Machine Intelligence 2

3 Stochastic Optimization

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Stochastic Optimization

Simulated Annealing

Mean-Field Annealing

Stochastic optimization

Supervised & unsupervised learning → evaluation of cost function E^T

- real-valued arguments: gradient based techniques (e.g. ICA weights)
- discrete arguments: ?? (e.g. for cluster assignment)

$\Rightarrow$ simulated annealing

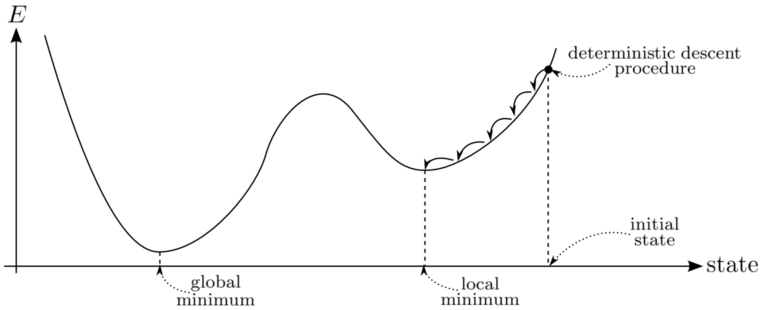
Setting

- discrete variables $s_i, \; i = 1, \ldots, N$ (e.g. $s_i \in \{+1, -1\}$ or $s_i \in \mathbb{N}$)
- short-hand notation: $\underline{\mathrm{s}}$ ("state") – often $\{\underline{\mathrm{s}}\}$ not a vector space (but called state space)
- **cost function:** $E : \underline{\mathbf{s}} \mapsto E_{(\underline{\mathbf{s}})} \in \mathbb{R}$ – not restricted to learning problems

Goal: find state $\underline{\mathrm{s}}^*$, such that:

$$E \stackrel{!}{=} \min \qquad \text{(desirable global minimum of } E\text{)}$$

Optimizing cost functions with local optima



- Deterministic descent may converge to local minima
- Grid-search, random search, multiple initializations
  $\rightsquigarrow$ *Simulated Annealing*

Simulated Annealing

History: "Naturalistic" stochastic optimization

$\rightsquigarrow$ mimicking freezing and crystallization

(atom configurations in crystals often close to global minima of the energy)

$\rightsquigarrow$ slow cooling (glass, unordered vs. crystal, ordered) $\Rightarrow$ annealing

$\Rightarrow$ slowly lower temperature while maintaining thermal equilibrium

$\Rightarrow$ computational temperature T or *noise parameter* $\beta = \dfrac{1}{T}$

Simulated Annealing

`initialization:` $\underline{\mathbf{s}}_0$, β_0 small ($\rightsquigarrow$ high temperature)

`BEGIN Annealing loop` $(t = 1, 2, \dots)$

$\underline{\mathbf{s}}_t = \underline{\mathbf{s}}_{t-1}$ (initialization of inner loop)

`BEGIN State update loop` (M iterations)

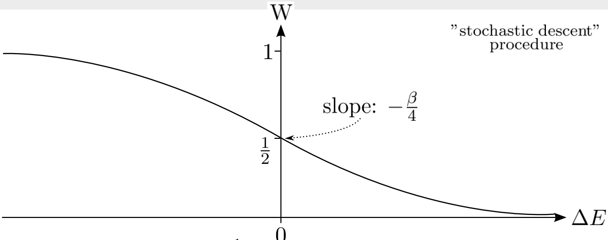
- `choose a new candidate state` $\underline{\mathbf{s}}$ randomly (local to $\underline{\mathbf{s}}_t$ – e.g. "bitflip")
- `calculate difference in cost:` $\Delta E = E_{(\underline{\mathbf{s}})} - E_{(\underline{\mathbf{s}}_t)}$
- `switch` $\underline{\mathbf{s}}_t$ `to` $\underline{\mathbf{s}}$ `with probability` $\mathrm{W}_{(\underline{\mathbf{s}}_t \to \underline{\mathbf{s}})} = \frac{1}{1+\exp(\beta_t \Delta E)}$ otherwise keep the previous state $\underline{\mathbf{s}}_t$

`END State update loop`

$\beta_t = \tau \beta_{t-1}$ ($\tau > 1 \implies$ increase of β)

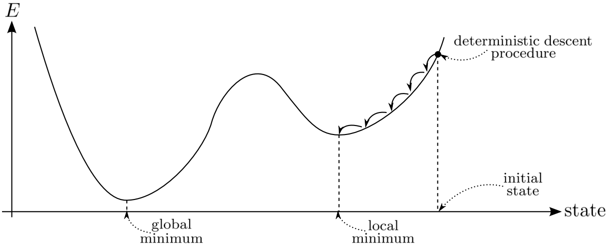
`END Annealing loop`

Transition probability



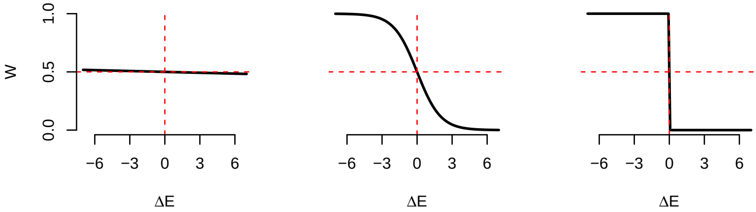
$$W_{(\underline{\mathbf{s}}_t \to \underline{\mathbf{s}})} = \frac{1}{1+\exp(\beta_t \Delta E)}, \quad \Delta E = E_{(\underline{\mathbf{s}})} - E_{(\underline{\mathbf{s}}_t)}$$

cost function with local optima:

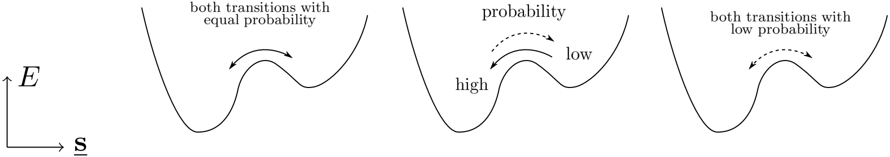


Annealing

limiting cases for high vs. low temperature:



low β (high temperature) | intermediate β | high β



Annealing schedule & convergence

Convergence to the global optimum is guaranteed if: $\beta_t \sim \ln t$

- $\Rightarrow$ robust optimization procedure
- $\Rightarrow$ but: $\beta_t \sim \ln t$ is **too slow** for practical problems
- $\Rightarrow$ therefore: $\beta_{t+1} = \tau \beta_t, \quad \tau \in [1.01, 1.30]$ (exponential annealing)
- $\Rightarrow$ additionally: the `State Update loop` has to be iterated often enough, e.g. $M = 500 - 2000$ ($\rightsquigarrow$ thermal equilibrium)

Examples

1. Finding the global optimum of cost function (with continuous variables)

$\Rightarrow$ https://www.youtube.com/watch?v=iaq_Fpr4KZc

2. Solving Sudoku with Simulated Annealing

- initially fill columns randomly (without replacement)
- rows/3x3-boxes violate the Sudoku rules
- choose random column and two rows: switch the 2 numbers (stochastically)
- $s_i \in \{1, 2, \ldots, 9\} \implies (9!)^9 \geq 10^{50}$ states
- cost function $E_{(\underline{\mathbf{s}})}$ total number of doubles in all rows/boxes (normalized)
- multiple global optima and also local optima
- 1000 steps per `State Update loop`

$\Rightarrow$ https://www.youtube.com/watch?v=E8tkpzDne7I (from 2:19)

The Gibbs distribution

- for constant β: noisy state change via Markov process $\underline{\mathbf{s}}_{t'}$
- t': iteration count of the `State Update loop`
- $\Pi_{(\underline{\mathbf{s}},t')}$: probability distribution across states

$$\Pi_{(\underline{\mathbf{s}},t')} \rightarrow \underbrace{P_{(\underline{\mathbf{s}})}}_{\text{stationary distribution}} \quad \text{for } t' \rightarrow \infty \text{ (and constant } \beta\text{)}$$

$\rightarrow P(\underline{\mathbf{s}})$ can be calculated analytically!

Calculation of the stationary distribution

Assumption of *detailed balance:*

$$\underbrace{\text{probability of transition } \underline{s} \to \underline{s}'}_{P_{(\underline{s})} \mathrm{W}_{(\underline{s} \to \underline{s}')}} = \underbrace{\text{probability of transition } \underline{s}' \to \underline{s}}_{P_{(\underline{s}')} \mathrm{W}_{(\underline{s}' \to \underline{s})}}$$

$$\frac{P_{(\underline{s})}}{P_{(\underline{s}')}} = \frac{\mathrm{W}_{(\underline{s}' \to \underline{s})}}{\mathrm{W}_{(\underline{s} \to \underline{s}')}} = \frac{1 + \exp\left\{\beta\left(E_{(\underline{s})} - E_{(\underline{s}')}\right)\right\}}{1 + \exp\left\{\beta\left(E_{(\underline{s}')} - E_{(\underline{s})}\right)\right\}} = \frac{1 + \exp(\beta \Delta E)}{1 + \exp(-\beta \Delta E)}$$

$$= \exp(\beta \Delta E) \frac{1 + \exp(-\beta \Delta E)}{1 + \exp(-\beta \Delta E)} = \exp(\beta \Delta E)$$

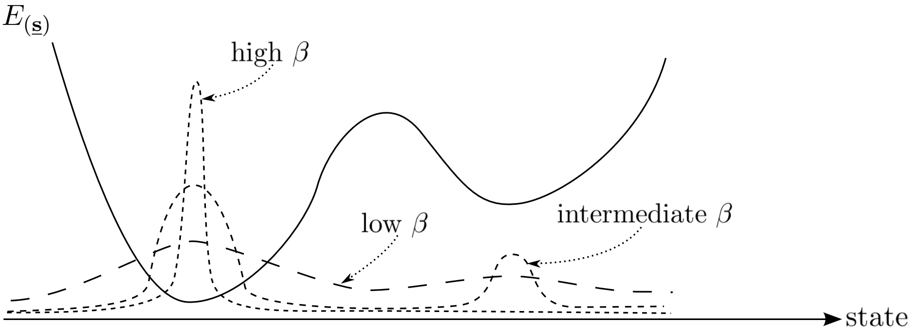
this condition is fulfilled for:

$$P_{(\underline{s})} = \frac{1}{Z} \exp(-\beta E) \qquad \text{(Gibbs-Boltzmann-distribution)}$$

normalization constant / partition function: $Z = \sum_{\underline{s}} \exp(-\beta E)$

Cost vs. probability distribution

$$P_{(\underline{\mathbf{s}})} = \frac{1}{Z} \exp(-\beta E) \qquad \text{(Gibbs-Boltzmann-distribution)}$$



$\beta \downarrow$: broad, "delocalized" distribution

$\beta \uparrow$: distribution localized around (global) minima

Mean-field annealing

Simulated Annealing

- $\rightarrow$ stochastic optimization: computationally expensive (sampling!)
- $\rightarrow$ stationary distribution $P_{(\underline{\mathbf{s}})}$ known (for each β_t), why not evaluate?
- $\rightarrow$ however: maxima of $P_{(\underline{\mathbf{s}})}$ equally hard to obtain as minima of $E_{(\underline{\mathbf{s}})}$
- $\rightarrow$ moments? for $\beta \rightarrow \infty$: $\langle \underline{\mathbf{s}} \rangle_P$ converges to $\underline{\mathbf{s}}^*$ of minimal cost ($P_{(\underline{\mathbf{s}})}$ singular)
- $\rightarrow$ but: moments of $P_{(\underline{\mathbf{s}})}$ can – in general – not be calculated analytically

Approximation by Mean-Field Annealing

- $\Rightarrow$ idea: approximate $P_{(\underline{\mathbf{s}})}$ by a computationally tractable distribution $Q_{(\underline{\mathbf{s}})}$
- $\Rightarrow$ this distribution is then used to calculate the first moment $\langle \underline{\mathbf{s}} \rangle_Q$
- $\Rightarrow$ the first moment is tracked during the annealing schedule β_t
- $\Rightarrow$ hope: $\langle \underline{\mathbf{s}} \rangle_Q \rightarrow \underline{\mathbf{s}}^*$ for $\beta_t \rightarrow \infty$

Factorizing distribution

Distribution $Q_{(\underline{\mathbf{s}})}$ to approximate $P_{(\underline{\mathbf{s}})}$

$$Q_{(\underline{\mathbf{s}})} \quad = \quad \frac{1}{Z_Q} \exp\left\{-\beta E_Q\right\} \quad = \quad \frac{1}{Z_Q} \exp\left\{ -\beta \sum_k \underbrace{e_k}_{\text{parameters}} \mathrm{s}_k \right\}$$

- Gibbs distribution with costs E_Q linear in the state variable $\underline{\mathbf{s}}_k$
- factorizing distribution $Q_{(\underline{\mathbf{s}})} = \Pi_k Q_k(s_k)$ with $Q_k(s_k) = \frac{1}{Z_{Q_k}} \exp(-\beta e_k \mathrm{s}_k)$
- $Q_{(\underline{\mathbf{s}})}$ factorizing $\iff$ s_k independent $\implies$ $\langle \Pi_k s_k \rangle_Q = \Pi_k \langle s_k \rangle_Q$ $\left(\substack{\text{moments}\\ \text{factorize}}\right)$
- $\left\langle s_k \right\rangle_Q = \frac{\sum\limits_{s_k} s_k \exp(-\beta e_k s_k)}{\sum\limits_{s_k} \exp(-\beta e_k s_k)}$

$\rightarrow$ family of distributions parametrized by the *mean fields* e_k

$\rightarrow$ determine e_k such that this approximation is as good as possible

Mean-field approximation

Quantities

$$P_{(\underline{\mathbf{s}})} = \frac{1}{Z_p} \exp(-\beta E_p)$$

true distribution

$$Q_{(\underline{\mathbf{s}})} = \frac{1}{Z_Q} \exp\Big(-\beta \overbrace{\sum_k e_k s_k}^{E_Q} \Big)$$

approximation: family of factorizing distributions

e_k : *mean fields* — parameters to be determined

Good approximation of P by Q

$\rightarrow$ minimization of the KL-divergence:

$$\mathrm{D_{KL}}(Q||P) = \sum_{\underline{\mathbf{s}}} Q_{(\underline{\mathbf{s}})} \ln \frac{Q_{(\underline{\mathbf{s}})}}{P_{(\underline{\mathbf{s}})}} \stackrel{!}{=} \min_{\underline{\mathbf{e}}}$$

Minimization of KL-divergence

$$\mathrm{D_{KL}}(Q||P) = \sum_{\underline{\mathbf{s}}} Q_{(\underline{\mathbf{s}})} \ln \frac{Q_{(\underline{\mathbf{s}})}}{P_{(\underline{\mathbf{s}})}} \overset{!}{=} \min_{\underline{\mathbf{e}}} \qquad \begin{aligned} P_{(\underline{\mathbf{s}})} &= \tfrac{1}{Z_p} \exp(-\beta E_p) \\ Q_{(\underline{\mathbf{s}})} &= \tfrac{1}{Z_Q} \exp\Big(-\beta \sum_k e_k s_k\Big) \end{aligned}$$

$$\begin{aligned}
\tfrac{\partial}{\partial e_l} \mathrm{D_{KL}} &= \tfrac{\partial}{\partial e_l} \Big\{ \beta \sum_{\underline{\mathbf{s}}} Q_{(\underline{\mathbf{s}})} E_p - \beta \sum_{\underline{\mathbf{s}}} Q_{(\underline{\mathbf{s}})} E_Q + \ln Z_p - \ln Z_Q \Big\} \\
&= \beta \tfrac{\partial}{\partial e_l} \big\langle E_p \big\rangle_Q \underbrace{- \beta \frac{\partial}{\partial e_l} \Big(\sum_{\underline{\mathbf{s}}} Q_{(\underline{\mathbf{s}})} \sum_k e_k s_k \Big)}_{-\beta \sum_k e_k \frac{\partial}{\partial e_l} \langle s_k \rangle_Q - \beta \langle s_l \rangle_Q} \underbrace{- \frac{1}{Z_Q} \sum_{\underline{\mathbf{s}}} \frac{\partial}{\partial e_l} \exp\Big(-\beta \sum_k e_k s_k\Big)}_{+\beta \langle s_l \rangle_Q} \\
&= \beta \tfrac{\partial}{\partial e_l} \big\langle E_p \big\rangle_Q - \beta \sum_k e_k \tfrac{\partial}{\partial e_l} \big\langle s_k \big\rangle_Q \qquad \overset{!}{=} \qquad 0, \qquad l = 1, \ldots, N
\end{aligned}$$

Result

$$\frac{\partial}{\partial e_l} \big\langle E_p \big\rangle_Q - \sum_k e_k \frac{\partial}{\partial e_l} \big\langle s_k \big\rangle_Q = 0$$

s_k are independent under Q :

$$\frac{\partial}{\partial e_l} \big\langle E_p \big\rangle_Q - e_l \frac{\partial}{\partial e_l} \big\langle s_l \big\rangle_Q = 0$$

$$\big\langle s_k \big\rangle_Q = \frac{\sum\limits_{s_k} s_k \exp(-\beta e_k s_k)}{\sum\limits_{s_k} \exp(-\beta e_k s_k)}$$

$\rightarrow$ coupled deterministic system of equations for $\{e_k\}$
$\rightarrow$ iterative solution procedure (usually no analytic result)

Mean-field annealing

Algorithm

`initialization:` $\langle \underline{\mathbf{s}} \rangle_0, \beta_0$

`BEGIN Annealing loop`

`Repeat`

- calculate mean-fields: $e_k, \quad k = 1, \ldots, N$
- calculate moments: $\left\langle s_k \right\rangle_Q, \quad k = 1, \ldots, N$

`Until` $|e_k^{\text{old}} - e_k^{\text{new}}| < \varepsilon$

increase β

`END Annealing loop`

$\Rightarrow$ inner loop: fixed-point iteration for the mean-fields e_k ($\rightsquigarrow$ EM-like)

$\Rightarrow$ deterministic (fast) rather than stochastic (slow) optimization method (given that mean-field equations can be easily evaluated, dep. on E_p)

$\Rightarrow$ moments $\left\langle s_k \right\rangle$ in general not from state space but $\left\langle s_k \right\rangle \rightarrow s_k^*$ for $\beta \rightarrow \infty$

Example (Ising model) – Setting and first Moments

Quadratic cost function $E(\underline{\mathbf{s}})$ with binary variables $s_k \in \mathcal{S} = \{+1, -1\}$,

$$E_p(\underline{\mathbf{s}}) = -\frac{1}{2} \sum_{\substack{i=1, j=1 \\ i \neq j}}^{N} W_{ij} s_i s_j,$$

real symmetric matrix $\underline{\mathbf{W}}$, no self-coupling

$\rightarrow$ Expressions required for the mean-field algorithm can be calculated:

$$\langle s_k \rangle_Q = \frac{\sum\limits_{s_k \in \mathcal{S}} s_k \exp(-\beta e_k s_k)}{\sum\limits_{s_k \in \mathcal{S}} \exp(-\beta e_k s_k)} = \frac{(+1)\exp(-\beta e_k) + (-1)\exp(\beta e_k)}{\exp(-\beta e_k) + \exp(\beta e_k)}$$

$$= \boxed{\tanh(-\beta e_k)}$$

Example (Ising model) – Mean-fields

$$
\begin{aligned}
0 &= \frac{\partial}{\partial e_k} \langle E_p \rangle_Q - e_k \frac{\partial}{\partial e_k} \langle s_k \rangle_Q \\
&= \frac{\partial}{\partial e_k} \left\langle -\frac{1}{2} \sum_{\substack{i=1, j=1 \\ i \neq j}}^{N} W_{ij} s_i s_j \right\rangle_Q - e_k \frac{\partial}{\partial e_k} \langle s_k \rangle_Q \\
&= -\frac{1}{2} \frac{\partial}{\partial e_k} \sum_{\substack{i=1, j=1 \\ i \neq j}}^{N} W_{ij} \langle s_i \rangle_Q \langle s_j \rangle_Q - e_k \frac{\partial}{\partial e_k} \langle s_k \rangle_Q \\
&= -\sum_{\substack{i=1 \\ i \neq k}}^{N} W_{ik} \langle s_i \rangle_Q \frac{\partial}{\partial e_k} \langle s_k \rangle_Q - e_k \frac{\partial}{\partial e_k} \langle s_k \rangle_Q
\end{aligned}
$$

$$
\Longrightarrow \boxed{e_k = -\sum_{\substack{i=1 \\ i \neq k}}^{N} W_{ik} \langle s_i \rangle_Q}
$$

(will be applied in exercise sheet 9)

Example (Ising model) – Fixed point iteration

Inner loop in mean-field annealing algorithm:

`Repeat`

- calculate mean-fields: $e_k = -\sum_{\substack{i=1 \\ i \neq k}}^{N} W_{ik} \langle s_i \rangle_Q, \quad k = 1, \ldots, N$
- calculate moments: $\langle s_k \rangle_Q = \tanh(-\beta e_k), \quad k = 1, \ldots, N$

`Until` $|e_k^{\text{old}} - e_k^{\text{new}}| < \varepsilon$

$\rightsquigarrow$ fixed-point iteration for mean-fields will converge