MM Algorithm

2012-9-25

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The MM algorithm is not an algorithm, but a **strategy** for constructing optimization algorithms.

An 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.

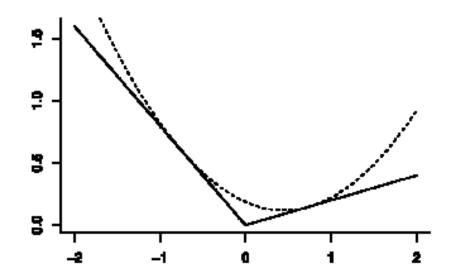
In minimization MM stands for **majorize/minimize**, and in maximization MM stands for **minorize/maximize**.

The **EM algorithm** from statistics is a special case.

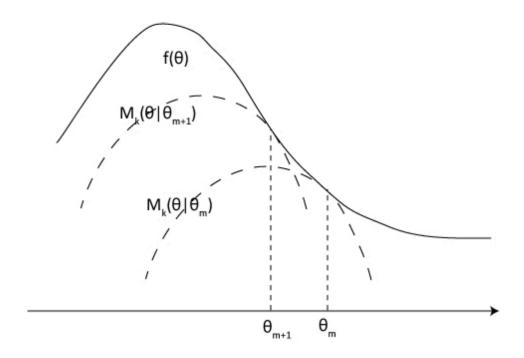
- We first focus on the **minimization** problem, in which MM = majorize/minimize.
- A function $g(\theta|\theta^{(k)})$ is said to **majorize** the function $f(\theta)$ at $\theta^{(k)}$ provided

$$f(\theta) \le g(\theta|\theta^{(k)})$$
 for all θ
 $f(\theta^{(k)}) = g(\theta^{(k)}|\theta^{(k)})$

- We choose a majorizing function $g(\theta|\theta^{(k)})$ and **minimize** it (rather than minimizing $f(\theta)$). Denote $\theta^{(k+1)} = \arg\min_{\theta} g(\theta|\theta^{(k)})$. Iterate until $\theta^{(k)}$ converges.
- Descent property: $f(\theta^{(k+1)}) \le g(\theta^{(k+1)}|\theta^{(k)}) \le g(\theta^{(k)}|\theta^{(k)}) = f(\theta^{(k)}).$



- In a **maximization** problem, MM = minorize/maximize.
- To maximize $f(\theta)$, we **minorize** it by a surrogate function $g(\theta|\theta^{(k)})$ and maximize $g(\theta|\theta^{(k)})$ to produce the next iterate $\theta^{(k+1)}$.
- A function $g(\theta|\theta^{(k)})$ is said to minorize the function $f(\theta)$ at $\theta^{(k)}$ provided that $-g(\theta|\theta^{(k)})$ majorizes $-f(\theta)$.



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 $\theta = (\theta_1, \dots, \theta_p)$,

$$g(\theta \mid \theta^{(k)}) = \sum_{j=1}^{p} q_j(\theta_j),$$

where $q_i(.)$ 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.

- Numerical stability: warranted by the descent property
- **Simplicity:** substitute a simple optimization problem for a difficult optimization problem.
 - 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 (Example 4).
 - It can generate an algorithm that avoids large matrix inversion (5).
- Iteration is the price we pay for simplifying the original problem.

- **(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) pay attentions to the **convexity** of the objective function and **inequalities**.
- (MM) easier to understand and sometimes easier to apply than EM algorithms.

Inequalities to construct majorizing/minorizing function -7/??

• Property of convex function: $\kappa(\theta)$ is called convex if for any θ_1 , θ_2 $\lambda \in [0, 1]$

$$\kappa (\lambda \theta_1 + (1 - \lambda)\theta_2)) \le \lambda \kappa(\theta_1) + (1 - \lambda)\kappa(\theta_2)$$

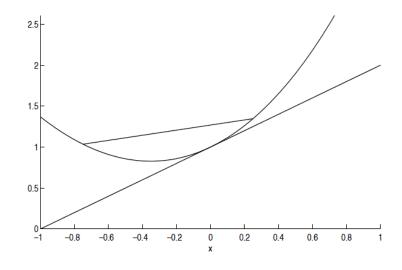
• Jensen's Inequality: For a convex function $\kappa(x)$ and any random variable X,

$$\kappa \left[\mathrm{E}(X) \right] \leq \mathrm{E} \left[\kappa(X) \right]$$

• Supporting hyperplanes: If $\kappa(.)$ is convex and differentiable, then

$$\kappa(\theta) \ge \kappa(\theta^{(k)}) + \left[\nabla \kappa(\theta^{(k)})\right]' (\theta - \theta^{(k)}),$$

and equality holds when $\theta = \theta^{(k)}$.



• **Quadratic upper bound:** Suppose a convex function $\kappa(\theta)$ is twice differentiable and have bounded curvature, so we can find a positive definite matrix M such that $M - \nabla^2 \kappa(\theta)$ is nonnegative definite. Then we can majorize $\kappa(\theta)$ by a quadratic function with sufficient high curvature and tangent to $\kappa(\theta)$ at $\theta^{(k)}$, i.e.,

$$\kappa(\theta) \le \kappa(\theta^{(k)}) + \left[\nabla \kappa(\theta^{(k)})\right]'(\theta - \theta^{(k)}) + \frac{1}{2}(\theta - \theta^{(k)})'M(\theta - \theta^{(k)})$$

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

$$\bigwedge_{i=1}^{m} \prod_{i=1}^{m} x_i \leq \frac{1}{m} \sum_{i=1}^{m} x_i,$$

and the equality holds iff $x_1 = x_2 = \ldots = x_m$.

• Cauchy-Schwartz Inequality: For *p*-vectors *x* and *y*,

$$x'y \le ||x|| \cdot ||y||,$$

where $||x|| = \sqrt{\sum_{i=1}^{p} x_i^2}$ is the norm of the vector.

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

$$-\log\left\{\mathrm{E}\left[\frac{a(Y)}{b(Y)}\right]\right\} \le \mathrm{E}\left[-\log\frac{a(Y)}{b(Y)}\right].$$

• If Y has the density b(y), then $\mathbf{E}[a(Y)/b(Y)] = 1$, so the left-hand side above vanishes and we obtain

$$E[\log a(Y)] \le E[\log b(Y)],$$

which is sometimes known as the **information inequality** (Kullback-Leibler information).

• It is this inequality that guarantees that a minorizing function is constructed in the E-step of any EM algorithm, making every EM algorithm an MM algorithm. We have the decomposition

$$h^{(k)}(\theta) \equiv \mathbb{E}\{\log f(Y_{\text{obs}}, Y_{\text{mis}}|\theta)|Y_{\text{obs}}, \theta^{(k)}\} = \mathbb{E}\{\log c(Y_{\text{mis}}|Y_{\text{obs}}, \theta)|Y_{\text{obs}}, \theta^{(k)}\} + \log g(Y_{\text{obs}}|\theta)$$

By the information inequality,

$$E\{\log c(Y_{mis}|Y_{obs},\theta)|Y_{obs},\theta^{(k)}\} \le E\{\log c(Y_{mis}|Y_{obs},\theta^{(k)})|Y_{obs},\theta^{(k)}\}$$

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

$$\log g(Y_{\text{obs}}|\theta) \ge h^{(k)}(\theta) - \mathbb{E}\{\log c(Y_{\text{mis}}|Y_{\text{obs}}, \theta^{(k)})|Y_{\text{obs}}, \theta^{(k)}\}$$
 (1)

• **Note:** The second term of (1) does not depend on θ .

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

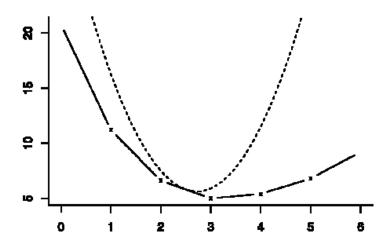
$$f(\theta) = \sum_{i=1}^{n} |y_i - \theta|.$$

• The quadratic function

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

majorizes $|y_i - \theta|$ at the point $\theta^{(k)}$.

- Hence, $g(\theta|\theta^{(k)}) = \sum_{i=1}^{n} h_i(\theta|\theta^{(k)})$ majorizes $f(\theta)$.
- Note: The majorization relation between functions is closed under the formation of sums, nonnegative products, limits, and composition with an increasing function.



• The **minimum** of the sum of the quadratic

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

occurs at

$$\theta^{(k+1)} = \frac{\sum_{i=1}^{n} w_i^{(k)} y_i}{\sum_{i=1}^{n} w_i^{(k)}}$$

for
$$w_i^{(k)} = |y_i - \theta^{(k)}|^{-1}$$
.

• This algorithm works except when a weight $w_i^{(k)} = \infty$. It generalizes to **sample** quantiles, least L1 regression and quantile regression.

• Consider a sports league with n teams. Assign team i the skill level θ_i , where $\theta_1 = 1$ for identifiability reason. 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** $f(\theta) = \ln L(\theta)$ and then rank the teams on the basis of the estimates.

The form of the log-likelihood

$$f(\theta) = \sum_{i \neq j} b_{ij} \left[\ln \theta_i - \ln(\theta_i + \theta_j) \right]$$

suggests that we **linearize** on the term $-\ln(\theta_i + \theta_j)$ to **separate parameters**.

• By the supporting hyperplane property and the convexity of $-\ln(.)$,

$$-\ln y \ge -\ln x - x^{-1}(y - x).$$

• The above inequality produces the **surrogate**

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

• Because the parameters are separated, we can easily find the optimal point

$$\theta_i^{(k+1)} = \frac{\sum_{i \neq j} b_{ij}}{\sum_{i \neq j} (b_{ij} + b_{ji}) / (\theta_i^{(k)} + \theta_j^{(k)})}.$$

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

$$v_j(\theta^{(k)}) - v_j(\theta) \ge \left[\nabla v_j(\theta^{(k)})\right]' \left(\theta^{(k)} - \theta\right). \tag{2}$$

• Again, by the **supporting hyperplane property** and the convexity of $-\ln(x)$, we have $-\ln y + \ln x \ge -x^{-1}(y-x)$ and then

$$v_j(\theta^{(k)}) \left[-\ln v_j(\theta) + \ln v_j(\theta^{(k)}) \right] \ge v_j(\theta^{(k)}) - v_j(\theta). \tag{3}$$

• By (2) and (3),

$$v_j(\theta^{(k)}) \left[-\ln v_j(\theta) + \ln v_j(\theta^{(k)}) \right] + \left[\nabla v_j(\theta^{(k)}) \right]' \left(\theta - \theta^{(k)} \right) \ge 0,$$

and the equality holds when $\theta = \theta^{(k)}$.

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

$$g(\theta|\theta^{(k)}) = f(\theta) + \omega \sum_{i=1}^{q} \left[v_j(\theta^{(k)}) \ln \frac{v_j(\theta^{(k)})}{v_j(\theta)} + \left[\nabla v_j(\theta^{(k)}) \right]' \left(\theta - \theta^{(k)} \right) \right] \ge f(\theta)$$

- Note:
 - Majorization disposes of the inequality constraints.
 - The presence of $\ln v_j(\theta)$ ensures $v_j(\theta) \ge 0$.
- An initial point $\theta^{(0)}$ must be selected with all inequality constraints strictly satisfied. All iterates stay within the interior region but allows strict inequalities to become equalities in 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 $v_j(\theta) \ge 0$, these should be enforced by introducing **Lagrange** multipliers during the minimization of $g(\theta|\theta^{(k)})$.

• We have an $n \times 1$ vector Y of binary responses and an $n \times p$ matrix X of predictors. The logistic regression model assumes that

$$\pi_i(\theta) \equiv \Pr(Y_i = 1) = \frac{\exp(\theta' x_i)}{1 + \exp(\theta' x_i)}.$$

Then the **log likelihood** is

$$l(\theta) \equiv \sum_{i=1}^{n} Y_i \theta' x_i - \sum_{i=1}^{n} \log \left\{ 1 + \exp(\theta' x_i) \right\}.$$

• The **Hessian** can be obtained by direct differentiation:

$$\nabla^2 l(\theta) = -\sum_{i=1}^n \pi_i(\theta) \left[1 - \pi_i(\theta)\right] x_i x_i'. \tag{4}$$

• Since $\pi_i(\theta)$ [1 – $\pi_i(\theta)$] is bounded above by 1/4, we may define the negative definite matrix M = -1/4X'X such that $\nabla^2 l(\theta) - M$ is nonnegative definite. Thus,

$$g(\theta|\theta^{(k)}) = l(\theta^{(k)}) + \left[\nabla l(\theta^{(k)})\right]'(\theta - \theta^{(k)}) + \frac{1}{2}(\theta - \theta^{(k)})'M(\theta - \theta^{(k)})$$

is a quadratic lower bound of $l(\theta)$.

• The MM algorithm proceeds by **maximizing** $g(\theta|\theta^{(k)})$, giving

$$\begin{split} \theta^{(k+1)} &= \theta^{(k)} - M^{-1} \nabla l(\theta^{(k)}) \\ &= \theta^{(k)} + 4(X'X)^{-1} X' \left[Y - \pi(\theta^{(k)}) \right]. \end{split}$$

- Computational advantage of the MM algorithm over Newton-Raphson
 - MM: invert X'X only once.
 - NR: invert the Hessian (??) for every iteration.

Convergence rate

- NR: a quadratic rate $\lim \|\theta^{(k+1)} \hat{\theta}\|/\|\theta^{(k+1)} \hat{\theta}\|^2 = c$ (constant)
- MM: a linear rate $\lim \|\theta^{(k+1)} \hat{\theta}\| / \|\theta^{(k+1)} \hat{\theta}\| = c < 1$

Complexity of each iteration

- NR: require evaluation and inversion of Hessian, $O(p^3)$
- MM: separates parameters, O(p) or $O(p^2)$

Stability of the algorithm

- NR: behave poorly if started too far from an optimum point
- MM: guaranteed to increase/decrease the objective function at every iteration

In conclusion, well-designed MM algorithms tend to require more iterations but simpler iterations than Newton-Raphson; thus MM sometimes enjoy an advantage in computation speed. Numerical stability also enters the balance sheet.

- Quantile regression (Hunter and Lange, 2000)
- Survival analysis (Hunter and Lange, 2002)
- Paired and multiple comparisons (Hunter 2004)
- Variable selection (Hunter and Li, 2002)
- DNA sequence analysis (Sabatti and Lange, 2002)