The MM Algorithm

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Overview

Today, we cover:

- The MM Algorithm
- Last lecture from Optimization 1! Tomorrow Bayesian Computing.

Announcements

- HW3 posted and due 3/4 at 10:00AM

Readings:

- Hunter and Lange: A tutorial on MM algorithms, *The American Statistician*

EM as MM

The EM is a **minorization** approach. Instead of directly maximizing. the log-likelihood, which is hard, the algorithm constructs a minorizing function and optimizes that function instead.

A function g *minorizes* f over $\mathcal{X}$ at y if:

1. $g(x) \leq f(x)$ for all $x \in \mathcal{X}$
2. $g(y) = f(y)$

MM algorithm

- Stands for “Majorize-Minimization” or “Minorize-Maximization”, depending on whether the desired optimization is a minimization or a maximization
- Not actually an algorithm, but a strategy for constructing optimization algorithms
- EM is a special case

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Idea: MM algorithm operates by creating a **surrogate function** that minorizes or majorizes the objective function. When the surrogate function is optimized, the objective function is driven uphill or downhill as needed.

Definition of an MM algorithm for Minimization

We first focus on the **minimization** problem, in which MM = Majorize–Minimize.

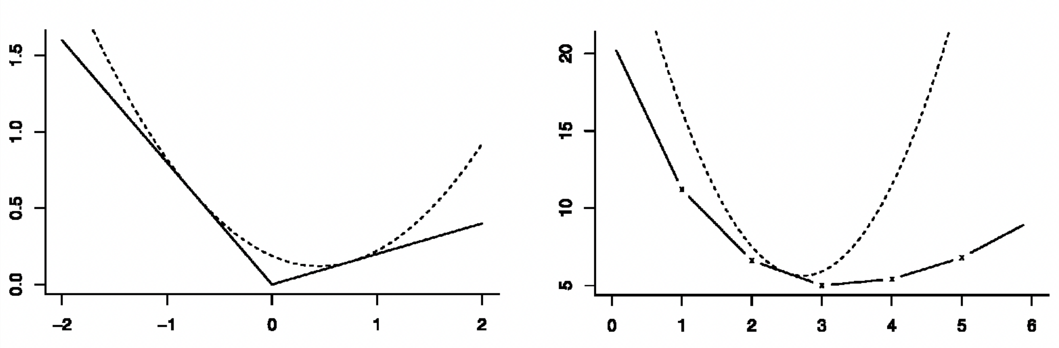
- A function $g(\theta|\theta^t)$ is said to **majorize** the function $f(\theta)$ at θ^t if

$$f(\theta) \leq g(\theta|\theta^t) \text{ for all } \theta \tag{1}$$

$$f(\theta^t) = g(\theta^t|\theta^t) \tag{2}$$

- We choose a majorizing function $g(\theta|\theta^t)$ and **minimize** it, instead of minimizing $f(\theta)$. Denote $\theta^{t+1} = \arg\min_\theta g(\theta|\theta^t)$. Iterate until θ^t converges.
- **Descent property**: $f(\theta^t) \leq g(\theta^{t+1}|\theta^t) \leq g(\theta^t|\theta^t) = f(\theta^t)$

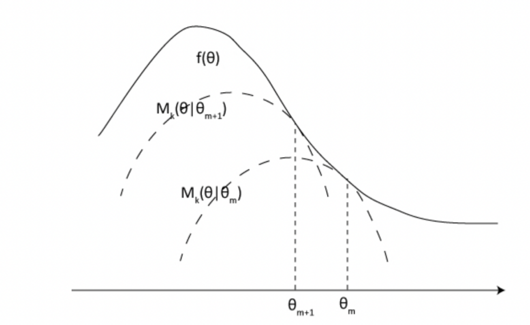
Definition of an MM algorithm for Minimization



MM algorithm for Maximization

In a **maximization** problem, MM = Minorize–Maximize.

- To maximize $f(\theta)$, we **minorize** it by a surrogate function $g(\theta|\theta^t)$ and maximize $g(\theta|\theta^t)$ to produce the next iteration θ^{t+1}
- $g(\theta|\theta^t)$ minorizes $f(\theta)$ at θ^t if $-g(\theta|\theta^t)$ majorizes $-f(\theta)$



Separation of high-dimensional parameter spaces

One of the key criteria in judging majorizing or minorizing functions is their **ease of optimization**.

- Successful MM algorithms in high-dimensional parameter spaces often rely on surrogate functions in which the individual parameter components are **separated**, i.e., for $\theta = (\theta_1, \ldots, \theta_p)$,

$$g(\theta|\theta^t) = \sum_{j=1}^{p} q_j(\theta_j)$$

where $q_j(\cdot)$ are univariate functions.

Because the p univariate functions may be **optimized one by one**, this makes the surrogate function easier to optimize at each iteration.

Advantages of the MM algorithm

- **Numerical stability**: warranted by the descent (or ascent) property
- **Simplicity**: Turn a difficult optimization problem into a simple one
    - It can turn a non-differentiable problem into a smooth problem (Example 2).
    - It can separate the parameters of a problem (Example 3).
    - It can linearize an optimization problem (Example 3).
    - It can deal gracefully with equality and inequality constraints (4).
    - It can generate an algorithm that avoids large matrix inversion (5).
- Iteration is the price we pay for simplifying the original problem.

EM algorithm vs. MM algorithm

- **EM**: The E-step creates a surrogate function by identifying a complete-data log-likelihood function and evaluating it with respect to the observed data. The M-step maximizes the surrogate function. Every EM algorithm is an example of an MM algorithm.
- **EM**: demands creativity in identifying the **missing data (complete data)** and technical skill in calculating an often complicated conditional expectation and then maximizing it analytically.
- **MM**: requires creativity in identifying the surrogate function, using proper inequalities.

Inequalities to construct majorizing/minorizing function

- **Property of convex function**: A function $f : R^p \to R$ is **convex** if for all $x_1, x_2 \in R^p$ and all $\alpha \in [0, 1]$,

$$f(\alpha x_1 + (1 - \alpha)x_2) \leq \alpha f(x_1) + (1 - \alpha)f(x_2)$$

- **Jensen's inequality**: for any convex function f and r.v. x,

$$f[E(x)] \leq E[f(x)]$$

- **Supporting hyperplanes**: If f is convex and differentiable, then

$$f(y) \geq f(x) + \nabla f(x)^\top (y - x), \forall x, y \in \mathbb{R}^p,$$

and equality holds when $y = x$.

Inequalities (continued)

- **Arithmetic-Geometric Mean Inequality**: For nonnegative $x_1, \ldots, x_m$,

$$\sqrt[m]{\prod_i^m x_i} \leq \frac{1}{m} \sum_{i=1}^m x_i,$$

  and the equality holds iff $x_1 = x_2 = \ldots = x_m$.
- **Cauchy-Schwartz Inequality**: for p-vectors x and y,

$$x^T y \leq ||x|| \cdot ||y||,$$

where $||x|| = \sqrt{\sum_i^p x_i^2}$ is the norm of the vector.

Inequalities (continued)

- **Quadratic upper bound**: If a convex function $f(x)$ is twice differentiable and has bounded curvature, then we can majorize $f(x)$ by a quadratic function with sufficiently high curvature and tangent to $f(x)$ at x^t. In algebraic terms, we can find a positive definite matrix M such that $M - \nabla^2 f(x)$ is nonnegative for all x, then

$$f(x) \leq f(x^t) + \nabla f(x^t)^T(x - x^t) + \frac{1}{2}(x - x^t)^T M(x - x^t)$$

provides a quadratic upper bound that majorizes $f(x)$.

Example 1: EM algorithms

- By **Jensen's inequality** and the convexity of the function $-\log(y)$, we have for probability densities $a(y)$ and $b(y)$ that

$$-\log\left\{E\left[\frac{a(y)}{b(y)}\right]\right\} \leq E\left[-\log\frac{a(y)}{b(y)}\right]$$

- Y has the density $b(y)$, then $E[a(y)/b(y)] = 1$. The left hand side vanishes, and we obtain

$$E[\log a(y)] \leq E[\log b(y)],$$

the Kullback-Leibler divergence.

- This inequality guarantees that a minorizing function is constructed in the E-step of any EM algorithm, making every EM algorithm an MM algorithm.

Example 1: EM algorithms, cont

- We have the **decomposition**

$$
\begin{aligned}
Q(\theta|\theta^t) &= E_z\left[\log p(y, z|\theta)|y, \theta^t\right] &(3)\\
&= E\left[\log p(z|y, \theta)|y, \theta^t\right] + \log p(y|\theta) &(4)
\end{aligned}
$$

BY KL divergence,

$$
E\left[\log p(z|y, \theta)|y, \theta^t\right] \leq E\left[\log p(z|y, \theta^t)|y, \theta^t\right] \forall\theta
$$

We obtain the **surrogate function** that minorizes the objective function

$$
\log p(y|\theta) \geq Q(\theta|\theta^t) - E\left[\log p(z|y, \theta^t)|y, \theta^t\right]
$$

Example 2: finding a sample median

- Consider the sequence of numbers $y_1, \dots y_n$. The sample median θ minimizes the **non-differentiable objective function**

$$f(\theta) = \sum_i^n |y_i - \theta|.$$

- The **quadratic function**

$$h_i(\theta|\theta^t) = \frac{(y_i - \theta)^2}{2|y_i - \theta^t|} + \frac{1}{2}|y_i - \theta^t|$$

majorizes $|y_i - \theta|$ at the point θ^t (Arithmetic-Geometric Mean Inequality).

- Hence, $g(\theta|\theta^t) = \sum_i^n h_i(\theta|\theta^t)$ majorizes $f(\theta)$.

Example 2: finding a sample median (continued)

We have the following objective function (a weighted sum of squares):

$$g(\theta|\theta^t) = \frac{1}{2}\sum_i^n \left[\frac{(y_i - \theta)^2}{|y_i - \theta^t|} + |y_i - \theta^t|\right]$$

- The **minimum** of $g(\theta|\theta^t)$ occurs at

$$\theta^{t+1} = \frac{\sum_i^n w_i^t y_i}{w_i^t}, w_i^t = |y_i - \theta^t|^{-1}$$

- This algorithm works except when a weight $w_i^t = \infty$. It generalizes to sample quantiles, LASSO, and quantile regression.

Example 2: finding a sample median (continued)

Do lab exercise 1

Finding a sample quantile

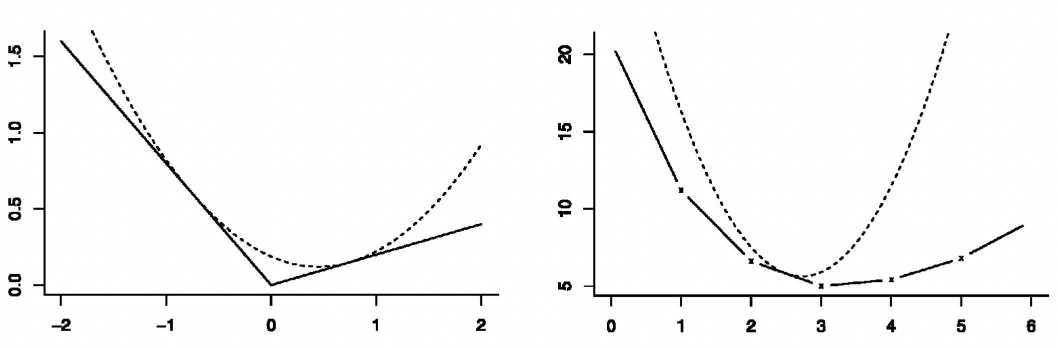
Median example generalizes to finding a sample quantile. A qth sample quantile of $y_1, \ldots, y_n$ is one that minimizes the function

$$f(\theta) = \sum_i p_q(y_i - \theta)$$

Where $p_q(\theta) = q\theta$ if $\theta \geq 0$ and $p_q(\theta) = -q(1-\theta)$ if $\theta < 0$. A majorizing function is

$$g_q(\theta|\theta^t) = \frac{1}{4}\sum_i^n \left[\frac{(y_i - \theta)^2}{|y_i - \theta^t|} + (4q-2)(y_i - \theta) + |y_i - \theta^t|\right]$$

Finding a sample quantile



Example 3: Bradley-Terry Ranking

Consider a sports league with n teams. Assign team i the skill level θ_i, where $\theta_1 = 1$ for identifiability. Bradley and Terry proposed the model

$$Pr(i \text{ beats } j) = \frac{\theta_i}{\theta_i + \theta_j}.$$

- If b_{ij} is the number of times i beats j, then the likelihood of the data is

$$L(\theta) = \prod_{i \neq j} \left(\frac{\theta_i}{\theta_i + \theta_j} \right)^{b_{ij}}.$$

We estimate θ by maximizing $f(\theta) = \log L(\theta)$ and then rank the teams on the basis of the estimates.

Example 3: Bradley-Terry Ranking

- The log-likelihood is $f(\theta) = \sum_{i \neq j} b_{ij}[\log \theta_i - \log(\theta_i + \theta_j)]$.
- We need to **linearize** the term $-\log(\theta_i + \theta_j)$ to **separate parameters**.

Example 3: Bradley-Terry Ranking (continued)

- By the **supporting hyperplane property** when f is convex and the convecity of $-\log(\cdot)$, we have

$$-\log(y) \geq -\log(x) - x^{-1}(y - x) = -\log(x) - y/x + 1$$

- The inequality indicates that

$$-\log(\theta_i + \theta_j) \geq -\log(\theta_i^t + \theta_j^t) - \frac{\theta_i + \theta_j}{\theta_i^t + \theta_j^t} + 1$$

Example 3: Bradley-Terry Ranking (continued)

- Thus, the **minorizing** function is

$$g(\theta|\theta^t) = \sum_{i \neq j} b_{ij} \left[\log \theta_i - \log(\theta_i^t + \theta_j^t) - \frac{\theta_i + \theta_j}{\theta_i^t + \theta_j^t} + 1 \right].$$

- The parameters are now **separated**. We can easily find the optimal point

$$\theta_i^t = \frac{\sum_{i \neq j} b_{ij}}{\sum_{i \neq j} (b_{ij} + b_{ji}) / (\theta_i^t + \theta_j^t)}$$

BT Ranking

Lab exercise 2

Example 4: Handling constraints

- Consider the problem of **minimizing** $f(\theta)$ subject to the **constraints** $v_j(\theta) \geq 0$ for $1 \leq j \leq q$, where each $v_j(\theta)$ is a concave, differentiable function.
- By the **supporting hyperplane property** and the convexity of $-v_j(\theta)$,

$$v_j(\theta^t) - v_j(\theta) \geq -[\nabla v_j(\theta^t)]^T(\theta - \theta^t)$$

- Again, by the **supporting hyperplane property** and the convexity of $-\log(\cdot)$, we have $-\log y + logx \geq -x^{-1}(y - x) \implies x(-\log y + \log x) \geq x - y$. Then:

$$v_j(\theta^t)[-\log v_j(\theta) + \log v_j(\theta^t)] \geq v_j(\theta^t) - v_j(\theta). \tag{5}$$

Example 4: Handling constraints

By (2) and (3) on the previous slide,

$$v_j(\theta^t)[-\log v_j(\theta) + \log v_j(\theta^t)] + [\nabla v_j(\theta^t)]^T(\theta - \theta^t) \geq 0$$

and the equality holds when $\theta = \theta^t$.

- Summing over j and multiplying by a positive tuning parameter ω, we construct the **surrogate function** that majorizes $f(\theta)$,

$$g(\theta|\theta^t) = f(\theta) + \omega \sum_{j=1}^{q} \left[v_j(\theta^t) \log \frac{v_j(\theta^t)}{v_j(\theta)} + [\nabla v_j(\theta^t)]^T(\theta - \theta^t) \right] \geq f(\theta)$$

Handling constraints (continued)

- Note:
  - **Majorization gets rid of the inequality constraints**!
  - The presence of $\log v_j(\theta)$ ensures $v_j(\theta) \geq 0$
- An initial point θ^0 must be selected with all inequality constraints strictly satisfied. All iterates stay within the interior region but allows strict inequalities to become equalities at the limit
- The minimization step of the MM algorithm can be carried out approximately by **Newton's method**.
- Where there are linear equality constraints $A\theta = b$ in addition to the inequality constraints $v_j(\theta) \geq 0$, these should be enforced by introducing Lagrange multipliers during the minimization of $g(\theta|\theta^t)$.

Comparing MM and Newton's Method

- **Convergence rate**
  - N: a quadratic rate $\lim ||\theta^{t+1} - \hat{\theta}||/||\theta^{t+1} - \hat{\theta}||^2 = c$
  - MM: a linear rate $\lim ||\theta^{t+1} - \hat{\theta}||/||\theta^{t+1} - \hat{\theta}|| = c < 1$
- **Complexity of each iteration**
  - N: requires evaluation and inversion of Hessian, $O(p^3)$
  - MM: separates parameters, $O(p)$ or $O(p^2)$
- **Stability of the algorithm**
  - N: behaves poorly if started too far from an optimum point
  - MM: guaranteed to increase/decrease the objective function at every iteration

Comparing MM and Newton's Method

In conclusion, well-designed MM algorithms tend to require more iterations but simpler iterations than Newton's method; thus MM sometimes enjoy an advantage in computation speed and numerical stability.

Resources

- Kenneth Lange lecture
- Example with NMF
- Lange examples of MM