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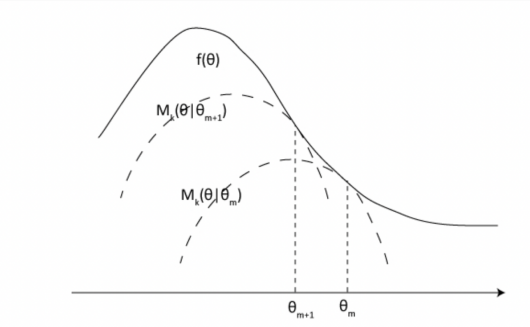
Idea: MM algorithm operates by creating a **surrogate function** that minorizes or majorizes the objective function. When the surrogate function is optimized, the objective function is driven uphill or downhill as needed.

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 $-f(\theta)$



Ascent property of minorization

1. $g(\theta|\theta^t) \leq f(\theta) \forall \theta$
2. $g(\theta^t|\theta^t) = f(\theta^t)$

Ascent property:

$$f(\theta^t) \geq g(\theta^{t+1}) \geq g(\theta^t|\theta^t) = f(\theta^t)$$

Definition of an MM algorithm for Minimization

Formal definition focuses on the **minimization** problem, in which MM = Majorize–Minimize.

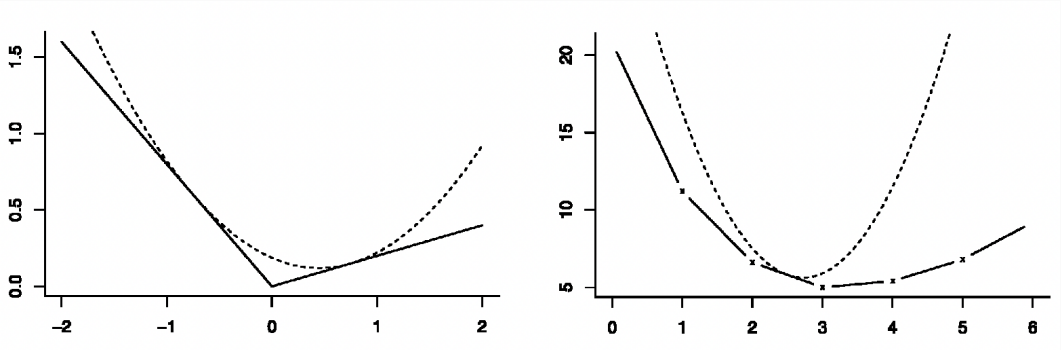
- A function $g(\theta|\theta^t)$ is said to **majorize** the function $f(\theta)$ at θ^t if

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

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

- 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



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

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

Inequalities to construct majorizing/minorizing function

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

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

Inequalities to construct majorizing/minorizing function

- **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: finding a sample median

- Consider the sequence of numbers $y_1, \ldots y_n$. 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 1: 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 1: finding a sample median (continued)

Do lab exercise 1

Finding a sample quantile

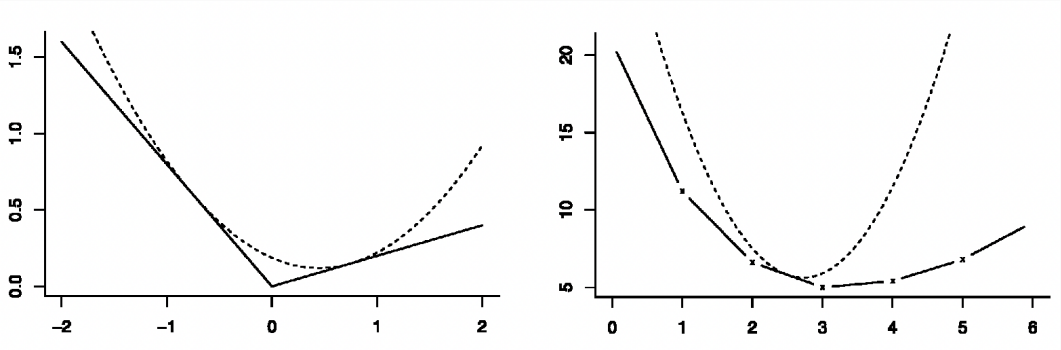
Median example generalizes to finding a sample quantile. A qth sample quantile of $y_1, \ldots, y_n$ is one that minimizes the function

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

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 2: 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 2: EM algorithms, cont

- We have the **decomposition**

$$Q(\theta|\theta^t) = E_z \left[\log p(y, z|\theta)|y, \theta^t\right] \tag{3}$$

$$= E\left[\log p(z|y, \theta)|y, \theta^t\right] + \log p(y|\theta) \tag{4}$$

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 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

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

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.

BT Ranking

Lab exercise 2

Resources

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