Computational statistics, lecture 6

Frank Miller, Department of Computer and Information Science, Linköping University

February 26, 2025

LINKÖPING UNIVERSITY

Today

(Literature: Givens and Hoeting, 3.3-3.4, 4.1-4.2.2; Gentle, 6.3, 6.6, 14.3)

- EM algorithm
- Stochastic optimization
  - Simulated annealing
  - Genetic algorithm
  - Stochastic Gradient Ascent
- Combinatorial optimization

- Optimization problem:
  - $\boldsymbol{x}$ p-dimensional vector, g: $\mathbb{R}^p \to \mathbb{R}$ function $\quad g$: $\mathbb{S} \to \mathbb{R}$
  - We search $\boldsymbol{x}^*$ with $g(\boldsymbol{x}^*) = \max g(\boldsymbol{x})$

EM algorithm

- EM = “Expectation-Maximization”
- Main application of this algorithm is in cases where not all data is observed
- E: Expectation will be taken over all (unobserved) data which lead to the observed data
- Algorithm is iterative:
  each iteration has an E step, followed by an M step

EM algorithm

- Let $\boldsymbol{X}$ be observed data, $\boldsymbol{Y}$ complete data, $\boldsymbol{\theta}$ unknown parameter-vector, $L(\boldsymbol{\theta}|\boldsymbol{x})$ likelihood to be maximized
- Iteration t $(t = 0,1, \ldots)$: $\boldsymbol{\theta}^{(t)}$
- Let $Q\left(\boldsymbol{\theta}\middle|\boldsymbol{x}; \boldsymbol{\theta}^{(t)}\right) = E\left\{\log L(\boldsymbol{\theta}|Y)|\boldsymbol{x}; \boldsymbol{\theta}^{(t)}\right\}$ be expectation of **log likelihood for complete data** conditional on observed data $\boldsymbol{X} = \boldsymbol{x}$
- EM algorithm:
  1. Initialize parameter-vector with a guess $\boldsymbol{\theta}^{(0)}$, $t = 0$
  2. **E step:** Compute $Q\left(\boldsymbol{\theta}\middle|\boldsymbol{x}; \boldsymbol{\theta}^{(t)}\right)$
  3. **M step:** Maximize $Q\left(\boldsymbol{\theta}\middle|\boldsymbol{x}; \boldsymbol{\theta}^{(t)}\right)$ with respect to $\boldsymbol{\theta}$ -> result is $\boldsymbol{\theta}^{(t+1)}$
  4. If not stopping criterion (e.g. $\left(\boldsymbol{\theta}^{(t+1)} - \boldsymbol{\theta}^{(t)}\right)^T \left(\boldsymbol{\theta}^{(t+1)} - \boldsymbol{\theta}^{(t)}\right) < \epsilon$) met, set `t <- t+1`, and go back to E step

EM algorithm: Example

- Effect of a drug to be measured and n patients (randomly chosen out of a population of patients) treated with the drug
- $X_i, i = 1, \ldots, n$, observed for each patient after drug-treatment
- Known that population consists of two groups:
  - One group responds well to the drug (i.e. larger X_i)
  - Another group responds only barely (smaller X_i)
- It is not known which patient belongs to which group

Observed: $\boldsymbol{X_i}$,

Unobserved: $\boldsymbol{Z_i} = \begin{cases} \mathbf{1}, \text{if patient } \boldsymbol{i} \text{ belongs to responder group} \\ \mathbf{0}, \text{otherwise} \end{cases}$

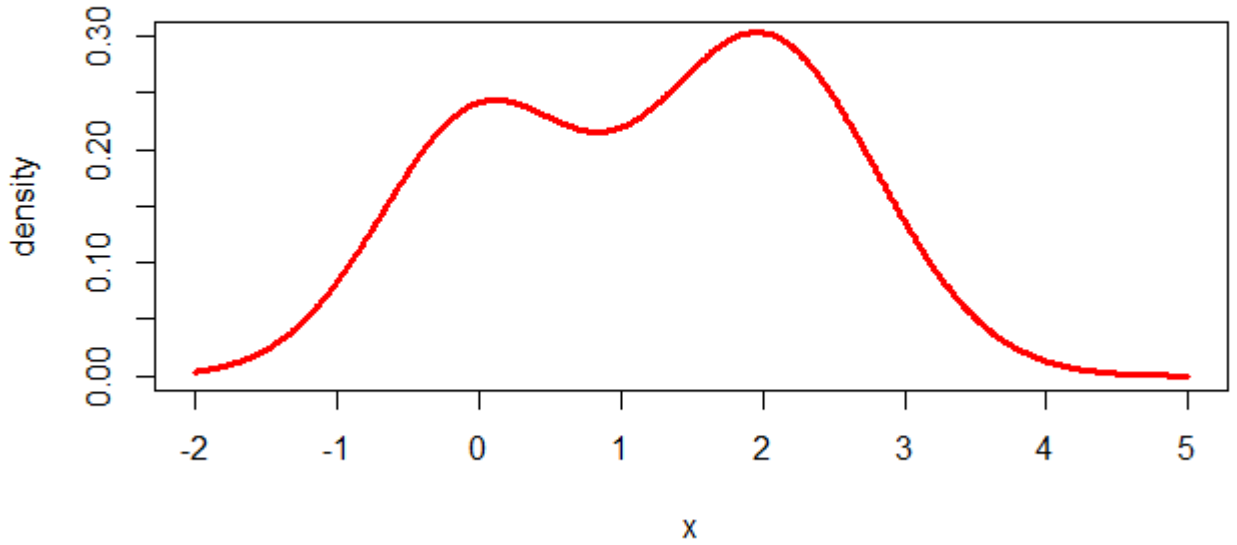
Complete data: $\boldsymbol{Y_i} = (\boldsymbol{X_i}, \boldsymbol{Z_i})$

EM algorithm: Example

- In this example, we assume that X_i has normal mixture density f for $c = 2$ groups (responder, non-responder)
- Generally, a normal mixture (also called GMM, Gaussian mixture model) has density f being sum of c weighted densities:
$$f(x) = \sum_{i=1}^{c} p_i \, \varphi(x; \mu_i; \sigma_i),$$
where p_i are weight or mixing coefficients ($p_i > 0;\ p_1 + \cdots + pc = 1$), and $\varphi(x; \mu; \sigma)$ being density of $N(\mu, \sigma^2)$
- Here for $c = 2$ groups ($p = p_1,\ p_2 = 1 - p$):
$$f(x) = p\varphi(x;\ \mu_1; \sigma_1) + (1 - p)\varphi(x; \mu_2; \sigma_2)$$
- 5 parameters to estimate from data: $p;\ \mu_1; \sigma_1; \mu_2; \sigma_2$

EM algorithm: Example

- $f(x) = p\varphi(x;\ \mu_1; \sigma_1) + (1-p)\varphi(x; \mu_2; \sigma_2)$
- Parameters: $p;\ \mu_1; \sigma_1; \mu_2; \sigma_2$



- Example here: $p = 0.4;\ \mu_1 = 0; \sigma_1 = 0.7; \mu_2 = 2; \sigma_2 = 0.8$

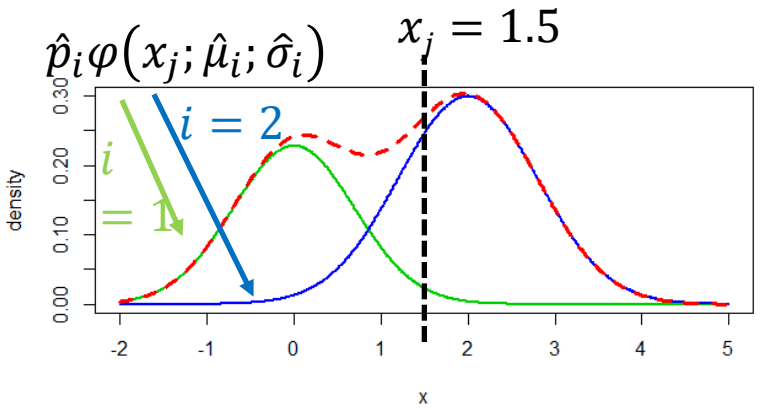
EM algorithm for normal mixtures

- The estimated probability that observation j belongs to group i (of c groups) is

E step

$$\hat{\pi}_{ij} = \frac{\hat{p}_i \varphi(x_j; \hat{\mu}_i; \hat{\sigma}_i)}{\sum_{k=1}^{c} \hat{p}_k \varphi(x_j; \hat{\mu}_k; \hat{\sigma}_k)},$$

where
$\varphi(\cdot; \mu; \sigma)$ is density of normaldist. with mean μ and sd σ



- Model parameters maximizing Q are:

M step

$$\hat{p}_i = \frac{1}{n}\sum_{j=1}^{n} \hat{\pi}_{ij},$$

$$\hat{\mu}_i = \frac{1}{\hat{p}_i n}\sum_{j=1}^{n} \hat{\pi}_{ij} \cdot x_j,$$

$$\hat{\sigma}_i^2 = \frac{1}{\hat{p}_i n}\sum_{j=1}^{n} \hat{\pi}_{ij} \cdot (x_j - \hat{\mu}_i)^2$$

Multivariate case similar, except:

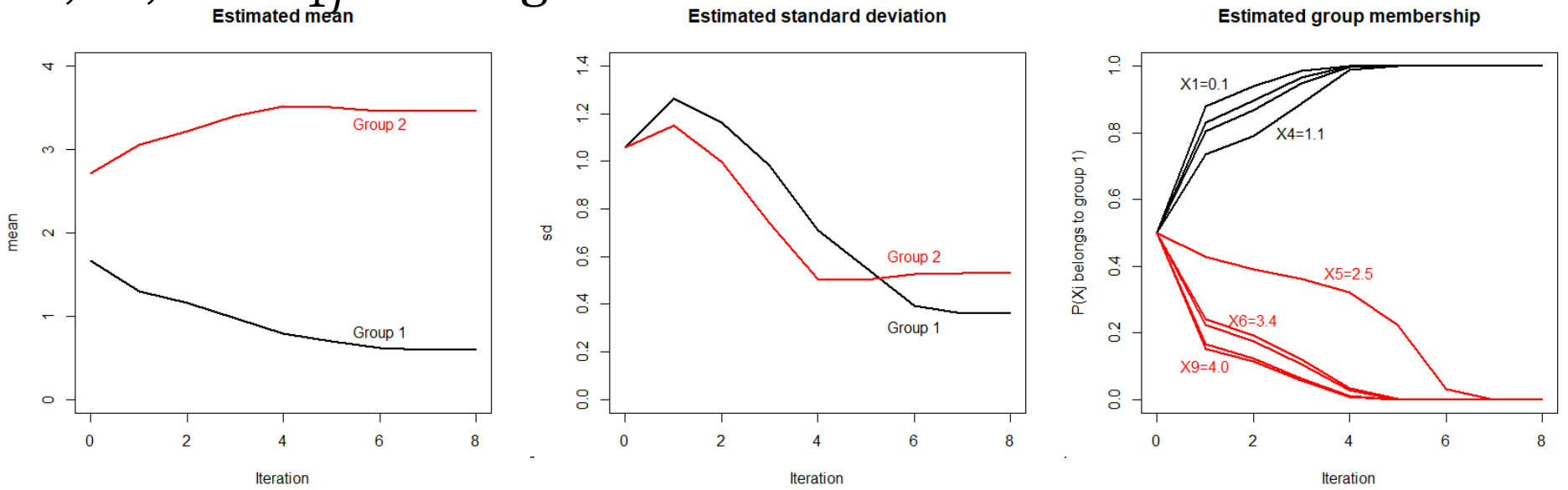
$$\hat{\boldsymbol{\mu}}_i = \frac{1}{\hat{p}_i n}\sum_{j=1}^{n} \hat{\pi}_{ij} \cdot \boldsymbol{x}_j,$$

$$\hat{\Sigma}_i = \frac{1}{\hat{p}_i n}\sum_{j=1}^{n} \hat{\pi}_{ij} \cdot (\boldsymbol{x}_j - \hat{\boldsymbol{\mu}}_i)(\boldsymbol{x}_j - \hat{\boldsymbol{\mu}}_i)^T$$

- $Q = \sum_{i=1}^{c}\sum_{j=1}^{n} \hat{\pi}_{ij}\{\log(\hat{p}_i) + \log \varphi(x_j; \hat{\mu}_i; \hat{\sigma}_i)\}$
- See Section (10.1 and) 10.2 of Lindholm, Wahlström, Lindsten, Schön (2022)

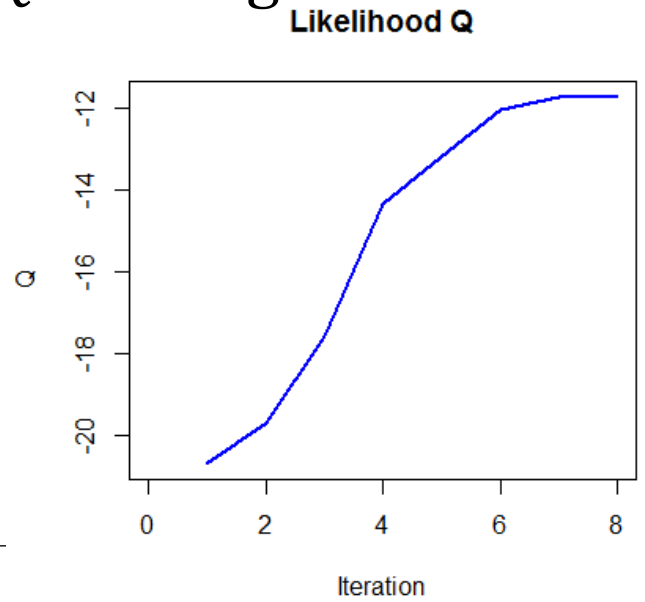
EM algorithm for normal mixtures

- Example for illustration: $n = 9$ observations obtained. Ordered data: 0.1, 0.5, 0.7, 1.1, 2.5, 3.4, 3.5, 3.9, 4.0
- EM algorithm terminates after 8 iterations with: $(p_1^{(8)}, \mu_1^{(8)}, \mu_2^{(8)}, \sigma_1^{(8)}, \sigma_2^{(8)}) = (0.444, 0.600, 3.460, 0.361, 0.532)$
- Mean, sd, and $\hat{\pi}_{1j}$ converge as follows:



EM algorithm for normal mixtures

- Example for illustration: $n = 9$ observations obtained. Ordered data: 0.1, 0.5, 0.7, 1.1, 2.5, 3.4, 3.5, 3.9, 4.0
- EM algorithm terminates after 8 iterations with: $(p_1^{(8)}, \mu_1^{(8)}, \mu_2^{(8)}, \sigma_1^{(8)}, \sigma_2^{(8)}) = (0.444, 0.600, 3.460, 0.361, 0.532)$
- Over the iterations, Q converges as follows:

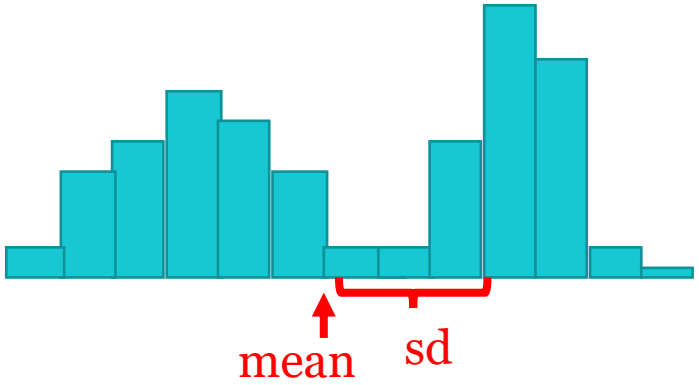


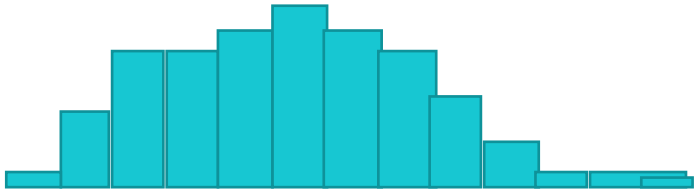
Q
-20.69286
-19.68185
-17.56861
-14.35840
-13.19032
-12.03445
-11.71313
-11.71272

```
emalg <- function(dat, eps=0.000001){
  n      <- length(dat)
  pi     <- rep(NA, n)          # initialize vector for prob. to belong to group 1
  # define reasonable starting values for parameters; here based on summary statistics for total dataset
  p      <- 0.5                 # starting value for mixing parameter
  sigma1 <- sd(dat)*2/3         # starting value for standard deviation in group taken as 2/3 of total sd
  sigma2 <- sigma1
  mu1    <- mean(dat)-sigma1/2 # starting values for means, taken a bit lower and a bit higher than overall mean
  mu2    <- mean(dat)+sigma1/2
  pv     <- c(p, mu1, mu2, sigma1, sigma2)  # parameter vector
  cc     <- eps + 100           # initialize convergence criterion to avoid stopping the while-loop directly
  while (cc>eps){
    pv1  <- pv                  # save previous parameter vector
    ### E step ###
    for (j in 1:n){
      pi1   <- p*dnorm(dat[j], mean=mu1, sd=sigma1)
      pi2   <- (1-p)*dnorm(dat[j], mean=mu2, sd=sigma2)
      pi[j] <- pi1/(pi1+pi2)
    }
    ### M step ###
    p      <- mean(pi)
    mu1    <- sum(pi*dat)/(p*n)
    mu2    <- sum((1-pi)*dat)/((1-p)*n)
    sigma1 <- sqrt(sum(pi*(dat-mu1)*(dat-mu1)/(p*n)))
    sigma2 <- sqrt(sum((1-pi)*(dat-mu2)*(dat-mu2)/((1-p)*n)))
    ######
    pv     <- c(p, mu1, mu2, sigma1, sigma2)
    cc     <- t(pv-pv1)%*%(pv-pv1)  # a convergence criterion, maybe not the best one
  }
  pv
}
data <- c(0.1, 0.5, 0.7, 1.1, 2.5, 3.4, 3.5, 3.9, 4.0) # example data and run of the algorithm
emalg(data)
```

Choice of starting values in example before

- We want to create automatically starting values which are meaningful for the data
- My heuristic rule to choose them in the R-code before:
  - Take total data and compute overall mean and sd
  - Overall sd is usually larger than sd's for groups
  - Therefore, I took 2/3* overall sd as starting values for the sd in both groups
  - For group means, starting values with 1 sd difference chosen



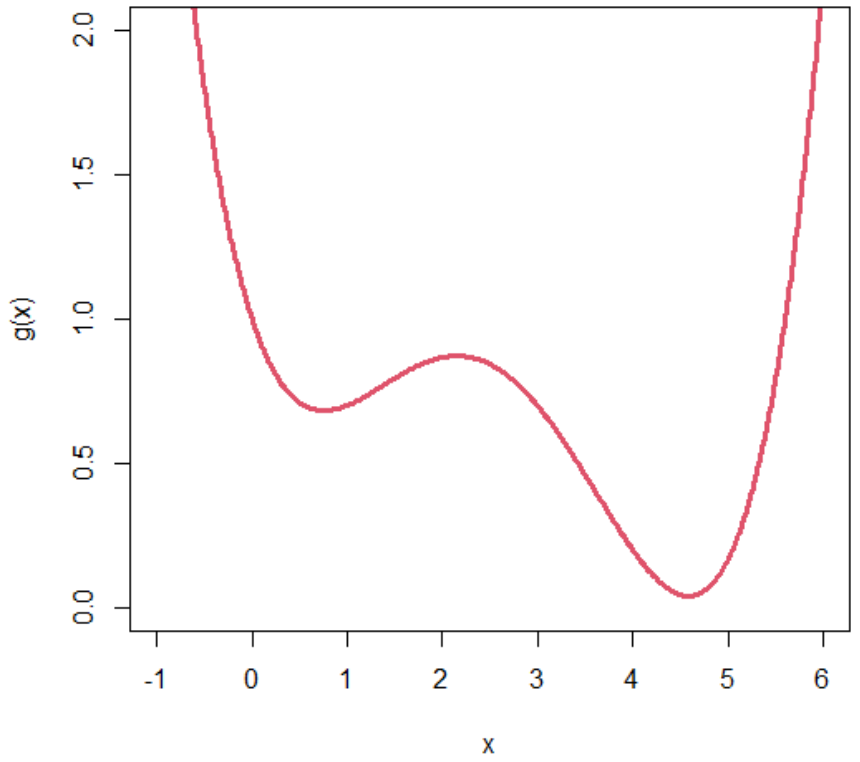


Choosing starting values, connection to K-means

- We can look at the data and guess the components in the mixture, their mean and variance
- We can use a heuristic rule to determine starting values (like in the example before)
- We can try a grid of starting parameter values
- Specifically, for the EM algorithm for normal mixtures, we can first run a classification algorithm and use its result as start for the EM algorithm

- Note (cp. course Machine Learning & Sec. 10.2 of Lindholm et al., 2022): The K-means algorithm can be seen as special case of the EM algorithm for normal mixtures when the variances tend to 0

Simulated annealing



AlphaOpt (2017). Introduction To Optimization: Gradient Free Algorithms (2/2) – Simulated Annealing, Nelder-Mead (0:15-1:35)

Simulated annealing

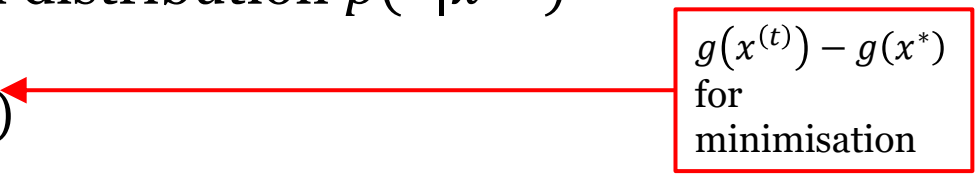
- Start value $x^{(0)}$; stage $j = 0, 1, 2, \ldots$ has m_j iterations; initial temperature τ_0; set $j = 0$
- Given iteration $x^{(t)}$, generate $x^{(t+1)}$ as follows:

1. Sample a candidate x^* from a proposal distribution $p(\cdot\,|x^{(t)})$
2. Compute $h\left(x^{(t)}, x^*\right) = \exp\left(\frac{g(x^*) - g\left(x^{(t)}\right)}{\tau_j}\right)$
3. Define next iteration $x^{(t+1)}$ according to

$$x^{(t+1)} = \begin{cases} x^*, \text{with probability } \min\{h\left(x^{(t)}, x^*\right), 1\} \\ x^{(t)}, \text{otherwise} \end{cases}$$

4. Set `t <- t+1` and repeat 1.-3. m_j times
5. Update $\tau_j = \alpha(\tau_{j-1})$ and $m_j = \beta(m_{j-1})$; set `j <- j+1`; go to 1

τ_j is temperature; function α should slowly decrease it; function β should be increasing



MCMC – Metropolis algorithm

From Lecture 4

- A general method to generate the Markov chain is the Metropolis-Hastings (MH) algorithm
- A starting value $x^{(0)}$ is generated from some starting distribution
- Given observation $x^{(t)}$, generate $x^{(t+1)}$ as follows:

Special case when g is symmetric: $g(x^*|x^{(t)}) = g(x^{(t)}|x^*)$

1. Sample a candidate x^* from a **symmetric** proposal $g(\cdot|x^{(t)})$
2. Compute the MH ratio $R(x^{(t)}, x^*) = \frac{f(x^*)}{f(x^{(t)})}$
3. Sample $x^{(t+1)}$ according to

$$x^{(t+1)} = \begin{cases} x^*, \text{with probability } \min\{R(x^{(t)}, x^*), 1\} \\ x^{(t)}, \text{otherwise} \end{cases}$$

4. If more observations needed, set `t <- t+1`; go to 1

Simulated annealing

- Initially, also “bad” proposals are accepted
- With decreasing temperature, accept only improvements
- This helps to explore first and avoids convergence to a local maximum too early
- Algorithm which has therefore chances to find the global optimum in presence of multiple local optima

- **`method="SANN"`** of R function **`optim`** is “a variant of simulated annealing” (documentation of **`optim`**)
  - Initial temperature can be important choice (can be changed e.g. by **`control=list(temp=0.01)`**; default 10 might be bad)

Simulated annealing: proposal distribution

- Step 1 in simulated annealing iteration rule:

1. Sample a candidate x^* from a proposal distribution $p(\cdot|x^{(t)})$

- Proposal distribution could be uniform distribution on a **neighborhood** of $x^{(t)}$; for a unidimensional optimisation problem:
  `xs <- xt + runif(n=1, min=-1, max=1)`
- Instead of Unif[-1,1], a distribution on a smaller or larger neighborhood could be used
- But also, normal distribution $N(0, \sigma^2)$ or other symmetric distribution around 0 might be added to $x^{(t)}$ instead
- For multidimensional cases, one could use iid components, a uniform distribution on a ball around $\boldsymbol{x}^{(t)}$, or a multivariate normal distribution with mean $\boldsymbol{x}^{(t)}$

Combinatorial optimization

- Generic optimization problem:
  - $\boldsymbol{x}$ p-dimensional vector, g: $\mathbb{R}^p \to \mathbb{R}$ function
  - We search $\boldsymbol{x}^*$ with $g(\boldsymbol{x}^*) = \max g(\boldsymbol{x})$

- Now, we consider also optimization problems which cannot exactly be formulated according to the generic one
- Especially, function g might be defined on another space than $\mathbb{R}^p$

- Generalized optimization problem:
  - $\boldsymbol{x}$ p-dimensional vector, g: $\mathbb{S} \to \mathbb{R}$ function for some set $\mathbb{S}$
  - We search $\boldsymbol{x}^*$ with $g(\boldsymbol{x}^*) = \max g(\boldsymbol{x})$

Example: Multiple linear regression

- Generalized optimization problem:
  - $\boldsymbol{x}$ p-dimensional vector, g: $\mathbb{S} \to \mathbb{R}$ function for some set $\mathbb{S}$
  - We search $\boldsymbol{x}^*$ with $g(\boldsymbol{x}^*) = \max g(\boldsymbol{x})$

- Multiple linear regression with q predictors
- Desired to choose best model based on criterion like AIC
- There are 2^q possible models
- If q small, AIC of all models can be computed (exhaustive search); for q larger, this is impossible (e.g. q=50, $1ms$ to compute an AIC → more than 35 000 years needed!)
- One model can be represented as element of $\mathbb{S} = \{0, 1\}^q$ (1=predictor included in model, 0 otherwise)

Example: Multiple linear regression

- Generalized optimization problem:
  - $\boldsymbol{x}$ p-dimensional vector, g: $\mathbb{S} \to \mathbb{R}$ function for some set $\mathbb{S}$
  - We search $\boldsymbol{x}^*$ with $g(\boldsymbol{x}^*) = \max g(\boldsymbol{x})$
- Optimization problem: Which model gives best AIC?
- Model 1: (1, 0, 0, 0, 1, 1, 0, 1, ...)
  Model 2: (1, 1, 1, 0, 1, 1, 0, 0, ...)
- Which models are ”close” to each other? (Need metric on $\mathbb{S} = \{0, 1\}^q$)
  What is a neighborhood of a model?

- Apply simulated annealing e.g. with neighborhood being all models which differ by one predictor (for proposal dist.)
- Uniform distribution on neighborhood can be used

Example: Multiple linear regression

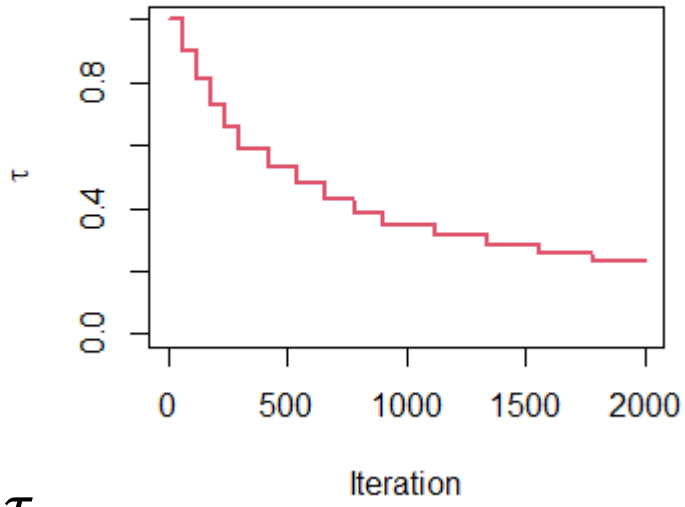
- Generalized optimization problem:
  - $\boldsymbol{x}$ p-dimensional vector, g: $\mathbb{S} \to \mathbb{R}$ function for some set $\mathbb{S}$
  - We search $\boldsymbol{x}^*$ with $g(\boldsymbol{x}^*) = \max g(\boldsymbol{x})$

- Arbitrary starting model generated (e.g. uniform distribution on $\mathbb{S} = \{0, 1\}^q$, `xs <- rbinom(q, size=1, prob=0.5)`)

- See example in Givens and Hoeting (2013), Section 3.3, with 27 predictors

Convergence of simulated annealing

- To achieve convergence to a global optimum (possibly in presence of local optima) in theory, one needs:
  - Run iterations for each fixed temperature long enough such that convergence to stationary distribution achieved
  - Cool temperature slowly enough such that iterations have time to escape from local optima
- Example from Givens and Hoeting (2013; p.73):
  - 5 stages with 60 iterations, then
  - 5 stages with 120 iterations, then
  - 5 stages with 220 iterations
  - From one stage to the next, τ is decreased by 10%, `tau <- 0.9*tau`; final τ is $0.9^{15} = 0.206$*initial τ



Simulated annealing: + and –

+ Very easy to implement
+ Theoretical property is good: theoretically, we can guarantee convergence to a global optimum even in the presence of local optima
+ Can even handle some non-standard optimization problems
– In practice, convergence can be “maddeningly slow”
– One needs to play around with cooling schedule to ensure convergence in practice

Genetic algorithms

- Example: Optimization problem $g: \mathbb{S} = \{0, 1\}^q \rightarrow \mathbb{R}$
- Several candidate solutions are considered in parallel at each iteration
- All candidate solutions at an iteration are called *generation* (size of generation often 10-200)
- One candidate solution is called *individual* having a *chromosome*
- Generation i (at iteration i):
  Individual 1: (1, 0, 0, 0, 1, 1, 0, 1, 0, 1)
  Individual 2: (1, 1, 1, 0, 1, 1, 0, 0, 0, 1)
  …
  Individual n: (1, 0, 1, 0, 0, 1, 1, 0, 1, 1)
- Each individual has a *fitness* (e.g., *fitness*=g)

Genetic algorithms

- Step 1: **Select** parents (at random, e.g. probability proportional to fitness)
  - Individual 1: (1, 0, 0, 0, 1, 1, 0, 1, 0, 1), fitness 10
    Individual 2: (0, 1, 1, 1, 1, 1, 1, 0, 0, 0), fitness 4.5
- Step 2: Apply genetic operator of **crossover**
  - New indiv. 1: (1, 0, 0, 1, 1, 1, 1, 0, 0, 0)
    New indiv. 2: (0, 1, 1, 0, 1, 1, 0, 1, 0, 1)
  - Pick randomly a position where the chromosome of two parents is splitted (e.g. uniform distribution on all q-1 possible split positions)
- Step 3: **Mutate** some genes:
  - (1, 0, 0, 0, 1, 1, 0, 0, 0, 1) -> (1, 0, 0, 0, 1, **0**, 0, 0, 0, 1)
  - Change each gene with probability μ, independently; μ should not be too small or too large; e.g. μ=0.01 in example from Givens and Hoeting (2013)

Steepest ascent (steepest descent)

- Iteration: $\boldsymbol{x}^{(t+1)} = \boldsymbol{x}^{(t)} + \alpha^{(t)}\, \boldsymbol{g}'\left(\boldsymbol{x}^{(t)}\right)$

- Optimization problem (finite sum case):
  - $\boldsymbol{x}$ p-dimensional vector, g_i: $\mathbb{R}^p \to \mathbb{R}$ functions
  - We search $\boldsymbol{x}^*$ with $g(\boldsymbol{x}^*) = \max g(\boldsymbol{x})$, where $g = \sum_{i=1}^{n} g_i$

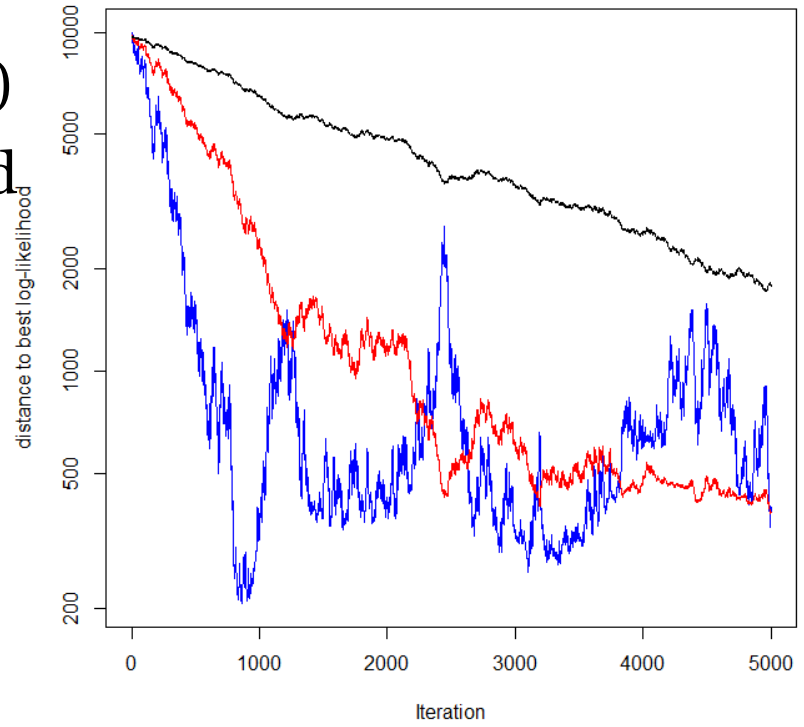
- If n large: Takes time to evaluate gradient $\boldsymbol{g}' = \sum_{i=1}^{n} \boldsymbol{g}'_i$

Stochastic steepest ascent

- Iteration:
  - Choose $i \in \{1, \ldots, n\}$ randomly
  - $\boldsymbol{x}^{(t+1)} = \boldsymbol{x}^{(t)} + \alpha^{(t)} \boldsymbol{g'}_i\left(\boldsymbol{x}^{(t)}\right)$
- $\alpha^{(t)}$ is a predefined sequence, either
  - constant step size $\alpha^{(t)} = \alpha$ or
  - decreasing step size e.g. $\alpha^{(t)} = \alpha/t$
- Convergence (to a local optimum) can be shown if step size fullfills $\sum_{t=1}^{\infty} \alpha^{(t)} = \infty$ and $\sum_{t=1}^{\infty} (\alpha^{(t)})^2 < \infty$ (example: $\alpha^{(t)} = \alpha/t$)

Stochastic steepest ascent: step size, runtime

- Example: Two-parameter MLE comp. (n=1 000 000)
- We monitor distance of current to max. log likelihood
- **Here constant step size** $\alpha^{(t)} = \alpha$
- Choice of step size is critical
- $\alpha = 0.0006$, $\alpha = 0.002$, $\alpha = 0.006$
- Which step size is best,
  - if you have time for 5000 iterations?
  - if you have time for 500, or for 50000 iterations?
- Stochastic steepest ascent: 50000 iterations took 7 s
- Steepest ascent with alpha-halving: 112 iterations took 52 s
- 3320 iterations of stochastic steepest ascent same time as 1 iteration of steepest ascent



Stochastic steepest ascent: mini-batches

- Instead of sampling a single i, a batch of size m can be sampled in each iteration
- Iteration:
  - Choose $\{i_1, \ldots, i_m\} \subseteq \{1, \ldots, n\}$ randomly
  - $\boldsymbol{x}^{(t+1)} = \boldsymbol{x}^{(t)} + \alpha^{(t)} \sum_{j=1}^{m} \boldsymbol{g'}_{i_j}\left(\boldsymbol{x}^{(t)}\right)$
- Decreases risk of large random oscillations
- Especially interesting when algorithm performed on a parallel computer