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# Locally-informed proposals in Metropolis-Hastings algorithm with applications

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# Markov chain

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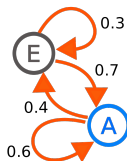
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## Definition

A Markov chain is a stochastic process describing a sequence on some countable state space  $S$  in which the probability of each event depends only on the state of previous event.

## Definition

Such a chain is uniquely defined by a stochastic transition matrix  $\mathbf{P}$  and a initial distribution  $\mu$ .



**Figure:** A diagram representing a two-state Markov chain, source: wiki.

# Properties

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## Definition (Irreducibility)

A Markov chain is irreducible if there is a possibility to reach every state from every state.

## Definition (Aperiodicity)

A state is aperiodic if there is a possibility of coming back to it after each step. A Markov chain is aperiodic when every state is irreducible and a state is aperiodic.

# Ergodic chains

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## Definition (Stationarity)

A probability distribution  $\pi = (\pi_1, \dots, \pi_N)$  is called stationary if it satisfies

$$\pi_j = \sum_{i \in S} \pi_i p_{ij},$$

## Definition (Ergodicity)

A Markov chain is ergodic when it is irreducible and aperiodic.

## Theorem

*Let  $\{X_k\}$  be a ergodic Markov chain with a transition matrix  $P$ , then:*

$$\lim_{k \rightarrow \infty} p_{ij}(k) = \pi_j.$$

# Metropolis-Hastings algorithm

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Construct a MC, which has a stationary distribution  $\pi$  ( $\pi_i > 0$ ). Assume that  $\mathbf{Q}$  is stochastic matrix which corresponds to an irreducible and aperiodic Markov chain and  $\mathbf{Q}_{i,j} > 0 \iff \mathbf{Q}_{j,i} > 0$ . Let us consider a matrix defined as:

$$\mathbf{P}_{i,j} = \begin{cases} \mathbf{Q}_{i,j} \min \left( 1, \frac{\pi_j \mathbf{Q}_{j,i}}{\pi_i \mathbf{Q}_{i,j}} \right) & \text{if } i \neq j, \\ 1 - \sum_{j \in S \setminus \{i\}} \mathbf{P}_{i,j} & \text{if } i = j. \end{cases} \quad (1)$$

## Theorem

*A matrix defined in (1) is stochastic, irreducible, aperiodic and has a stationary distribution  $\pi$ .*

# Metropolis-Hastings algorithm

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## Algorithm Metropolis-Hastings algorithm

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- 1: Choose a state  $i \in S$ .
  - 2:  $X_0 \leftarrow i$
  - 3: **for**  $k = 0, 1, \dots$  **do**
  - 4:     Sample  $j \sim \mathbf{Q}_i = (\mathbf{Q}_{i,1}, \mathbf{Q}_{i,2}, \dots, \mathbf{Q}_{i,N})$ .
  - 5:     Sample  $U \sim \text{Unif}(0, 1)$ .
  - 6:     **if**  $U \leq \min\left(1, \frac{\pi_j \mathbf{Q}_{j,i}}{\pi_i \mathbf{Q}_{i,j}}\right)$  **then**
  - 7:          $X_{k+1} \leftarrow j$
  - 8:     **else**
  - 9:          $X_{k+1} \leftarrow X_k$
  - 10:    **end if**
  - 11: **end for**
-

# Traveling salesman problem

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## Definition (TSP)

Given a list of cities and the distances between each pair of cities, what is the shortest possible route that visits each city exactly once and returns to the origin city?

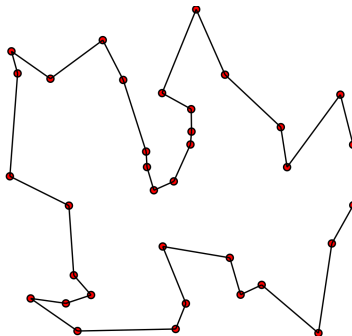


Figure: Traveling salesman problem, source: wiki.



# Traveling salesman problem

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## Definition (Traveling salesman problem)

Given an undirected weighted graph  $G = (V, E)$ ,  $|V| = n$  find a permutation  $\sigma_{\min}$  of vertices such that

$$\sigma_{\min} = \arg \min_{\sigma \in S_n} \left( \sum_{i=1}^{n-1} w_{\sigma(i), \sigma(i+1)} + w_{\sigma(n), \sigma(1)} \right),$$

where  $S_n$  is a set of all permutations of vertices and  $w_{i,j}$  is distance (weight) between cities  $i$  and  $j$ .

# Softmax

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## Definition

For a given vector  $\mathbf{x} = (x_1, x_2, \dots, x_d)^T \in \mathbb{R}^d$  a softmax function  $s : \mathbb{R}^d \rightarrow [0, 1]^d$  is defined as

$$s(\mathbf{x})_i = \frac{e^{x_i}}{\sum_{j=1}^d e^{x_j}},$$

$$s(\mathbf{x}) = (s(\mathbf{x})_1, s(\mathbf{x})_2, \dots, s(\mathbf{x})_d).$$

$$\sigma_{\min} = \arg \min_{\sigma \in S_n} (w_{\sigma}) = \arg \max_{\sigma \in S_n} \frac{e^{-w_{\sigma}}}{\sum_{\sigma' \in S_n} e^{-w_{\sigma'}}},$$

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$$\pi_{\sigma} = \frac{e^{-w_{\sigma}}}{\sum_{\sigma' \in S_n} e^{-w_{\sigma'}}}$$

$$\frac{\pi_{\sigma'} Q_{\sigma', \sigma}}{\pi_{\sigma} Q_{\sigma, \sigma'}} = e^{-(w_{\sigma'} - w_{\sigma})} \cdot \frac{Q_{\sigma', \sigma}}{Q_{\sigma, \sigma'}}.$$

$$\log \left( \frac{\pi_{\sigma'} Q_{\sigma', \sigma}}{\pi_{\sigma} Q_{\sigma, \sigma'}} \right) = -(w_{\sigma'} - w_{\sigma}) + \log(Q_{\sigma', \sigma}) - \log(Q_{\sigma, \sigma'}).$$

# Candidates

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## Definition

A neighbour  $\sigma'$  of a permutation  $\sigma$  is a permutation, that for some  $k, l$  it satisfies  $\sigma'(k) = \sigma(l)$ ,  $\sigma'(l) = \sigma(k)$  and  $\sigma'(i) = \sigma(i)$  for the rest of indices.

These neighbours are the original tour with two swapped indices. This let us consider a smaller space – there are  $\binom{n}{2} = \frac{n(n-1)}{2} \approx n^2$  neighbours if the number of vertices is  $n$ .

# Random candidates (RN)

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Sample neighbours uniformly. It is equivalent to choosing random indices to swap.

$$Q_{\sigma,\sigma'} = \begin{cases} \frac{1}{|S_\sigma|} & \text{if } \sigma \in S_\sigma, \\ 0 & \text{if } \sigma \notin S_\sigma. \end{cases}$$

where  $S_\sigma$  is a set of all possible neighbours of  $\sigma$ .

# Random candidates (RN)

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When given a tour  $\sigma$  and its neighbour  $\sigma'$  they differ only on those edges where swap is happening, let us say  $k, l$ . So for this situation we have tours:

$$\begin{aligned}\sigma &= (\dots, \sigma(k-1), \sigma(k), \sigma(k+1), \dots, \\ &\quad \dots, \sigma(l-1), \sigma(l), \sigma(l+1), \dots) \\ \sigma' &= (\dots, \sigma(k-1), \sigma(l), \sigma(k+1), \dots, \\ &\quad \dots, \sigma(l-1), \sigma(k), \sigma(l+1), \dots)\end{aligned}$$

To compute difference  $-(w_{\sigma'} - w_{\sigma})$  we need to remove weights  $w_{\sigma(k-1), \sigma(k)}$ ,  $w_{\sigma(k), \sigma(k+1)}$ ,  $w_{\sigma(l-1), \sigma(l)}$ ,  $w_{\sigma(l), \sigma(l+1)}$  and add  $w_{\sigma(k-1), \sigma(l)}$ ,  $w_{\sigma(l), \sigma(k+1)}$ ,  $w_{\sigma(l-1), \sigma(k)}$ ,  $w_{\sigma(k), \sigma(l+1)}$ .

# Locally-informed proposals (LIP)

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The idea is to balance the increase in the probability of neighbour with decrease of reverse probability, such that it will be easy to compute.

$$Q_{\sigma,\sigma'} \propto e^{\frac{-(w_{\sigma'}-w_{\sigma})}{\tau}}.$$

The distribution is chosen in such a way, so that we can easily group up the terms in acceptance criterion:

$$\frac{\pi_{\sigma'} Q_{\sigma',\sigma}}{\pi_{\sigma} Q_{\sigma,\sigma'}} = e^{-(w_{\sigma'}-w_{\sigma})} \cdot \frac{e^{\frac{-(w_{\sigma}-w_{\sigma'})}{\tau}}}{e^{\frac{-(w_{\sigma'}-w_{\sigma})}{\tau}}} \cdot \frac{C_{\sigma'}}{C_{\sigma}} = e^{(-(w_{\sigma'}-w_{\sigma})(1-\frac{2}{\tau}))} \cdot \frac{C_{\sigma'}}{C_{\sigma}}$$

# Example

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Let us set  $k = 2$  and  $l = 7$ , then the set of indices to consider is  $\{1, 2, 3, 6, 7, 8\}$  and the permutations:

$$\sigma = (1, \mathbf{2}, 3, 4, 5, 6, \mathbf{7}, 8, 9, \dots)$$

$$\sigma' = (1, \mathbf{7}, 3, 4, 5, 6, \mathbf{2}, 8, 9, \dots).$$



# Example

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	2	3	4	5	6	7	8	9	10
1	(1,2)	(1,3)	(1,4)	(1,5)	(1,6)	(1,7)	(1,8)	(1,9)	...
2		(2,3)	(2,4)	(2,5)	(2,6)	(2,7)	(2,8)	(2,9)	...
3			(3,4)	(3,5)	(3,6)	(3,7)	(3,8)	(3,9)	...
4				(4,5)	(4,6)	(4,7)	(4,8)	(4,9)	...
5					(5,6)	(5,7)	(5,8)	(5,9)	...
6						(6,7)	(6,8)	(6,9)	...
7							(7,8)	(7,9)	...
8								(8,9)	...
9									...

Table: Neighbour representation.

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The idea is to describe a probability of state using a cooling parameter  $t_k$  such that it reminds the cooling of a metal and may change with each step:

$$\pi_i = \frac{e^{\frac{-E_i}{t_k}}}{C},$$

where  $C$  is normalizing constant. The quotient of probabilities then is:

$$\frac{\pi_j}{\pi_i} = e^{\frac{E_i - E_j}{t_k}}$$

# Initial condition

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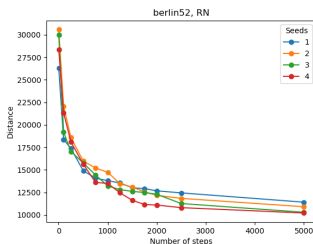
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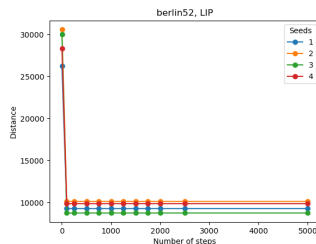
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(a) Random neighbours.



(b) Locally-informed proposals.

Figure: Different initial states for *berlin52*.

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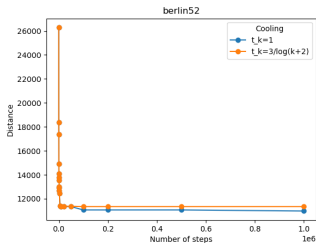
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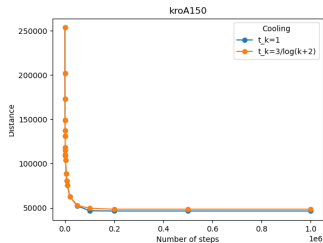
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(a) berlin52.



(b) kroA150.

Figure: Different cooling parameters for *berlin52* and *kroA150*.

# Temperature

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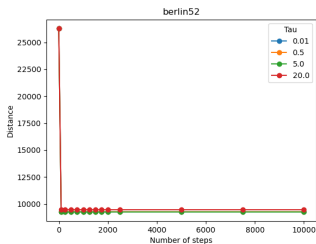
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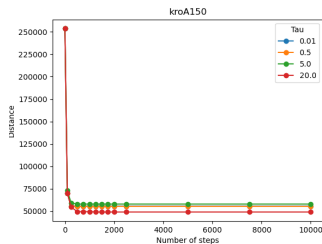
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(a) berlin52.



(b) kroA150.

Figure: Different temperature parameters for *berlin52* and *kroA150*.

# Algorithms comparison

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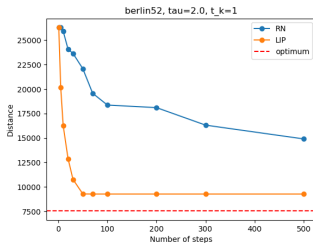
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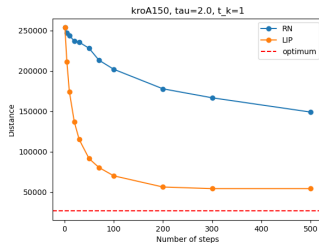
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(a) berlin52,  $t_k = 1$ .



(b) kroA150,  $t_k = 1$ .

**Figure:** Comparing RN and LIP for *berlin52* and *kroA150* with low number of iterations.

# Algorithms comparison

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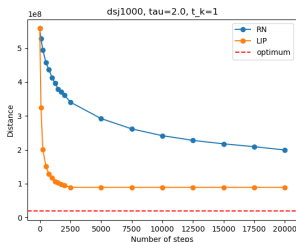
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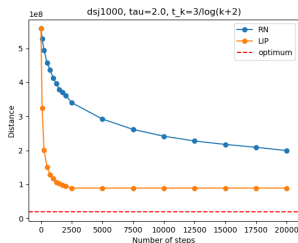
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(a)  $dsj1000$ ,  $t_k = 1$ .



(b)  $dsj1000$ ,  $t_k = \frac{3}{\log(k+2)}$ .

**Figure:** Comparing RN and LIP for  $dsj1000$  with different cooling parameters.

# Algorithms comparison

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	RN			LIP		
dataset	dist.	time [s]	ratio	dist.	time [s]	ratio
berlin52	11344	1.32	1.50	9276	116	1.23
kroA150	62467	1.24	2.36	53988	454	2.04
att532	165445	1.38	5.98	78150	2462	2.82
dsj1000	199343433	1.5	10.68	89105687	6439	4.78

Table: Methods comparison,  $t_k = 1$ , 20000-th step.



# Algorithms comparison

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	RN			LIP		
dataset	step	distance	time [s]	step	distance	time [s]
berlin52	20000	11344	1.32	27	11198	0.22
kroA150	20000	62467	1.24	139	62459	3.64
att532	20000	165445	1.38	199	165247	24.65
dsj1000	20000	199343433	1.5	256	199338468	80.54

**Table:** Amount of time and number of steps required for LIP algorithm to reach the result of RN after 20000 steps,  $t_k = 1$ .

# Conclusions

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- LIP algorithm is decreasing the distance quicker than RN,
- LIP converges to some value, which is always smaller than the RN,
- LIP reaches better results in feasible time,
- Only first hundreds iterations matter,
- LIP algorithm is considerably slower for a longer run.

# Improvements

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- Use of interning in *Python3*,
- use of concurrency,
- sampling from  $Q_\sigma$  using MCMC methods,
- better tuning of temperature and cooling parameters.

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Thank you for your attention.