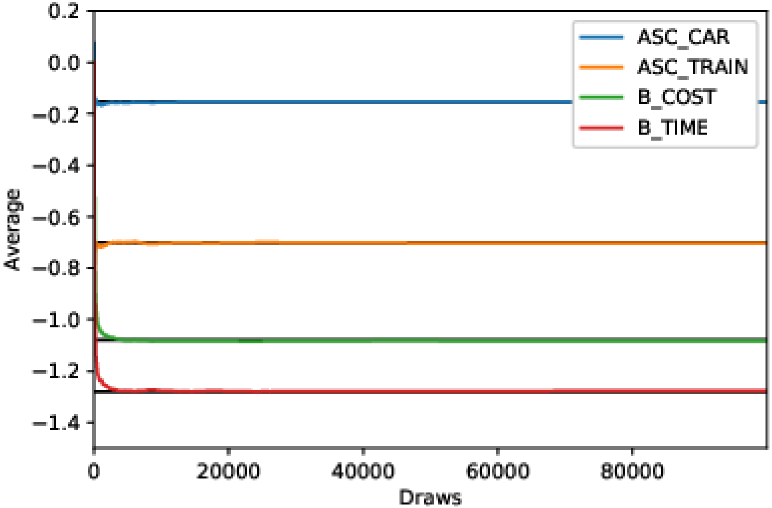
Two competing effects

- **Small step size λ:** high acceptance, but small moves $\Rightarrow$ slow exploration.
- **Large step size λ:** large moves, but low acceptance $\Rightarrow$ many repeats.

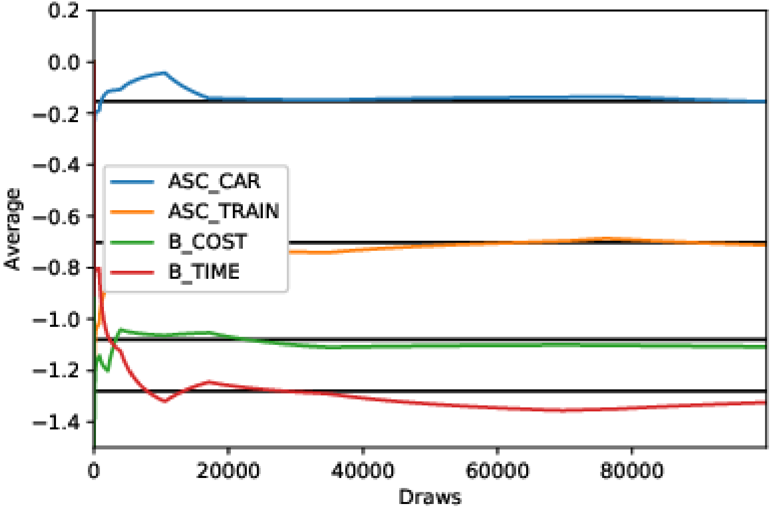
Key message

Acceptance rate alone is not a performance metric. We want good mixing: the chain should explore the target distribution efficiently.

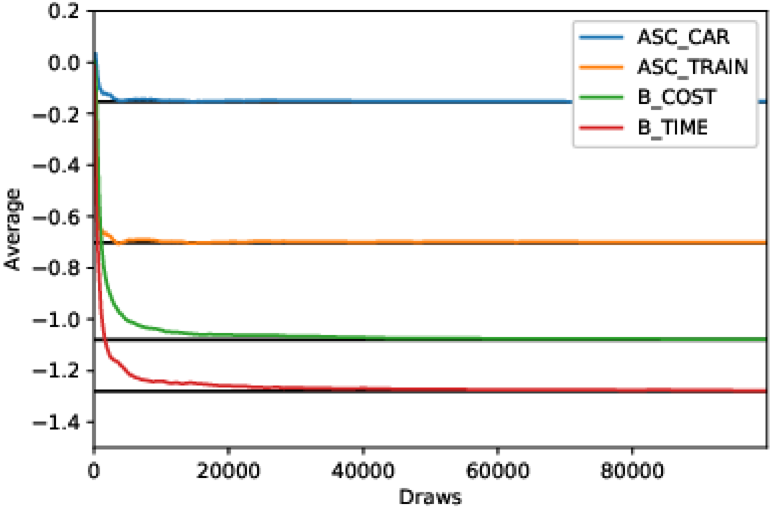
Step: $\lambda = 0.1$ — Accept rate: 7%



Step: $\lambda = 1$ — Accept rate: 0.02%

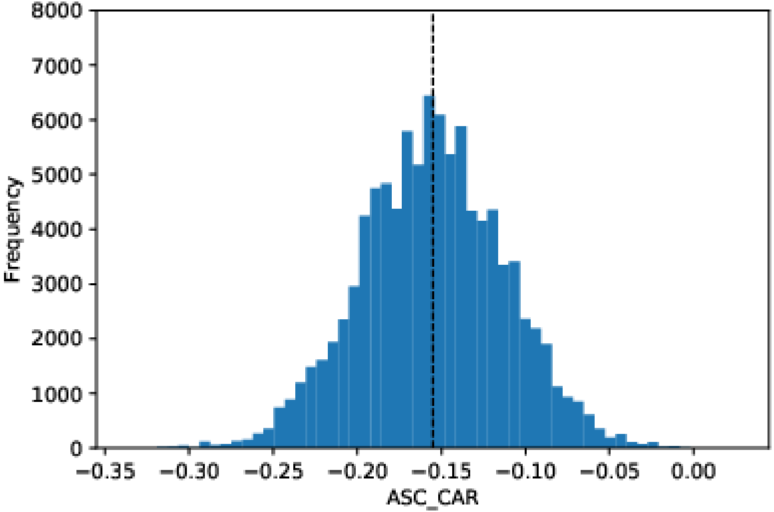


Step: $\lambda = 0.01$ — Accept rate: 78.2%



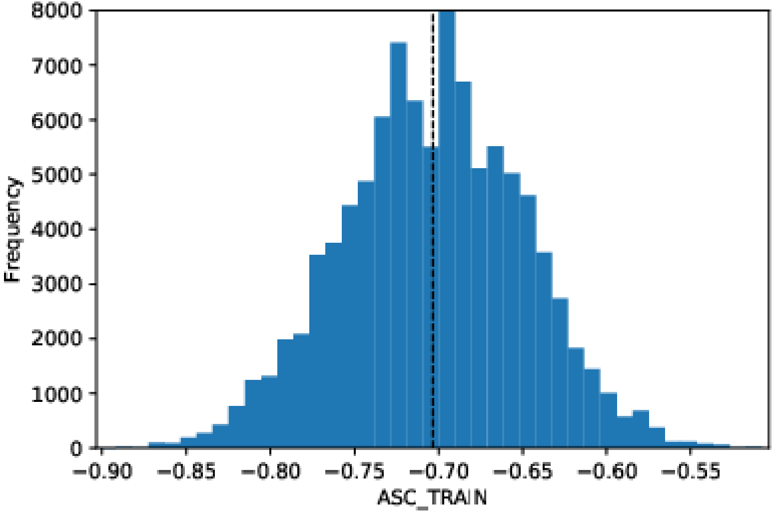
Distribution of the parameter: ASC_CAR

$\lambda = 0.1$, 2000 dropped



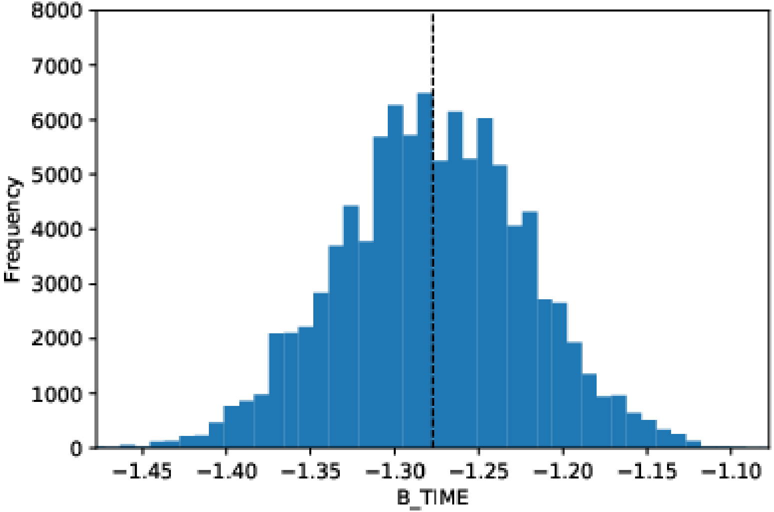
Distribution of the parameter: ASC_TRAIN

$\lambda = 0.1$, 2000 dropped



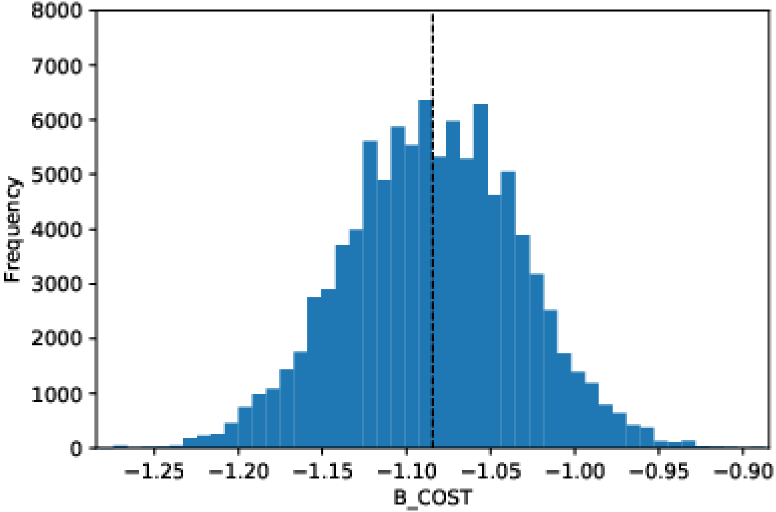
Distribution of the parameter: B_TIME

$\lambda = 0.1$, 2000 dropped



Distribution of the parameter: B_COST

$\lambda = 0.1$, 2000 dropped



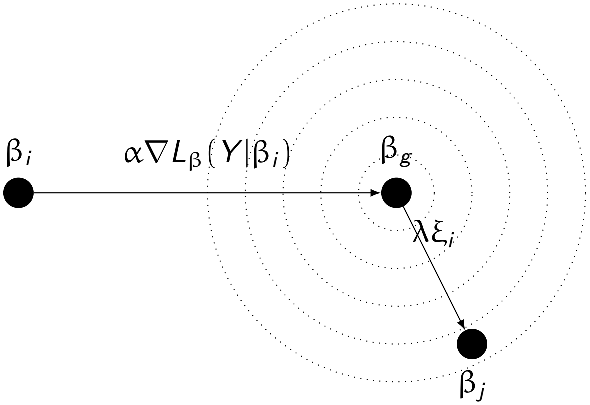
Markov chain: gradient based

Idea

- The gradient $\nabla L_\beta(Y|\beta)$ of the likelihood is an ascent direction.
- Instead of performing a random walk around β_i, we perform a random walk around
$$\beta_g = \beta_i + \alpha \nabla L_\beta(Y|\beta_i).$$
- Motivation: we want to bias the search towards higher values of the likelihood.

Markov chain: gradient based

Idea

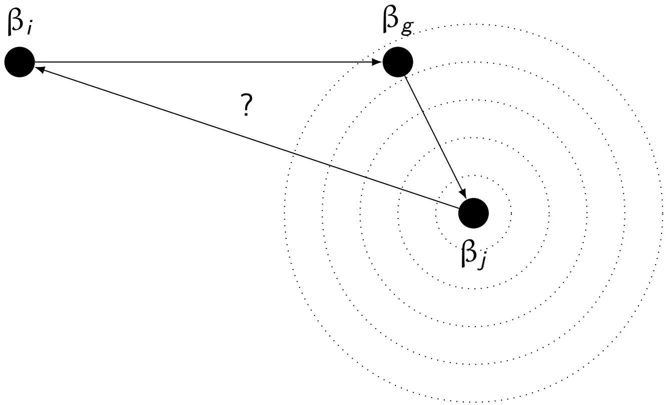


Reject criterion of MH

- Forward transition probability:

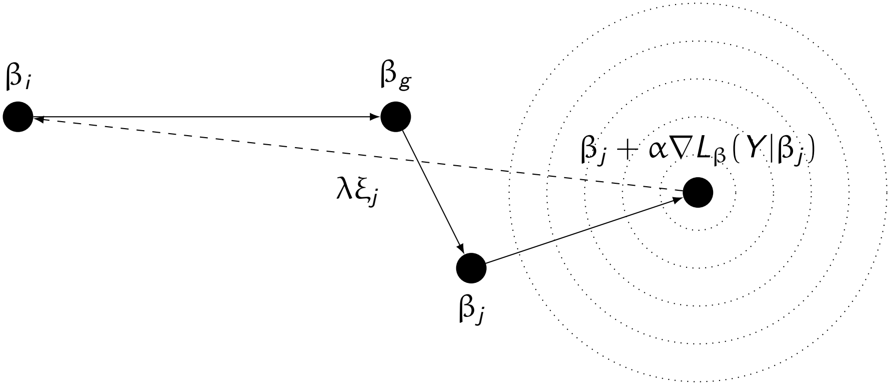
$$Q_{ij} = \phi(\xi_i).$$

- Backward transition probability:

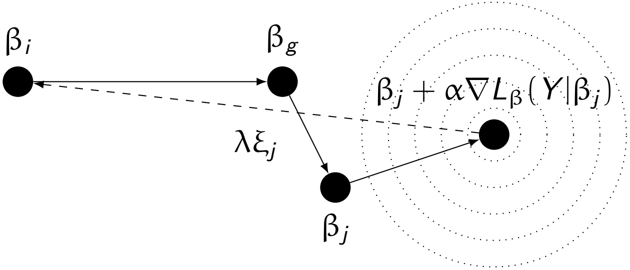


Reject criterion of MH

Backward transition probability



Reject criterion of MH



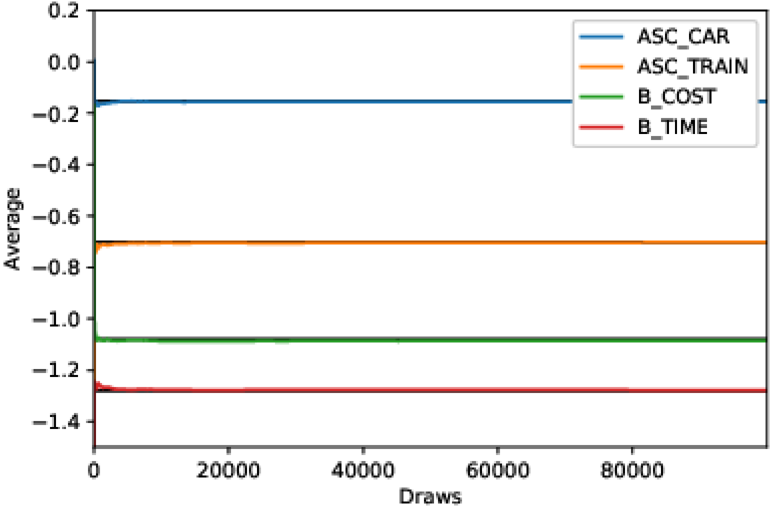
$$\beta_i = \beta_j + \alpha \nabla L_\beta(Y|\beta_j) + \lambda\xi_j$$

$$Q_{ji} = \phi(\xi_j) = \phi\left(\frac{\beta_i - \beta_j - \alpha \nabla L_\beta(Y|\beta_j)}{\lambda}\right)$$

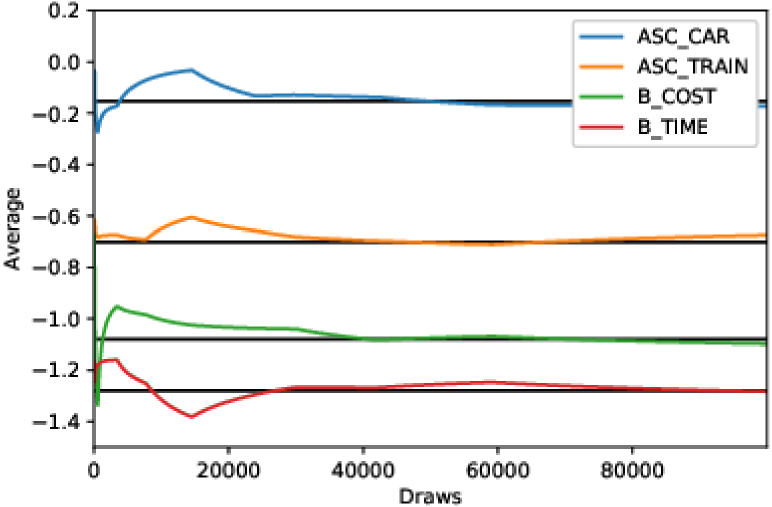
Python code

```
beta = firstBeta
loglike, g, _, _ = biogeme.calculateLikelihoodAndDerivatives(beta)
betaGrad = beta + stepGradient * g
logPosterior =  logPosteriorDensity(beta, loglike)

T = 5000
draws = []
for total in range(T):
    ksi = np.random.normal(size=len(beta))
    next = betaGrad + stepRandomWalk * ksi
    nextLoglike, nextg, _, _ = biogeme.calculateLikelihoodAndDerivatives(next)
    nextGrad = next + stepGradient * nextg
    logPosteriorNext = logPosteriorDensity(next, nextLoglike)

    logQij = lognormpdf(ksi)

    ksiback = (beta - nextGrad) / stepRandomWalk
    logQji = lognormpdf(ksiback)

    diff = logPosteriorNext + logQji - logPosterior - logQij
    r = np.random.uniform()
    if np.log(r) <= diff:
        beta = next
        loglike = nextLoglike
        g = nextg
        betaGrad = nextGrad
        logPosterior = logPosteriorNext
    draws += [beta]
```

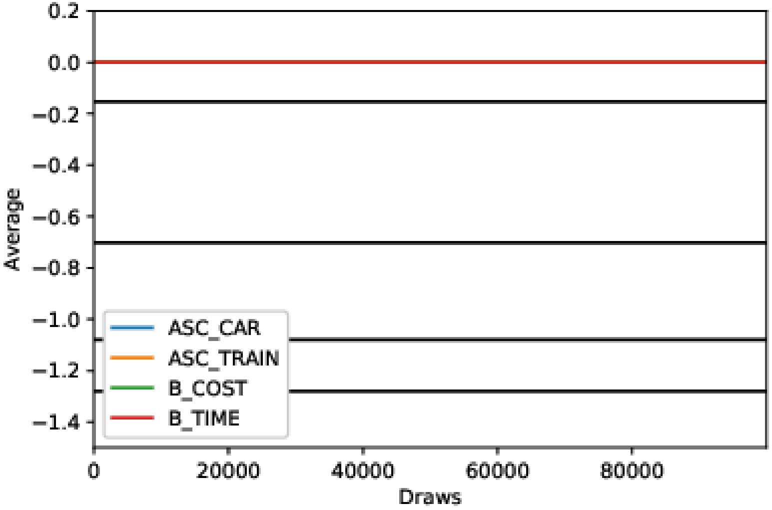
Step: $\lambda = 0.1$ — Accept rate: 8.6%



Step: $\lambda = 1$ — Accept rate: 0.01%

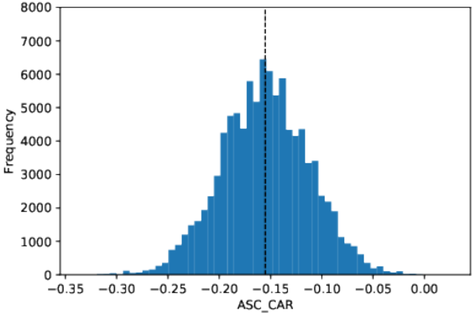


Step: $\lambda = 0.01$ — Accept rate: 0%

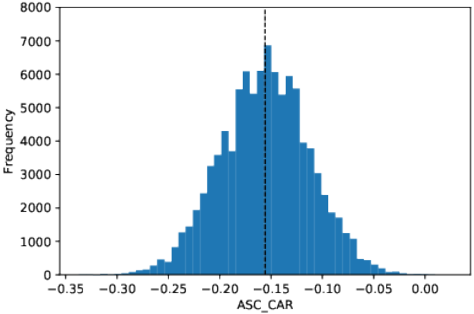


Distribution of the parameter: ASC_CAR

$\lambda = 0.1$, 2000 dropped



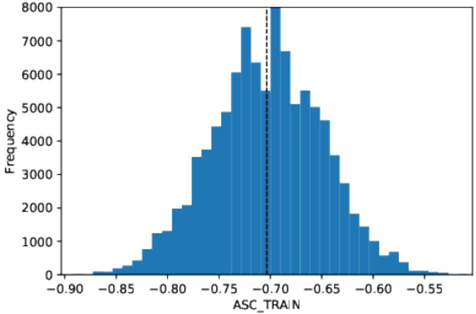
Random walk



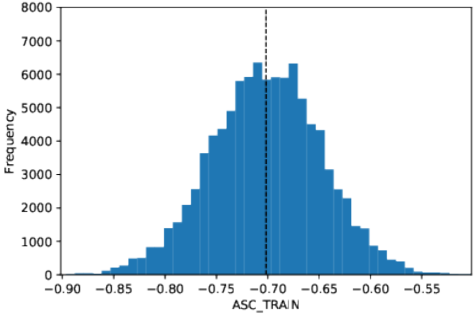
Gradient based

Distribution of the parameter: ASC_TRAIN

$\lambda = 0.1$, 2000 dropped



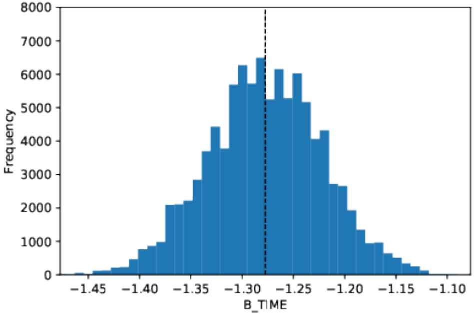
Random walk



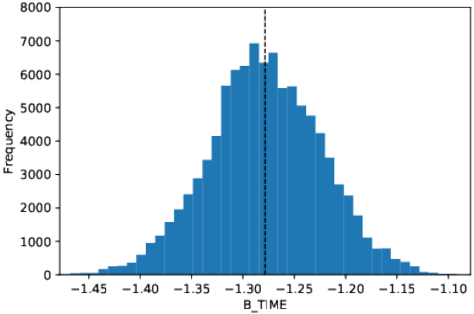
Gradient based

Distribution of the parameter: B_TIME

$\lambda = 0.1$, 2000 dropped



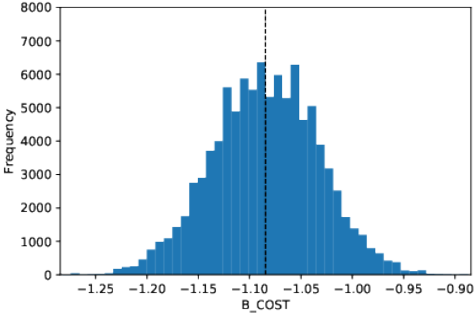
Random walk



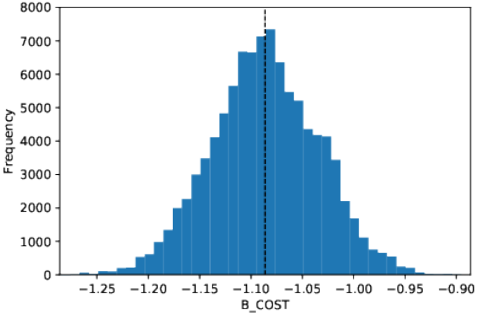
Gradient based

Distribution of the parameter: B_COST

$\lambda = 0.1$, 2000 dropped



Random walk



Gradient based

Mixed strategy: idea

Why mix proposal mechanisms?

- Random-walk proposals explore locally but can be slow.
- Gradient-based proposals move toward high-density regions but may get stuck or be unstable.
- A mixed strategy combines robustness and efficiency.

Key principle

At each iteration, we randomly choose <u>how</u> to propose the next state.

Mixed strategy: proposal mechanism

Two proposal kernels

From the current state β_i:

- **Random walk (probability p):**

$$\beta_j = \beta_i + \lambda\xi, \qquad \xi \sim N(0, I).$$

- **Gradient-based move (probability $1-p$):**

$$\beta_g = \beta_i + \alpha\nabla L_\beta(Y \mid \beta_i), \qquad \beta_j = \beta_g + \lambda\xi.$$

Two-stage randomness

1. Choose the move type.
2. Draw the Gaussian noise ξ.

Mixed strategy: Metropolis–Hastings

Mixture proposal density

The proposal density is a mixture:

$$Q_{ij} = p\, Q_{ij}^{\mathrm{RW}} + (1-p)\, Q_{ij}^{\mathrm{Grad}}.$$

The backward density Q_{ji} is defined analogously.

Acceptance probability

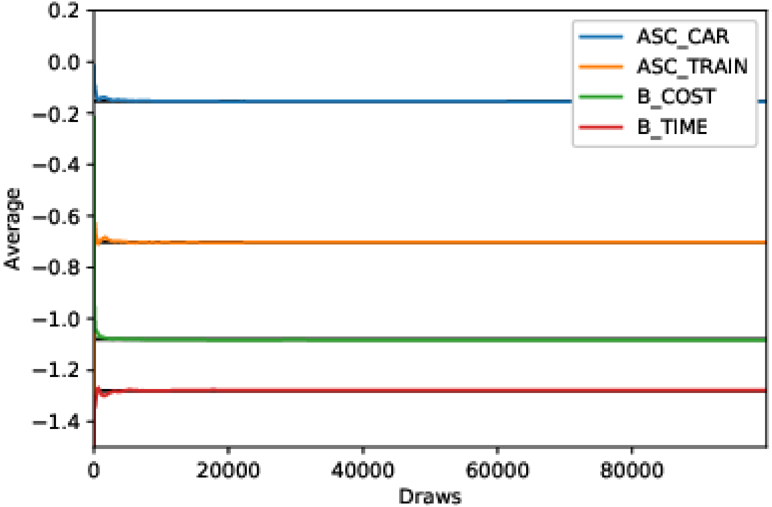
The Metropolis–Hastings acceptance rule is unchanged:

$$\alpha_{ij} = \min\left(\frac{b_j Q_{ji}}{b_i Q_{ij}}, 1\right).$$

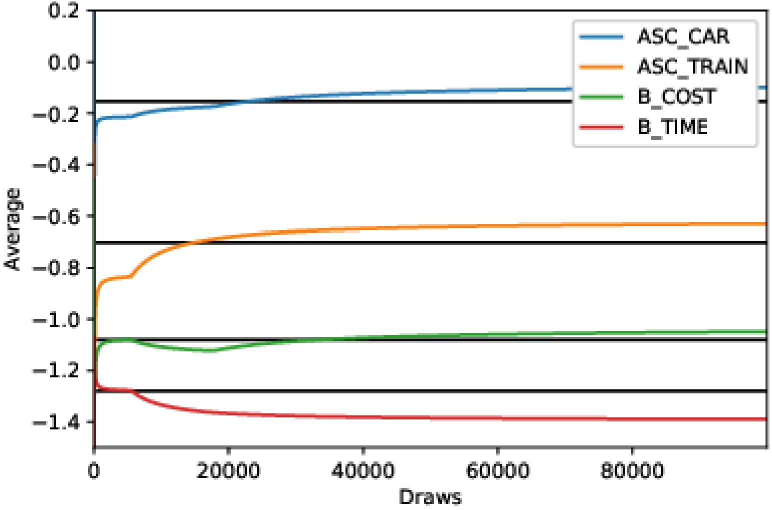
Key point

Metropolis–Hastings remains valid as long as the same mixture density is used consistently in forward and backward transitions.

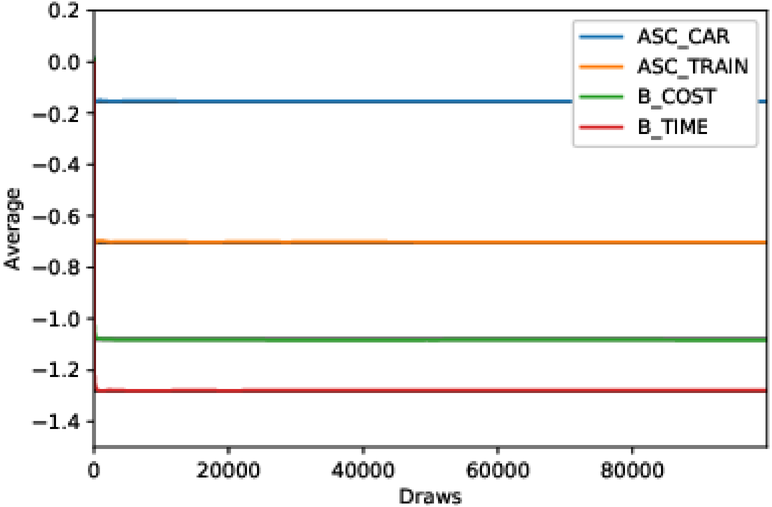
Step: $\lambda = 0.1$ — Accept rate: 8.3%



Step: $\lambda = 1$ — Accept rate: 0.009%

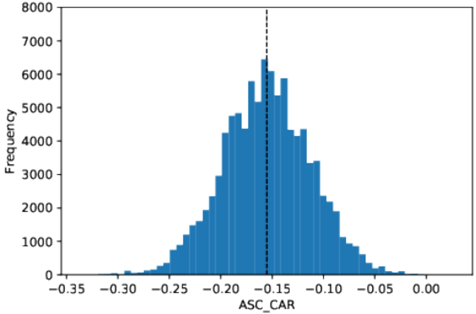


Step: $\lambda = 0.01$ — Accept rate: 63.24%

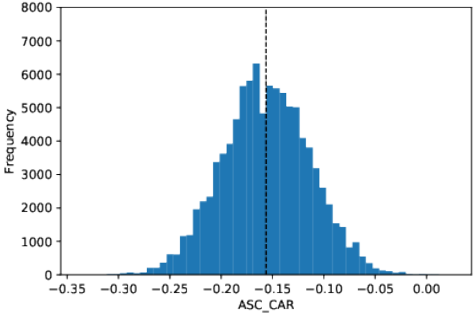


Distribution of the parameter: ASC_CAR

$\lambda = 0.1$, 2000 dropped



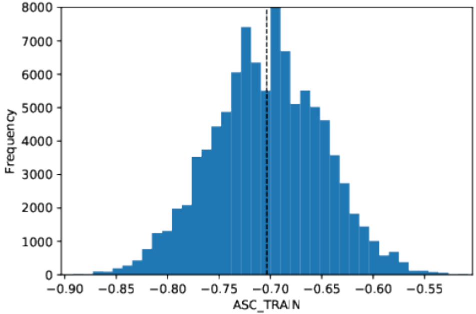
Random walk



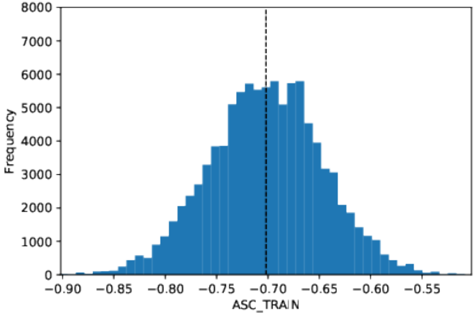
Mixed

Distribution of the parameter: ASC_TRAIN

$\lambda = 0.1$, 2000 dropped



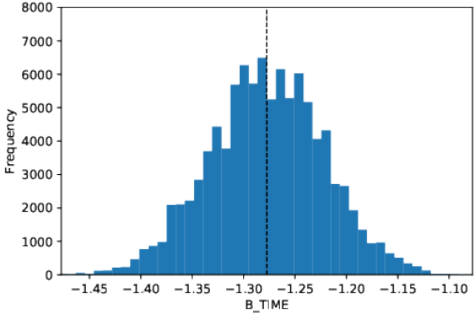
Random walk



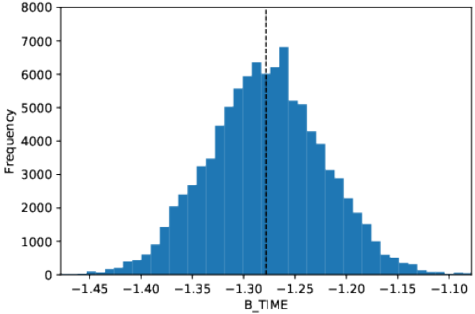
Mixed

Distribution of the parameter: B_TIME

$\lambda = 0.1$, 2000 dropped



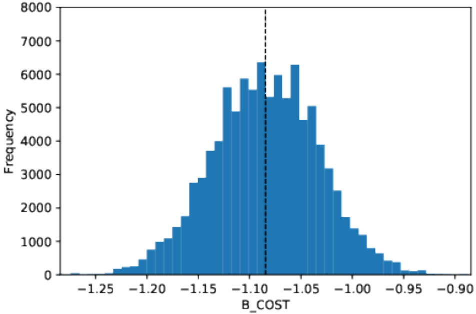
Random walk



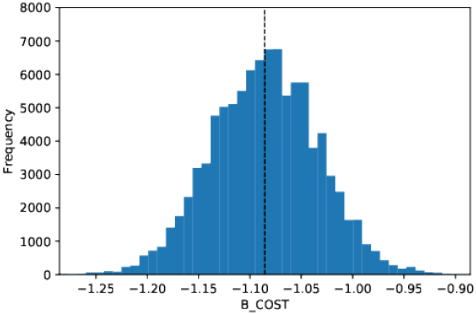
Mixed

Distribution of the parameter: B_COST

$\lambda = 0.1$, 2000 dropped



Random walk



Mixed

Practical considerations

Multiple starting points

- Generate multiple Markov chains.
- Initialize each sequence with a different value.

Stationarity

- Chains must have reached stationarity.
- How do we detect it?

Correlation

- Within sequences.
- Across sequences.
- It may generate inefficiencies in the simulation.

Sequences management

Generate S sequences of length N'

$s = 1$

$s = 2$

$s = 3$

$s = 4$

Sequences management

Warm-up: drop half of each sequence

$s = 1$

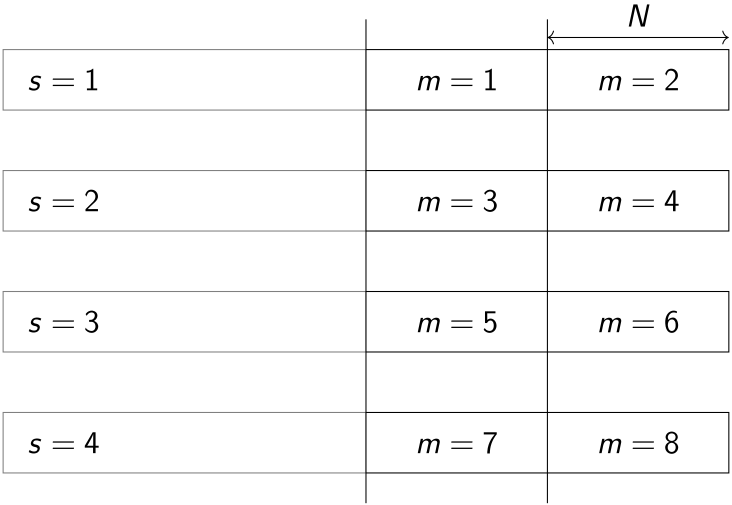
$s = 2$

$s = 3$

$s = 4$

Sequences management

Split each sequence into two to obtain M sequences of length $N = N'/4$



Between-sequence variance

Let θ be the parameter of interest, and θ_{nm} draw n from sequence m.

$$B = \frac{N}{M-1}\sum_{m=1}^{M}(\bar{\theta}_m - \bar{\theta})^2,$$

where

$$\bar{\theta}_m = \frac{1}{N}\sum_{n=1}^{N}\theta_{nm} \quad \text{mean of each sequence}$$

$$\bar{\theta} = \frac{1}{M}\sum_{m=1}^{M}\bar{\theta}_m \qquad \text{mean of the mean}$$

Within-sequence variance

$$W = \frac{1}{M} \sum_{m=1}^{M} v_m^2$$

where

$$v_m^2 = \frac{1}{N-1} \sum_{n=1}^{N} (\theta_{nm} - \bar{\theta}_m)^2.$$

How long should the sequences be?

Potential scale reduction (Gelman–Rubin)

$$\widehat{R}_N = \sqrt{\frac{N-1}{N} + \frac{1}{N}\frac{B}{W}}.$$

Interpretation

- $\widehat{R}_N \to 1$ as N increases (when chains have mixed).
- Choose N such that $\widehat{R}_N \leqslant 1.1$.

See Gelman et al. (2013) Section 11.4.

Practical considerations: warm-up and stationarity

Warm-up (burn-in)

- Early iterations depend strongly on initialization.
- Discard an initial part of each chain before collecting statistics.

Stationarity (informal)

- After warm-up, the chain should behave as if it were sampling from the target.
- Diagnostics help detect lack of mixing / non-stationarity.

Practical considerations: multiple chains

Why multiple chains?

- Run several chains from dispersed starting points.
- Compare their behavior to detect convergence problems.

Gelman–Rubin diagnostic

- $\widehat{R}$ compares between-chain and within-chain variability.
- Values close to 1 indicate that chains mix similarly.

Autocorrelation and effective sample size

Why MCMC is different from i.i.d. simulation

Successive draws from a Markov chain are typically correlated:

$$\mathrm{Corr}(X_t, X_{t+k}) \neq 0.$$

Consequence

Correlation reduces the amount of information in T iterations. We summarize this by the effective sample size (ESS):

$$\mathrm{ESS} \leqslant T.$$

Practical takeaway

More iterations are not always better: we want low autocorrelation and good mixing.

Practical considerations: quick checklist

What to monitor

- trace plots (drift? jumps? sticking?),
- acceptance rate (too low? too high?),
- $\widehat{R}$ across chains,
- ESS / autocorrelation (how much independent information?).

Rule of thumb

If diagnostics disagree, trust the most conservative one and run longer / retune.

Outline

Gibbs sampling

Motivation

- Draw from multivariate distributions.
- Main difficulty: deal with correlations.

Metropolis-Hastings

- Let $X = (X^1, X^2, \ldots, X^n)$ be a random vector with pmf (or pdf) $p(x)$.
- Assume we can draw from the conditionals:

$$\Pr(X^i | X^j = x^j,\ j \neq i),\ i = 1, \ldots, n.$$

- Markov process. Assume current state is x.
  - Draw randomly (equal probability) a coordinate i.
  - Draw r from the ith conditional.
  - New state: $y = (x^1, \ldots, x^{i-1}, r, x^{i+1}, \ldots, x^n)$.

Gibbs sampling

Transition probability

$$Q_{xy} = \frac{1}{n} \Pr(X^i = r | X^j = x^j,\ j \neq i) = \frac{p(y)}{n \Pr(X^j = x^j,\ j \neq i)}$$

- The denominator is independent of X^i.
- So Q_{xy} is proportional to $p(y)$.

Metropolis-Hastings

$$\alpha_{xy} = \min\left(\frac{p(y)\, Q_{yx}}{p(x)\, Q_{xy}}, 1\right) = \min\left(\frac{p(y) p(x)}{p(x) p(y)}, 1\right) = 1$$

The candidate state is always accepted.

Example: bivariate normal distribution

$$\begin{pmatrix} X \\ Y \end{pmatrix} \sim N\left(\begin{pmatrix} \mu_X \\ \mu_Y \end{pmatrix}, \begin{pmatrix} \sigma_X^2 & \rho\sigma_X\sigma_Y \\ \rho\sigma_X\sigma_Y & \sigma_Y^2 \end{pmatrix}\right)$$

Marginal distribution:

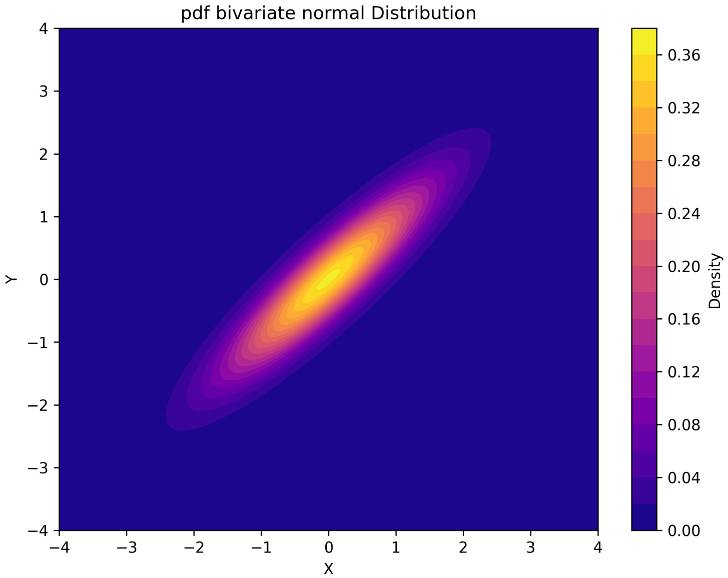
$$Y|(X = x) \sim N\left(\mu_Y + \frac{\sigma_Y}{\sigma_X}\rho(x - \mu_X), (1 - \rho^2)\sigma_Y^2\right)$$

Apply Gibbs sampling to draw from:

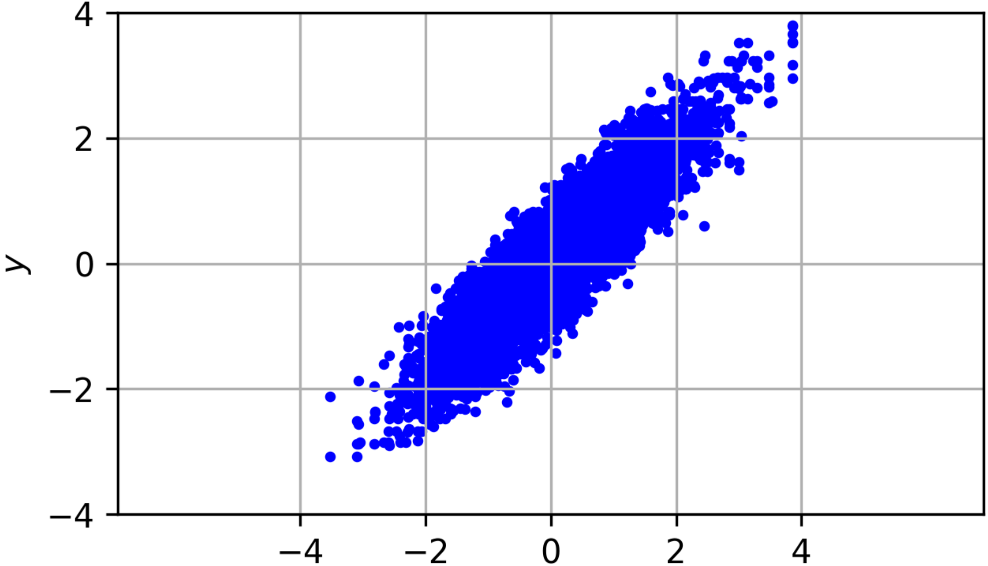
$$N\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & 0.9 \\ 0.9 & 1 \end{pmatrix}\right)$$

Note: just for illustration. Should use Cholesky factor.

Example: pdf


pdf bivariate normal Distribution
4
3
2
1
0
−1
−2
−3
−4
Y
−4
−3
−2
−1
0
1
2
3
4
X
0.36
0.32
0.28
0.24
0.20
0.16
0.12
0.08
0.04
0.00
Density

Example: draws from Gibbs sampling



Outline

Simulated annealing

Combinatorial optimization

$$\min_{x \in \mathcal{F}} f(x)$$

where the feasible set $\mathcal{F}$ is a large finite set of vectors.

Set of optimal solutions

$$\mathcal{X}^* = \{x \in \mathcal{F} | f(x) \leqslant f(y),\ \forall y \in \mathcal{F}\} \text{ and } f(x^*) = f^*,\ \forall x^* \in \mathcal{X}^*.$$

Probability mass function on $\mathcal{F}$

$$p_\lambda(x) = \frac{e^{-\lambda f(x)}}{\sum_{y \in \mathcal{F}} e^{-\lambda f(y)}},\ \lambda > 0.$$

Simulated annealing

$$p_\lambda(x) = \frac{e^{-\lambda f(x)}}{\sum_{y \in \mathcal{F}} e^{-\lambda f(y)}}$$

- Equivalently

$$p_\lambda(x) = \frac{e^{\lambda(f^* - f(x))}}{\sum_{y \in \mathcal{F}} e^{\lambda(f^* - f(y))}}$$

- As $f^* - f(x) \leqslant 0$, when $\lambda \to \infty$, we have

$$\lim_{\lambda \to \infty} p_\lambda(x) = \frac{\delta(x \in \mathcal{X}^*)}{|\mathcal{X}^*|},$$

where

$$\delta(x \in \mathcal{X}^*) = \begin{cases} 1 & \text{if } x \in \mathcal{X}^* \\ 0 & \text{otherwise.} \end{cases}$$

Example

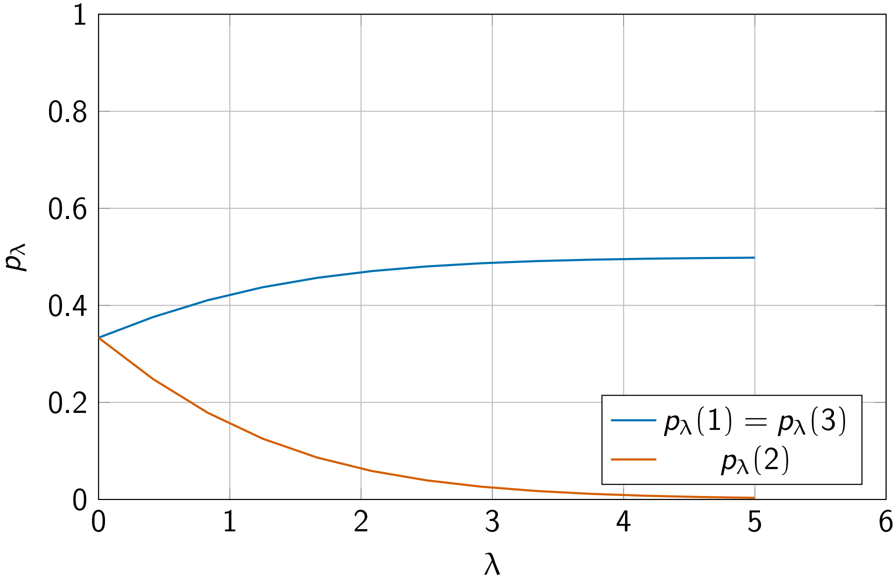
$$\mathcal{F} = \{1, 2, 3\}, \quad f(\mathcal{F}) = \{0, 1, 0\}.$$

$$p_\lambda(1) = \frac{1}{2 + e^{-\lambda}},$$

$$p_\lambda(2) = \frac{e^{-\lambda}}{2 + e^{-\lambda}},$$

$$p_\lambda(3) = \frac{1}{2 + e^{-\lambda}}.$$

Example



1
0.8
0.6
0.4
0.2
0
p_λ
0
1
2
3
4
5
6
λ
$p_\lambda(1) = p_\lambda(3)$
$p_\lambda(2)$

Simulated annealing

- If λ is large,
- we generate a Markov chain with stationary distribution $p_\lambda(x)$.
- The mass is concentrated on optimal solutions.
- As the normalizing constant is not needed, only $e^{\lambda(f^* - f(x))}$ is used.
- Construction of the Markov process through the concept of <u>neighborhood</u>.
- A <u>neighbor</u> y of x is obtained by simple modifications of x.
- The Markov process will proceed from neighbors to neighbors.
- The neighborhood structure must be designed such that the chain is irreducible, that is the whole space $\mathcal{F}$ must be covered.
- It must be designed also such that the size of the neighborhood is reasonably small.

Neighborhood

Metropolis-Hastings

- Denote $N(x)$ the set of neighbors of x.
- Define a Markov process where the next state is a randomly drawn neighbor.
- Transition probability:

$$Q_{xy} = \frac{1}{|N(x)|}$$

- Metropolis Hastings:

$$\alpha_{xy} = \min\left(\frac{p(y)Q_{yx}}{p(x)Q_{xy}}, 1\right) = \min\left(\frac{e^{-\lambda f(y)}|N(x)|}{e^{-\lambda f(x)}|N(y)|}, 1\right)$$

Neighborhood

Notes

- The neighborhood structure can always be arranged so that each vector has the same number of neighbors. In this case,

$$\alpha_{xy} = \min\left(\frac{e^{-\lambda f(y)}}{e^{-\lambda f(x)}}, 1\right)$$

- If y is better than x, the next state is automatically accepted.
- Otherwise, it is accepted with a probability that depends on λ.
- If λ is high, the probability is small.
- When λ is small, it is easy to escape from local optima.

Heuristic

Issue

- The number of iterations needed to reach a stationary state and draw an optimal solution may exceed the number of feasible solutions in the set.
- The acceptance probability is very small.
- Therefore, a complete enumeration works better.
- The method is used as a heuristic.

Takeaways

Core ideas

- MCMC draws from a target $\pi(x) \propto b(x)$ without computing normalizing constants.
- Metropolis–Hastings: propose with $q(\cdot \mid x)$, correct with an acceptance probability.
- Gibbs sampling: special case where proposals are always accepted.

Practice

- Tuning matters (step size, proposal design).
- Diagnose: warm-up, mixing, autocorrelation, $\widehat{R}$, ESS.
- Use draws for expectations and posterior predictive quantities.

Outline

Markov Chains

Andrey Markov, 1856–1922, Russian mathematician.

Markov Chains: glossary

Stochastic process

X_t, $t = 0, 1, \ldots,$, collection of r.v. with same support, or state space $\{1, \ldots, i, \ldots, J\}$.

Markov process: (short memory)

$$\Pr(X_t = i | X_0, \ldots, X_{t-1}) = \Pr(X_t = i | X_{t-1})$$

Homogeneous Markov process

$$\Pr(X_t = j | X_{t-1} = i) = \Pr(X_{t+k} = j | X_{t-1+k} = i) = P_{ij} \;\; \forall t \geqslant 1, k \geqslant 0.$$

Markov Chains

Transition matrix

$$P \in \mathbb{R}^{J \times J}.$$

Properties:

$$\sum_{j=1}^{J} P_{ij} = 1, \; i = 1, \ldots, J, \quad P_{ij} \geqslant 0, \; \forall i, j,$$

Ergodicity

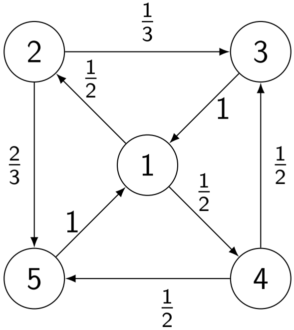
- If state j can be reached from state i with non zero probability, and i from j, we say that i communicates with j.
- Two states that communicate belong to the same class.
- A Markov chain is irreducible or ergodic if it contains only one class.
- With an ergodic chain, it is possible to go to every state from any state.

Markov Chains

Aperiodic

- P_{ij}^t is the probability that the process reaches state j from i after t steps.
- Consider all t such that $P_{ii}^t > 0$. The largest common divisor d is called the period of state i.
- A state with period 1 is aperiodic.
- If $P_{ii} > 0$, state i is aperiodic.
- The period is the same for all states in the same class.
- Therefore, if the chain is irreducible, if one state is aperiodic, they all are.

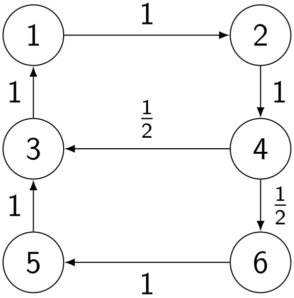
A periodic chain



$$P = \begin{pmatrix} 0 & \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & 0 & \frac{1}{3} & 0 & \frac{2}{3} \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 & \frac{1}{2} \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad d = 3.$$

$$P_{ii}^t > 0 \text{ for } t = 3, 6, 9, 12, 15 \ldots$$

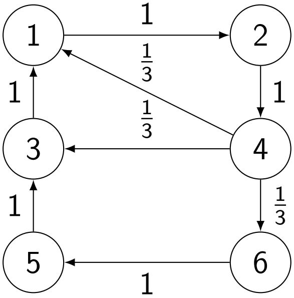
Another periodic chain



$$P = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \quad d = 2.$$

$$P_{ii}^t > 0 \text{ for } t = 4, 6, 8, 10, 12, \ldots$$

An aperiodic chain



$$P = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{3} & 0 & \frac{1}{3} & 0 & 0 & \frac{1}{3} \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \quad d = 1.$$

$P_{ii}^t > 0$ for $t = 3, 4, 6, 7, 8, 9, 10, 11, 12 \ldots$

Aperiodic chain

An equivalent definition

An irreducible Markov chain is said to be aperiodic if for some $t \geqslant 0$ and some state i, we have

$$\Pr(X_t = i | X_0 = i) > 0$$

and

$$\Pr(X_{t+1} = i | X_0 = i) > 0$$

Intuition

Oscillation

$$P = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

The chain will not "converge" to something stable.

Outline

Markov Chains

Stationary probabilities

$$\Pr(j) = \sum_{i=1}^{J} \Pr(j|i)\Pr(i)$$

- Stationary probabilities: unique solution of the system

$$\pi_j = \sum_{i=1}^{J} P_{ij}\pi_i, \quad \forall j = 1, \ldots, J. \tag{1}$$

$$\sum_{j=1}^{J} \pi_j = 1.$$

- Solution exists for any irreducible chain.

Example

- A machine can be in 4 states with respect to wear
  - perfect condition,
  - partially damaged,
  - seriously damaged,
  - completely useless.
- The degradation process can be modeled by an irreducible aperiodic homogeneous Markov process, with the following transition matrix:

$$P = \begin{pmatrix} 0.95 & 0.04 & 0.01 & 0.0 \\ 0.0 & 0.90 & 0.05 & 0.05 \\ 0.0 & 0.0 & 0.80 & 0.20 \\ 1.0 & 0.0 & 0.0 & 0.0 \end{pmatrix}$$

Example

Stationary distribution: $\left(\frac{5}{8}, \frac{1}{4}, \frac{3}{32}, \frac{1}{32}\right)$

$$\left(\frac{5}{8}, \frac{1}{4}, \frac{3}{32}, \frac{1}{32}\right) \begin{pmatrix} 0.95 & 0.04 & 0.01 & 0.0 \\ 0.0 & 0.90 & 0.05 & 0.05 \\ 0.0 & 0.0 & 0.80 & 0.20 \\ 1.0 & 0.0 & 0.0 & 0.0 \end{pmatrix} = \left(\frac{5}{8}, \frac{1}{4}, \frac{3}{32}, \frac{1}{32}\right)$$

- Machine in perfect condition 5 days out of 8, in average.
- Repair occurs in average every 32 days

From now on: Markov process = irreducible aperiodic homogeneous Markov process

Markov Chains

Detailed balance equations

Consider the following system of equations:

$$x_i P_{ij} = x_j P_{ji}, \quad i \neq j, \quad \sum_{i=1}^{J} x_i = 1 \tag{2}$$

We sum over i:

$$\sum_{i=1}^{J} x_i P_{ij} = x_j \sum_{i=1}^{J} P_{ji} = x_j.$$

If (2) has a solution, it is also a solution of (1). As π is the unique solution of (1) then $x = \pi$.

$$\pi_i P_{ij} = \pi_j P_{ji}, \quad i \neq j$$

The chain is said <u>time reversible</u>

Stationary distributions

Property of irreducible aperiodic Markov chains

$$\pi_j = \lim_{t \to \infty} \Pr(X_t = j) \quad j = 1, \ldots, J.$$

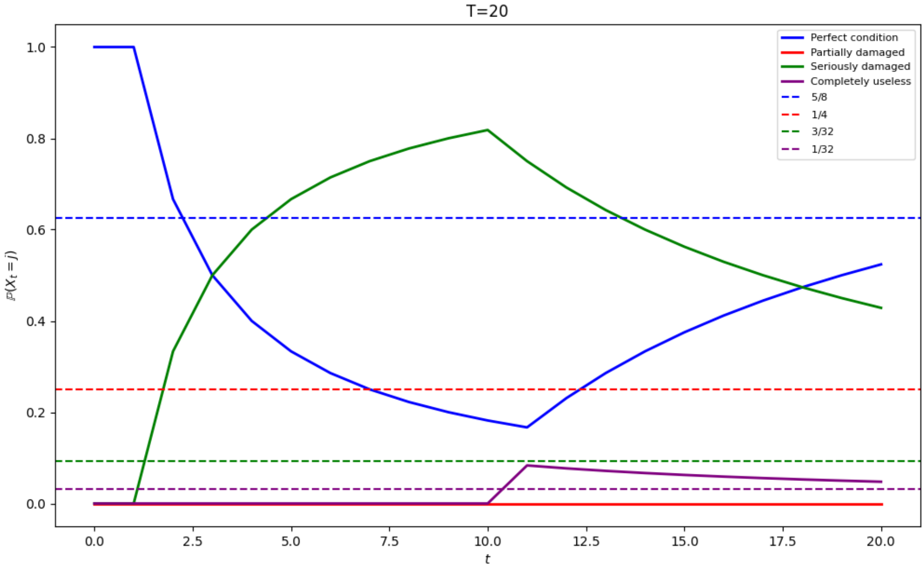
Ergodicity

- Let f be any function on the state space.
- Then, with probability 1,

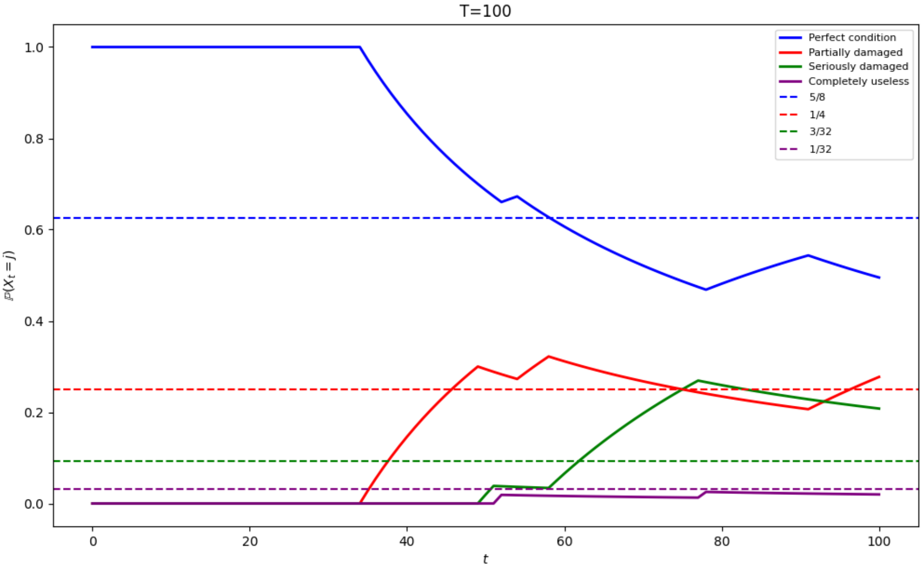
$$\lim_{T \to \infty} \frac{1}{T} \sum_{t=1}^{T} f(X_t) = \sum_{j=1}^{J} \pi_j f(j).$$

- Computing the expectation of a function of the stationary states is the same as to take the average of the values along a trajectory of the process.

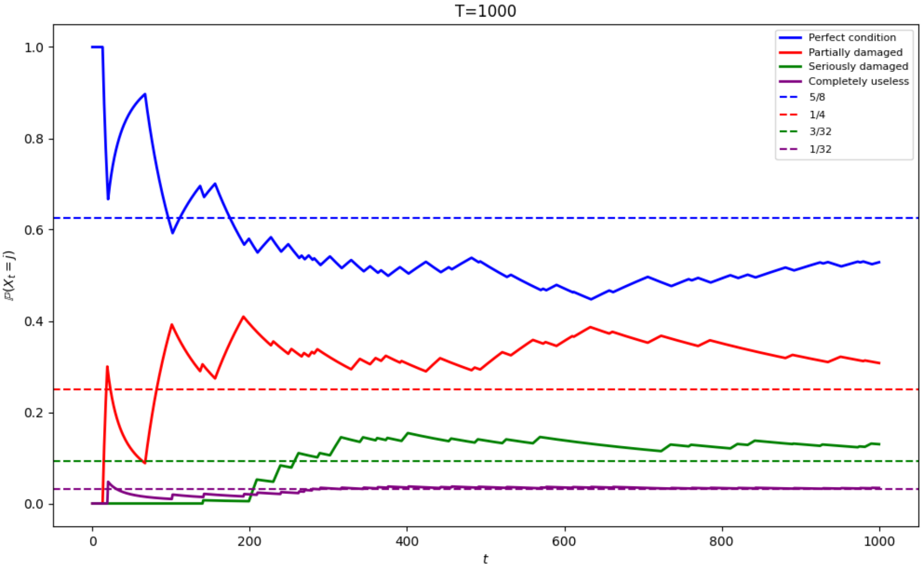
Example: $T = 20$


T=20
1.0
0.8
0.6
0.4
0.2
0.0
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
t
$\mathbb{P}(X_t = j)$
Perfect condition
Partially damaged
Seriously damaged
Completely useless
5/8
1/4
3/32
1/32

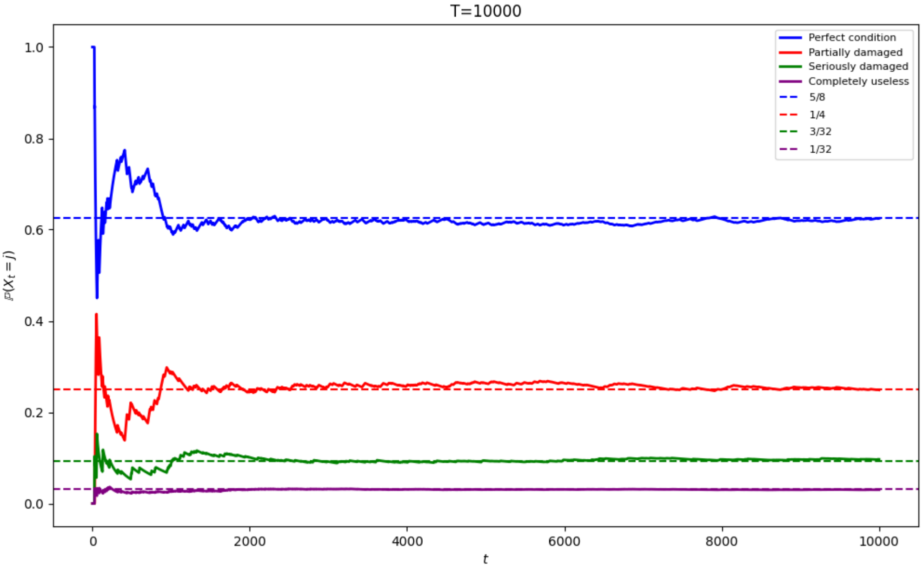
Example: $T = 100$



Example: $T = 1000$



Example: $T = 10000$



A periodic example

It does not work for periodic chains

$$P = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\Pr(X_t = 1) = \begin{cases} 1 & \text{if } t \text{ is odd} \\ 0 & \text{if } t \text{ is even} \end{cases}$$

$$\lim_{t \to \infty} \Pr(X_t = 1) \text{ does not exist}$$

Stationary distribution

$$\pi = \begin{pmatrix} 0.5 \\ 0.5 \end{pmatrix}$$

Python code

```
def lognormpdf(x,mu=None,S=None):
    """ log of gaussian pdf of x, when x ~ N(mu,sigma) """
    nx = x.size
    if mu is None:
        mu = np.array([0]*nx)
    if S is None:
        S = np.identity(nx)

    norm_coeff = nx*np.log(2*np.pi)+np.linalg.slogdet(S)[1]

    err = x-mu
    if (sp.issparse(S)):
        numerator = spln.spsolve(S, err).T.dot(err)
    else:
        numerator = np.linalg.solve(S, err).T.dot(err)

    return -0.5*(norm_coeff+numerator)
```