

Stochastic Optimization

This exercise sheet is about applying simulated annealing and a deterministic approximation thereof to a toy problem.

8.1 Simulated Annealing (5 points)

Simulated annealing can be used to optimize a *cost function* $E : \mathbf{s} \rightarrow \mathbb{R}$ where the state \mathbf{s} is a set of discrete state variables $s_i \in \{-1, +1\}$, $i = 1, \dots, N$. For a fully connected “network” with $N = 6$ binary nodes, this means that $\mathbf{s} \in \{-1, +1\}^6$, and we will use the cost (“energy”)

$$E(\mathbf{s}) = -\frac{1}{2} \sum_{i,j=1}^N w_{ij} s_i s_j,$$

where $w_{ij} = w_{ji} \in \mathbb{R}$, and $w_{ii} = 0$.
The probability that the network is in a state \mathbf{s} with energy $E(\mathbf{s})$ is given by

$$P(\mathbf{s}) = \frac{1}{Z} \exp(-\beta E(\mathbf{s})),$$

where the *partition function* Z guarantees $P(\mathbf{s})$ to be a valid probability mass function and is given as the *sum over all possible configurations*, i.e., $Z = \sum_{\mathbf{s}} \exp(-\beta E(\mathbf{s}))$.

Write a program that finds the optimal configuration \mathbf{s} for a given set of weights \mathbf{W} as follows (try to find reasonable parameters β_0 and τ to have a rather efficient implementation if possible):

Initialization:

- set $\beta_0, \tau > 1$, and t_{max} (make sure β_0 is small enough), try both $M = 1$ and $M = 500$
- set initial state \mathbf{s} randomly; \mathbf{W} arbitrary, but symmetrically and with zero diagonal

Optimization: for each iteration $t = 0, \dots, t_{max}$

- repeat the following M times (state update loop):
 - select node i randomly
 - determine the energies for the two options of state s_i and compute their difference

$$E_{s_i} = -\frac{1}{2} \sum_{j \in \mathcal{N}_i} w_{ij} s_i s_j \quad \text{and} \quad E_{-s_i} = -E_{s_i} \quad \rightarrow \quad \Delta E = E_{-s_i} - E_{s_i}$$
 where \mathcal{N}_i is the set of neighbors of node i , i.e. here the set of all other nodes
 - flip state s_i with probability $P(s_i \rightarrow -s_i) = (1 + e^{\beta_t \Delta E})^{-1}$
- increase β using $\beta_{t+1} = \tau \beta_t$

Plotting:

- Plot the temperature $T_t = \frac{1}{\beta_t}$ and the energy $E(\mathbf{s})$ over the iterations $t = 0, \dots, t_{max}$.
- Show the energy $E(\mathbf{s})$ for all possible 2^6 states using a bar plot. The sequence of the states is not relevant. Additionally, plot the probabilities $P(\mathbf{s})$ for different β as a bar plot. Choose the $\{\beta\}$ in a way, that the probability distributions differ discernibly.

8.2 Mean-Field Annealing (5 points)

Mean-field annealing is a deterministic approximation of simulated annealing. During optimization each node i corresponds to the first moment of s_i and **thus takes continuous** instead of binary values. The states s_i represent the mean with respect to the factorized distribution $Q(\mathbf{s}) \approx P(\mathbf{s})$. Consider again a fully connected network with $N = 6$ nodes. The cost (energy) function remains the same:

$$E(\mathbf{s}) = -\frac{1}{2} \sum_{i,j=1}^N w_{ij} s_i s_j,$$

where the $w_{ij} \in \mathbb{R}$ are symmetric, and $w_{ii} = 0$. The approximated probability of a state \mathbf{s} is now given by

$$Q(\mathbf{s}) = \frac{1}{Z_Q} \exp\left(-\beta \sum_j e_j s_j\right).$$

Write a program that finds the optimal configuration \mathbf{s} of the network for given weights \mathbf{W} . It should execute the following steps:

Initialization:

- β_0 small enough, $\tau > 1$, set t_{max} , ε small enough
- initial state \mathbf{s} randomly, \mathbf{W} from exercise above

Optimization: for each iteration $t = 0, \dots, t_{max}$

- repeat the following until convergence, i.e., $|\mathbf{e}_{new} - \mathbf{e}_{old}| < \varepsilon$
 - for $i = 1, \dots, N$:
 - * compute mean-field

$$e_i = - \sum_{j \in \mathcal{N}_i} w_{ij} s_j$$

where \mathcal{N}_i is the set of neighbors of node i , i.e. here the set of all other nodes.

* update the state using $s_i = \tanh(-\beta e_i)$

- Increase β using $\beta_{t+1} = \tau \beta_t$

Plotting:

- Plot the temperature $T_t = \frac{1}{\beta_t}$ and the energy E_t over the iterations $t = 0, \dots, t_{max}$.

Comparison: for simulated and mean-field annealing compare:

- the required number of iterations until convergence
- the total runtime (in dependence of different choices of M, τ, ε)
- the final result \mathbf{s} after iteration t_{max}

Total points: 10