Stochastic Simulation
Simulated annealing

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A general optimisation problem

- $f^\star = \min_{x \in \mathcal{S}} f(x)$
- The set $\mathcal{S}$ can be quite general
- $x^\star = \text{argmin}_{x \in \mathcal{S}} f(x)$
- Note $x^\star$ might not be unique so we can define the set $\mathcal{M}$ of minimising points
- $\mathcal{M} = \{x \in \mathcal{S} | f(x) = f^\star\}$ Assume $|\mathcal{M}| < \infty$, that is the cardinality of $\mathcal{M}$ (number of elements in $\mathcal{M}$) is finite
- This will typically be the case for discrete optimisation, where also $|\mathcal{S}| < \infty$.

Optimisation problem - probability distribution

We introduce a probability distribution over $\mathcal{S}$ to be

$$
\begin{aligned}
P_T(x) &= \frac{e^{-f(x)/T}}{\sum_{y\in\mathcal{S}} e^{-f(y)/T}} = \frac{e^{-f(x)/T}}{|M|e^{-f^\star/T} + \sum_{y\in\mathcal{S}\setminus\mathcal{M}} e^{-f(y)/T}} \\
&= \frac{e^{(f^\star - f(x))/T}}{|M| + \sum_{y\in\mathcal{S}\setminus\mathcal{M}} e^{(f^\star - f(y))/T}}
\end{aligned}
$$

- we have a probability function with an "easy" to calculate expression multiplied with a difficult to calculate constant
- For fixed T we can sample, states x with low "energy" (low valuels of $f(x)$) will be more frequent/likely
- As $T \to 0$ the distribution will degenerate to states with minimum energy

Simulated annealing

- Stochastic algorithm for optimisation
- Large scale (typically discrete) problems
- Attempts to find the global optimum in presence of multiple local optima

$$\min_{\boldsymbol{x}} f(\boldsymbol{x})$$

- One among many stochastic optimisation methods
  - a metaheuristic
- Simulated annealing one of the first, inspired from Metropolis-Hastings - Kirkpatrick paper Science 1983
- Alternatives: Stochastic gradient and several other

Physical inspiration (with apologies)

Steel and other materials can exist in several crystalline structures.

One - the ground state - has lowest energy.

The material may be “caught” in other states which are only locally stable.

This is likely to happen when welding, machining, etc.

By heating the material and **slowly** cooling, we ensure that the material ends in the ground state.

This process is called **annealing**.

P.d.f. of the state at fixed temperature

Use $X \in \mathcal{S}$ to denote the state of the system (e.g., positions of atoms).

Let $U(x)$ denote the energy of state $x \in \mathcal{S}$.

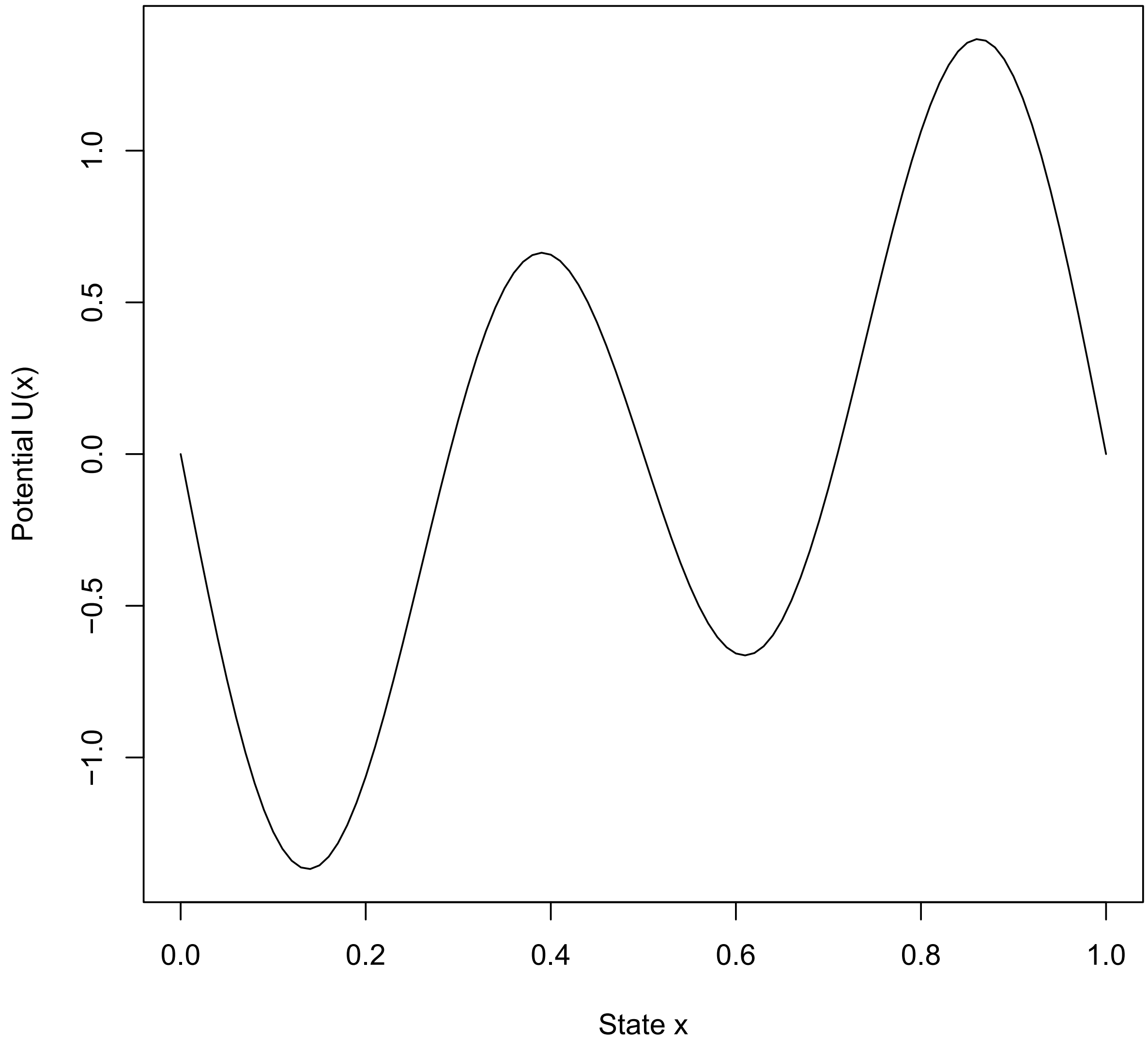
According to statistical physics, if the temperature is T, the p.d.f. of X is *the Canonical Distribution*

$$f(x, T) = c_T \cdot \exp\left(-\frac{U(x)}{T}\right)$$

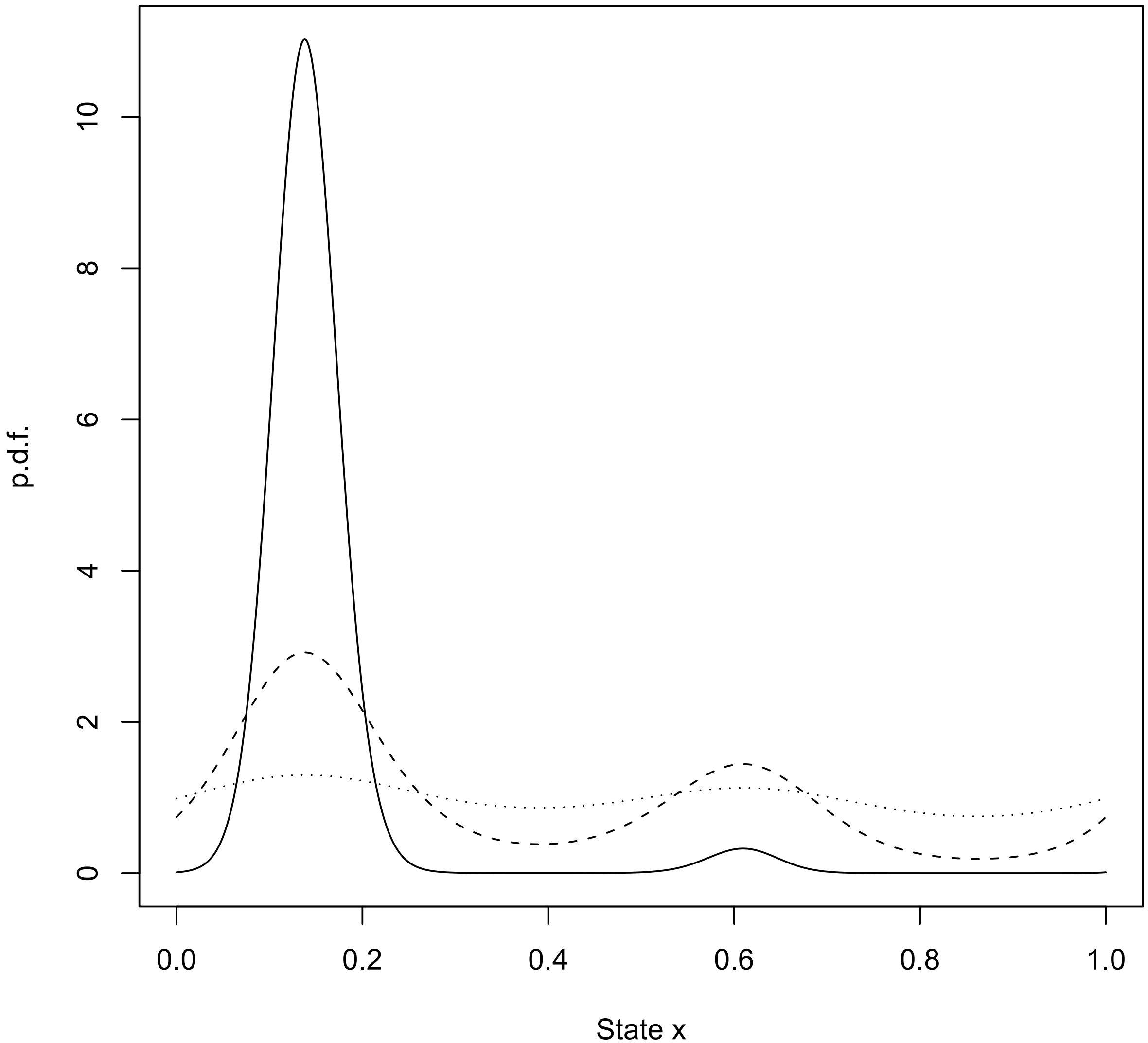
So states with low U are more probable; in particular at low T.

Note the normalization constant c_T is unknown; can be found by integration, but our algorithms will not require it.

Example energy potential



Corresponding p.d.f., for $T = 0.2, 1, 5$



An algorithm for Simulated Annealing

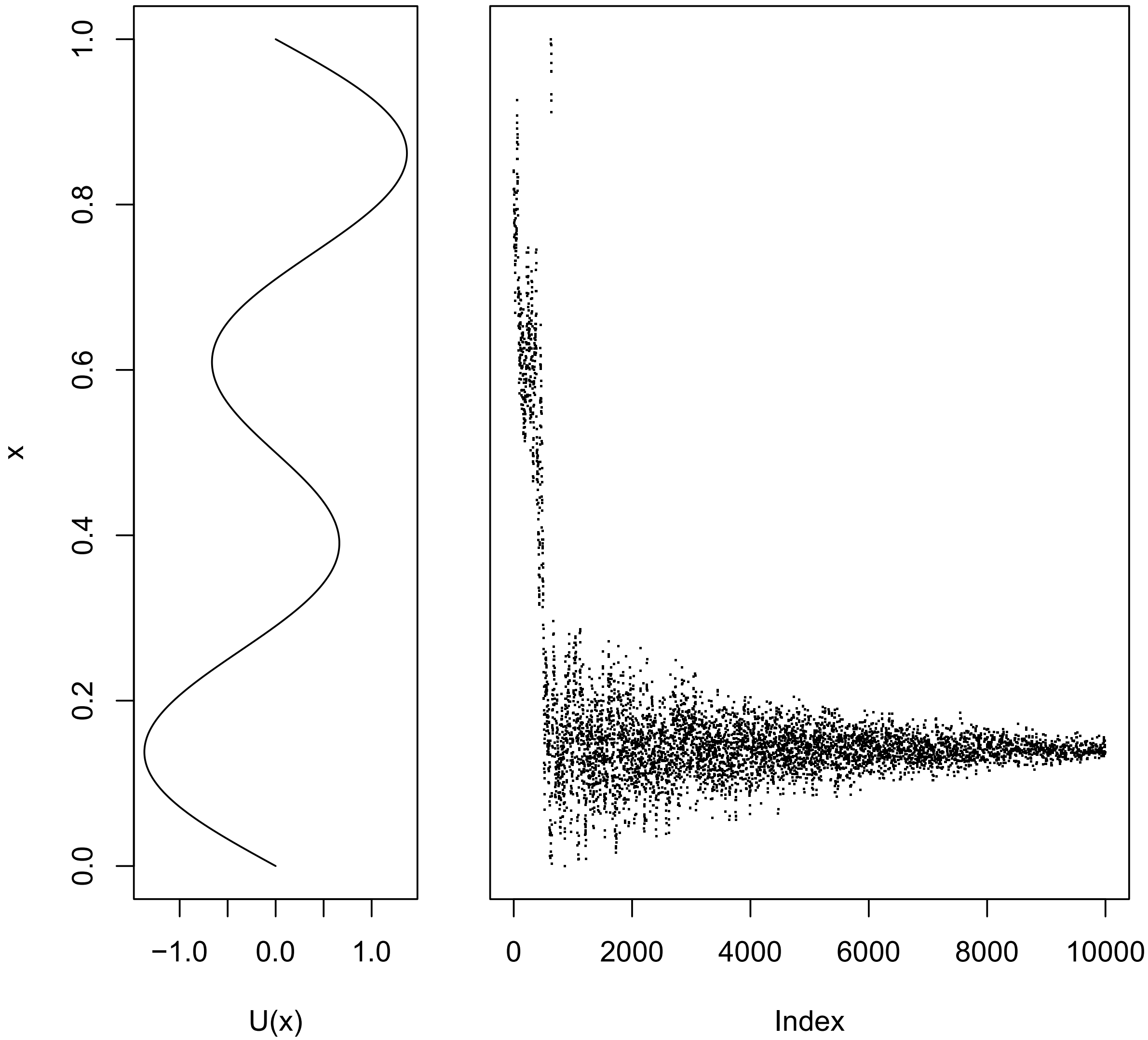
Let the temperature be a decreasing function of time or iteration number - k.

At each time step, update the state according to the random walk Metropolis-Hastings algorithm for MCMC, where the target p.d.f. is $f(x, T_i)$.

I.e., permute the state X_i randomly to generate a candidate Y_i. If the candidate has lower energy than the old state, accept. Otherwise, accept only with probability

$$\exp(-(U(Y_i) - U(X_i))/T_i)$$

for a symmetric proposal distribution (to keep the probabilistic interpreation)


x
1.0
0.8
0.6
0.4
0.2
0.0
−1.0
0.0
1.0
U(x)
0
2000
4000
6000
8000
10000
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Different issues

- Try with different schemes for lowering the temperature
- Alternative initial solutions
- Different candidate generation algorithms
- Refine with local search

Travelling salesman problem (TSP)

A basic problem in combinatorial optimisation

Given n stations, and an n-by-n matrix A giving the cost of going from station i to j.

Find a route S (a permutation of $1,\ldots,n$) which

- starts and ends at station 1, $S_1 = 1$
- has minimal total cost

$$\sum_{i=1}^{n-1} A(S_i, S_{i+1})$$

Cost matrix - an example

Town	Town to					
from	1	2	3	4	5	6
1	-	5	3	1	4	12
2	2	-	22	11	13	30
3	6	8	-	13	12	5
4	33	9	5	-	60	17
5	1	15	6	10	-	14
6	24	6	8	9	40	-

Cost matrix - an example

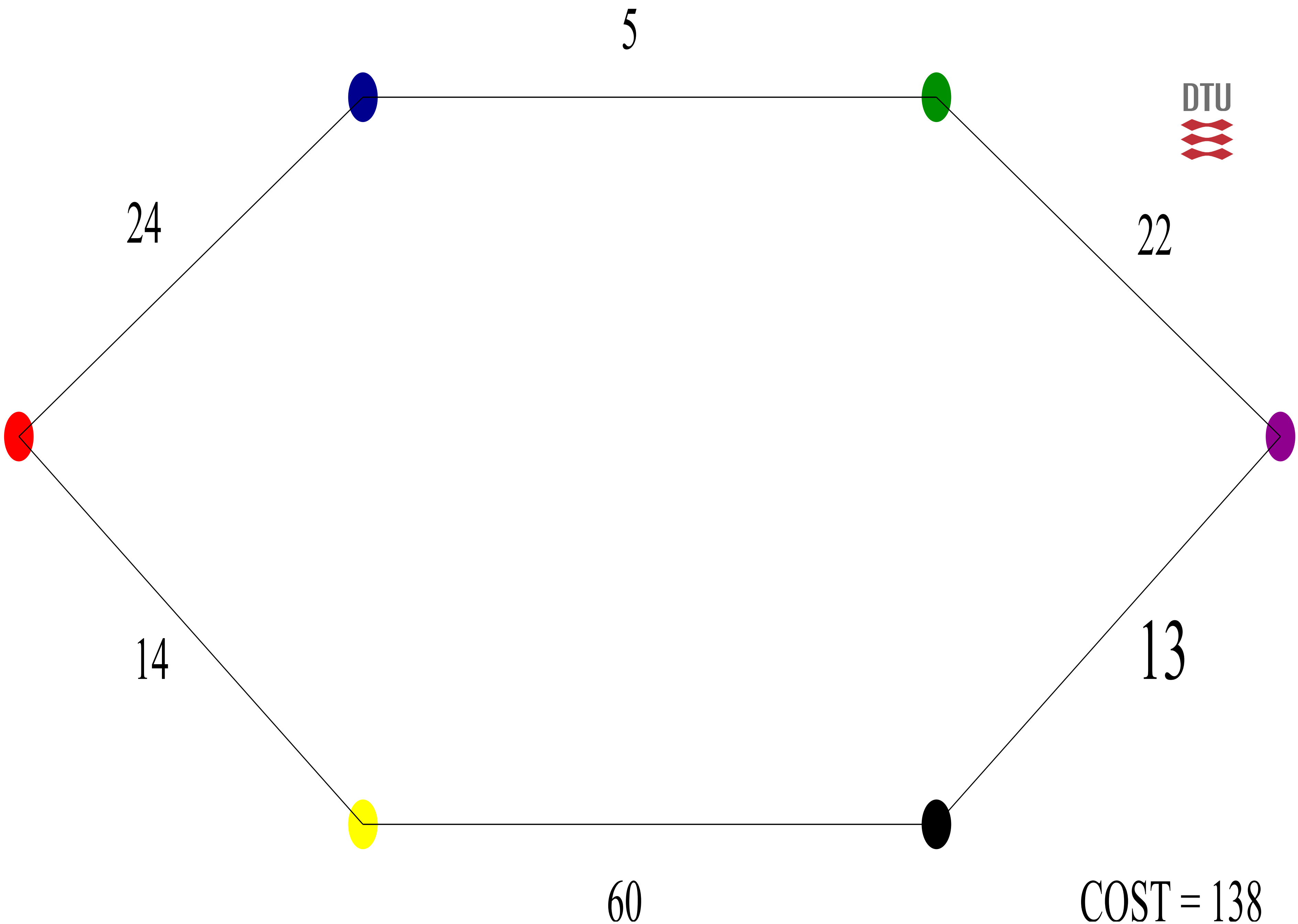
Town from	Town to 1	2	3	4	5	6
1	-	5	3	1	4	12
2	2	-	22	11	13	30
3	6	8	-	13	12	5
4	33	9	5	-	60	17
5	1	15	6	10	-	14
6	24	6	8	9	40	-

- Initial solution: $\{1, 2, 3, 4, 5, 6, 1\}$

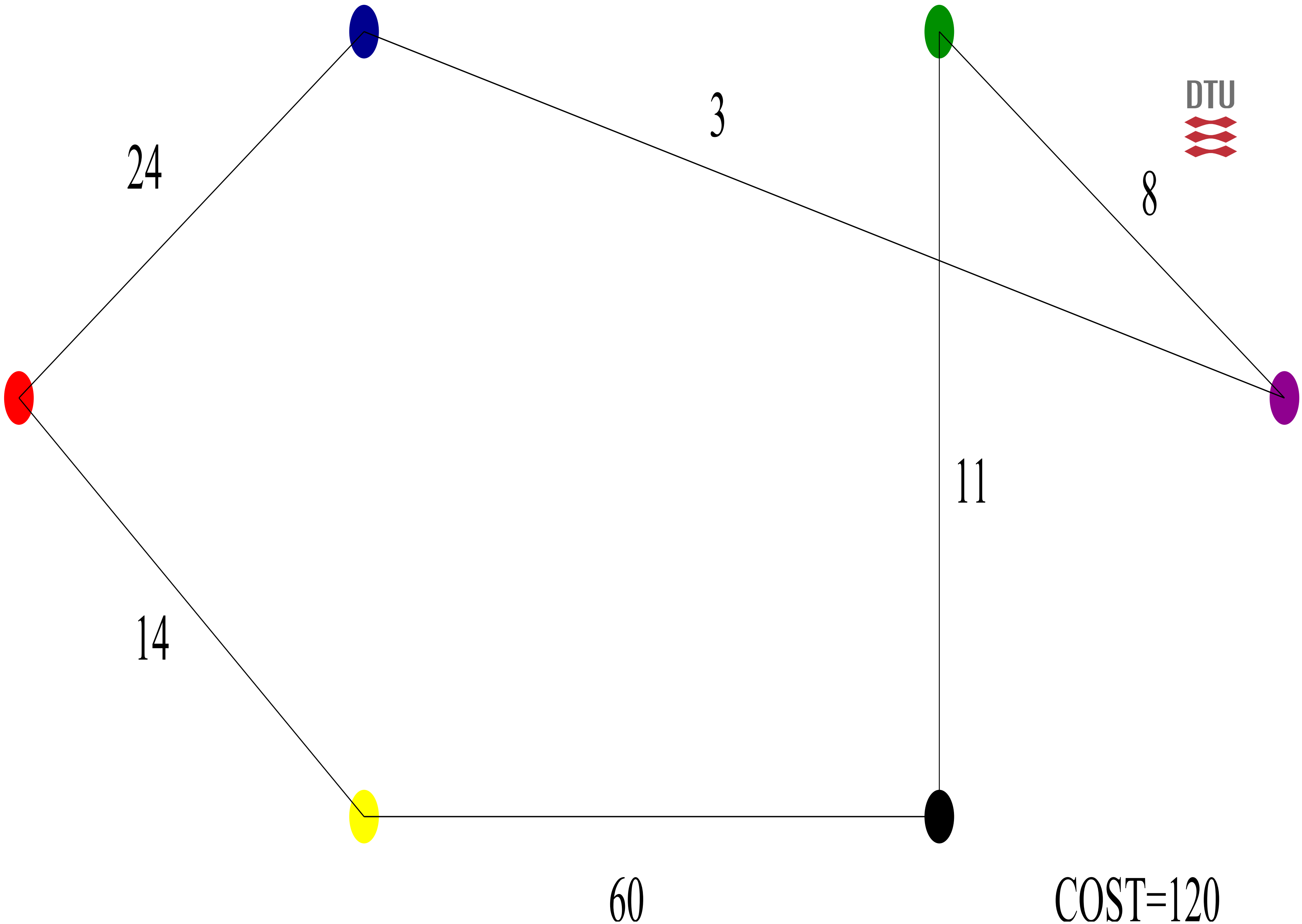
Cost matrix - an example

Town from	Town to 1	2	3	4	5	6
1	-	5	3	1	4	12
2	2	-	22	11	13	30
3	6	8	-	13	12	5
4	33	9	5	-	60	17
5	1	15	6	10	-	14
6	24	6	8	9	40	-

- Initial solution: $\{1, 2, 3, 4, 5, 6, 1\}$ initial cost: 5+22+13+60+14+24 = 138



COST = 138



COST=120

Exercise 7

1. Implement simulated annealing for the travelling salesman. As proposal, permute two random stations on the route. As cooling scheme, you can use e.g. $T_k = 1/\sqrt{1+k}$. or $T_k = -\log(k+1)$, feel free to experiment with different choices. The route must end where it started. Initialise with a random permutation of stations.
   (a) Have input be positions in the plane of the n stations. Let the cost of going $i \mapsto j$ be the Euclidian distance between station i and j.
   Plot the resulting route in the plane.
   Debug with stations on a circle.
   (b) Then modify your progamme to work with costs directly and apply it to the cost matrix from the course homepage.