EM Algorithm, Stochastic Optimization

732A90
Computational Statistics

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Stochastic and combinatorial optimization

- So far: Unconstrained optimization
  - Predictor variables are continuous
  - Response function is differentiable
- We discussed Steepest descent, Newton, BFGS, CG
- But: predictors can be discrete
  (scheduling problems, travelling salesman)
- But: outcome can be discrete, noisy or multi–modal

Stochastic and combinatorial optimization

Given a (large) set of states S, find

$$\min_{s \in S} f(s)$$

- Exhaustive search (shortest path algorithm)
- Often exhaustive search is NP–hard (TSP)
- Alternative: stochastic methods
  random search

Simulated annealing

Motivation from physics: cooling of metal

- Parameters:
  Energy of metal
  (decreasing, but not strictly monotonic)
  Temperature (decreasing)
- Aim: find global minimum energy

Simulated annealing

Initialize $k = 1$, θ_0, $T(1) = T_0$, $i = 0$
while $k < k_{max} + 1$ **do**
  generate new state ξ, compute $\Delta f = f(\xi) - f(\theta)$
  if $\Delta f < 0$ **then**
    accept ξ ($\theta_k = \xi$)
  else
    accept ξ ($\theta_k = \xi$) with $P(\Delta f, T(k))$
  end if
  $k = k + 1$
  {WE CAN ALSO HAVE A SEARCH LOOP FOR EACH $T(k)$ level}
end while

N. Metropolis, A. Rosenbluth, M. Rosenbluth, A. Teller, E. Teller, Equations of state calculations by fast computing machines. J. Chem. Phys. 21:1087-1092, 1953.

Simulated annealing

- https://www.youtube.com/watch?v=iaq_Fpr4KZc
- Generating new state:
  - Continuous: choose a new point a (random) distance from the current one
  - Discrete: similar or some rearrangement
- Selection probability: e.g $\exp(-\Delta f(x)/T)$: decreasing with $f(x)$, increasing with T
- Temperature function: constant, proportional to k, or

$$T(k+1) = b(k)T(k), \quad b(k) = (\log(k))^{-1}$$

Remember: A smaller value is better than one on the path to the global minimum! Always keep track of smallest found.

Simulated annealing: TSP example

Assume constant temperature

Choose initial configuration $(Town_1, \ldots, Town_n)$
$k = 1$
while $k < k_{max} + 1$ **do**
    Generate new configuration by rearrangement,

$$\begin{aligned}(1,2,3,4,5,6,7,8,9) &\rightarrow (1,6,5,4,3,2,7,8,9)\\(1,2,3,4,5,6,7,8,9) &\rightarrow (1,7,8,2,3,4,5,6,9)\end{aligned}$$

    Measure difference in path length (Δf) between old and new configuration
    if shorter path found **then**
        accept it
    else
        accept it with probability $P(\Delta f)$
    end if
    $k++$
end while

Genetic algorithm

- Inspiration from evolutionary theory: survival of the fittest
- Variables=genotypes
- Observation=organism, characterized by genetic code
- State space=population of organisms
- Objective function=fitness of organism

New points are obtained from old points by crossover and mutation, the population only retains the fittest organisms (with better objective function).

`https://en.wikipedia.org/wiki/List_of_genetic_algorithm_applications`

Genetic algorithm

Encoding points

1. Enumerate each element of the state space, S
2. Code for observation i is binary representation of i (or something else)

Mutation and recombination rules

Crossover: $(1010\ 1110, 1100\ 0110) \longrightarrow 1010\ 0110$

Inversion: $11001011 \longrightarrow 11010011$

Mutation: $11010111 \longrightarrow 1101\mathbf{1}111$

Clone: $11010111 \longrightarrow 11010111$

Genetic algorithm

Initialize $i = 0$, population $\mathbf{P}_0$ and calculate fitness
while end criteria not met **do**
    Choose individuals $\mathbf{T}_i$ from $\mathbf{P}_i$ for reproduction
    $\mathbf{T}'_i$ = crossover between individuals from $\mathbf{T}_i$
    $\mathbf{O}_i$ = randomly inverte, mutate, clone $\mathbf{T}'_i$
    Calculate fitness and obtain $\mathbf{P}_i$ from $\mathbf{O}_i$
    $i = i + 1$
end while

ALWAYS KEEP BEST INDIVIDUAL

Genetic algorithm: TSP example

Encoding and crossover

- Encode tours as $A_1, \ldots, A_n$ but

  Parent 1: FAB|ECGD   Parent 2: DEA|CGBF
  Child: FAB|CGBF   Child: DEA|ECGD

Instead

1. Remove FAB from DEACGBF $\longrightarrow$ DECG.
   Child becomes FABDECG.
2. Second child will be by taking prefix from Parent 2: DEAFBCG

Genetic algorithm: Mutations

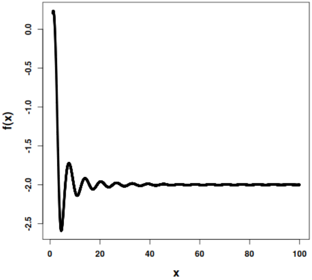
- If a population is small and only crossover: the input domain becomes limited and may converge to a local minimum.
- Large initial populations are computationally heavy.
- Mutations allow one to explore more of S: jump out of local minimum.
- In TSP: mutation move a city in the tour to another position.
- Reproduction: Among m tours selected at step 2, two best are selected for reproduction, two worst replaced by children.
- If m is large, some tours might never be parents, global solution may be missed. Random chance of reproduction?
- Mutation probability is usually small (unless you want to jump wildly)

Genetic algorithm: example

Minimize

$$f(x) := \frac{x^2}{e^x} - 2\exp(-(9\sin x)/(x^2 + x + 1))$$

- `fitness(x)`$= -f(x)$,
- `crossover(x,y)`$= (x + y)/2$,
- `mutate(x)`$= x + \epsilon; = x^2 \mod 30$
  (mod $\equiv$ %%—integer division)
- smallest fitness individual removed



- mutation probability: 0.5 worked well; 0.1: cannot change; 0.9: cannot stabilize

EM algorithm

Fundamental algorithm of computational statistics!

Model depends on the data which are observed (known) $\mathbf{Y}$ and **latent** (unobserved) data $\mathbf{Z}$.

The data's (**both** $\mathbf{Y}$'s and $\mathbf{Z}$'s) distribution depends on some parameters θ.

AIM: Find MLE of θ.

- All data is known: Apply unconstrained optimization (discussed in Lecture 2)
- Unobserved data
  - **Sometimes** it is possible to look at the marginal distribution of the observed data.
  - Otherwise: **EM algorithm**

EM algorithm

Let

$$Q(\theta, \theta^k) = \int \log p(\mathbf{Y}, \mathbf{z}|\theta) p(\mathbf{z}|\mathbf{Y}, \theta^k) \mathrm{d}\mathbf{z} = \mathrm{E}\left[\mathrm{loglik}(\theta|\mathbf{Y}, \mathbf{Z})|\theta^k, \mathbf{Y}\right]$$

1: $k = 0$, $\theta^0 = \theta^0$
2: **while** Convergence not attained **and** $k < k_{max} + 1$ **do**
3: **E–step**: Derive $Q(\theta, \theta^k)$
4: **M–step**: $\theta^{k+1} = \mathrm{argmax}_\theta \; Q(\theta, \theta^k)$
5: $k++$
6: **end while**

Example: Normal data with missing values (but here analytical approach is also possible)

EM algorithm: R

`732A90_ComputationalStatisticsHT2022_Lecture06codeSlide16.R`

EM algorithm: R

```
> Y<-rnorm(100)
> Y[sample(1:length(Y),20,replace=FALSE)]<-NA
> EM.Norm(Y,0.0001,100)
[1]    1.0000    0.1000 -997.5705
[1]    0.1341894    1.3227095 -128.2789837
[1]   -0.03897274    1.38734070 -126.86036252
[1]   -0.07360517    1.39307050 -126.80801589
[1]   -0.08053165    1.39392861 -126.80593837
[1]   -0.08191695    1.39408871 -126.80585537
> mean(Y,na.rm=TRUE)
[1] -0.08226328
> var(Y,na.rm=TRUE)
[1] 1.411775
```

Notice: can be done by studying marginal distribution of observed data.

EM algorithm: Applications

Mixture models Z is a latent variable, $P(Z = k) = \pi_k$

- Mixed data comes from different sources (e.g. for regression, classification)
- Clustering
  1. Density in each cluster is normally distributed.
  2. Cluster label is latent (we do not know what are the chances an observation is from the given cluster)

$$p(x) = \sum_{k=1}^{K} \pi_k \mathcal{N}\left(x|\vec{\mu}_k, \mathbf{\Sigma}_k\right) \quad \text{(informally)}$$

Direct MLE leads to numerical problems.
Introduce latent class variables and use EM.

EM algorithm: Gaussian mixtures

input: data $\vec{x}_1, \ldots, \vec{x}_n$; K clusters

Initialize $r = 0$, $(\vec{\mu}_1^0, \ldots, \vec{\mu}_K^0)$, $(\mathbf{\Sigma}_1^0, \ldots, \mathbf{\Sigma}_K^0)$

while end criteria not met **do**

 E-step ($\overline{z}_{jk}$: *responsibility* of cluster k explaining $\vec{x}_j$)

$$\overline{z}_{jk} = \frac{\mathcal{N}\left(x_j | \vec{\mu}_k^r, \mathbf{\Sigma}_k^r\right)}{\sum_{i=1}^{K} \pi_i \mathcal{N}\left(\vec{x}_j | \vec{\mu}_i^r, \mathbf{\Sigma}_i^r\right)}, \quad j = 1, \ldots, n$$

 M–step for $k = 1, \ldots, K$

$$n_k = \sum_{j=1}^{n} \overline{z}_{jk}, \qquad \pi_k^r = n_k / n,$$

$$\vec{\mu}_k^r = (n_k)^{-1} \sum_{j=1}^{n} \overline{z}_{jk} \vec{x}_j, \quad \mathbf{\Sigma}_k^r = (n_k)^{-1} \sum_{j=1}^{n} \overline{z}_{jk} (\vec{x}_j - \vec{\mu}_k^r)(\vec{x}_j - \vec{\mu}_k^r)^T$$

 evaluate log–likelihood

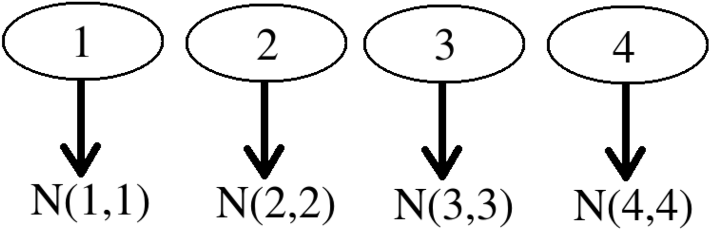
$$\log \mathcal{L}(\{\pi_k^r, \vec{\mu}_k^r, \mathbf{\Sigma}_k^r\}_{k=1}^K) = \sum_{j=1}^{n} \log \left(\sum_{k=1}^{K} \pi_k^r \mathcal{N}\left(\vec{x}_j | \vec{\mu}_k^r, \mathbf{\Sigma}_k^r\right) \right)$$

 $r = r + 1$

end while

See also Ch. 7.10.7, *EM for Mixture of Gaussians*, O. Simeon, *Machine Learning for Engineers*, Cambridge University Press, 2023 (there supervised log–loss optimized)

Gaussian mixtures: example



$P(1) = P(2) = P(3) = P(4) = 0.25$

1. draw class $Z \in \{1, 2, 3, 4\}$ uniformly
2. draw normal distribution $\mathcal{N}(Z, Z)$ with density $\phi_{Z,Z}(\cdot)$

We can write the mixture density as

$$f(x) = 0.25\phi_{1,1}(x) + 0.25\phi_{2,2}(x) + 0.25\phi_{3,3}(x) + 0.25\phi_{4,4}(x).$$

Stochastic gradient descent (SGD)—2016 slides

$$\text{Goal}: \ \text{maximize} \ \ g(\theta) = N^{-1} \sum_{j=1}^{N} g_j(\theta) \text{ for large } N$$

γ_i: learning rate

1: $\theta_0 = \theta_0$, $i = 0$
2: **while** stopping criterion not met **do**
3: subset $S_i \subseteq \{1, \ldots, N\}$, with $|S_i| = S$
4: update:

$$\theta_{i+1} = \theta_i + \frac{\gamma_i}{S} \sum_{j \in S_i} g_j(\theta)$$

5: $i++$
6: **end while**

Ch. 5.11; O. Simeone, Maching Learning for Engineers, 2023, Cambridge University Press, Cambridge

Variational inference (VI)

x: observed variable; z: latent variable;
Model: $p_\psi(x,z) = p_\psi(x|z)p_\psi(z)$

ψ: unknown parameters

$$\text{likelihood}: \; L(\psi) = p_\psi(x) = \int p_\psi(x,z)dz \;\; \text{not tractable}$$

$q_\theta(\cdot)$: known parametric family of distributions
$q_{\theta_\psi}(z) \approx p_\psi(z|x)$ in Kullback-Leibler divergence sense,

$$q_{\theta_\psi^*}(z) = \arg\min_{\theta_\psi} \mathrm{KL}(q_{\theta_\psi}(z), p_\psi(z|x))$$

Variational inference (VI)

$$\mathrm{KL}(q_\theta(z), p_\psi(z|x)) := \int \log q_\theta(z) q_\theta(z) dz - \int \log p_\psi(z|x) q_\theta(z) dz$$
$$= \int \log q_\theta(z) q_\theta(z) dz - \int \log p_\psi(z,x) q_\theta(z) dz + \log p_\psi(x)$$
$$\geq \int \log q_\theta(z) q_\theta(z) dz - \int \log p_\psi(z,x) q_\theta(z) dz =: (-1) ELBO(q_\theta)$$

$ELBO$: evidence lower bound, as $\log p_\psi(x) \geq ELBO(q_\theta)$

estimate $ELBO(q_\theta)$ using that $q_\theta(z)$ is a distribution
maximize $ELBO(q_\theta)$ w.r.t. θ (minimizes KL),

$$p_\psi(x) = p_\psi(z|x) p_\psi(z,x) \approx q_{\theta^*_\psi}(z) p_\psi(z,x)$$

Summary

Random walk over the state space in search of minimum

1. Follow decreasing path
2. **BUT** with a certain probability go to higher values, to avoid local minima traps.
3. **Never forget** best found conformation!

4. Simulated annealing, Genetic algorithm, **EM algorithm**, SGD, VI