MM Algorithm

September 7, 2020

Overview of the MM algorithm

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** can be thought as a special case of MM.

Definition of an MM algorithm for Minimization

- 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

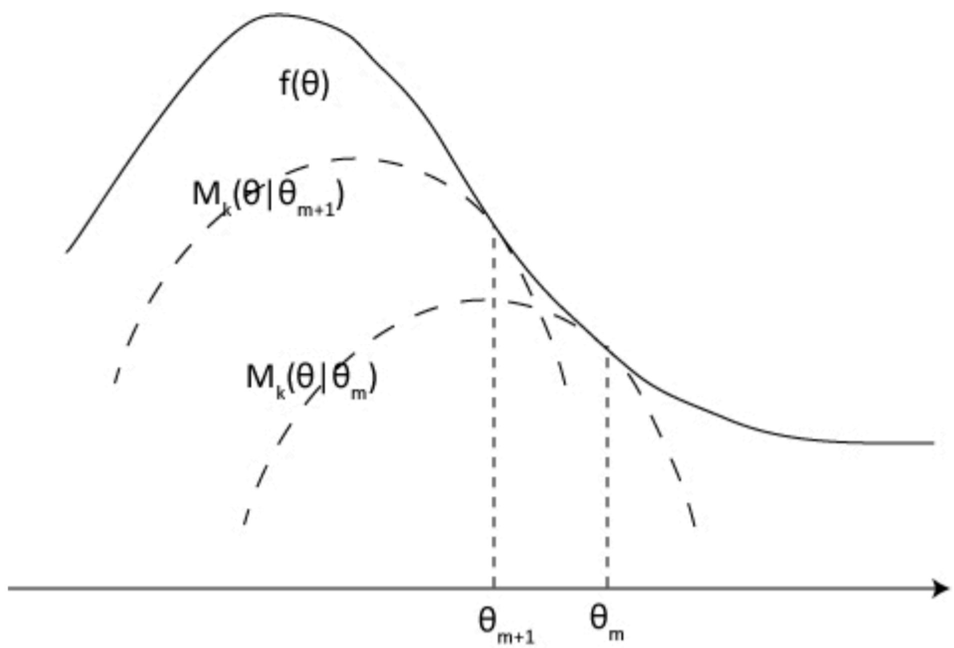
$$f(\theta) \leq g(\theta|\theta^{(k)}) \quad \text{for all} \quad \theta$$
$$f(\theta^{(k)}) = g(\theta^{(k)}|\theta^{(k)})$$

- 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:** $f(\theta^{(k+1)}) \leq g(\theta^{(k+1)}|\theta^{(k)}) \leq g(\theta^{(k)}|\theta^{(k)}) = f(\theta^{(k)})$.

Definition of an MM algorithm for Maxmization

- 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 $\theta = (\theta_1, \ldots, \theta_p)$,

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

where $q_j(.)$ 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 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 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)** 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

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

$$\kappa\left(\lambda\theta_1 + (1-\lambda)\theta_2)\right) \leq \lambda\kappa(\theta_1) + (1-\lambda)\kappa(\theta_2)$$

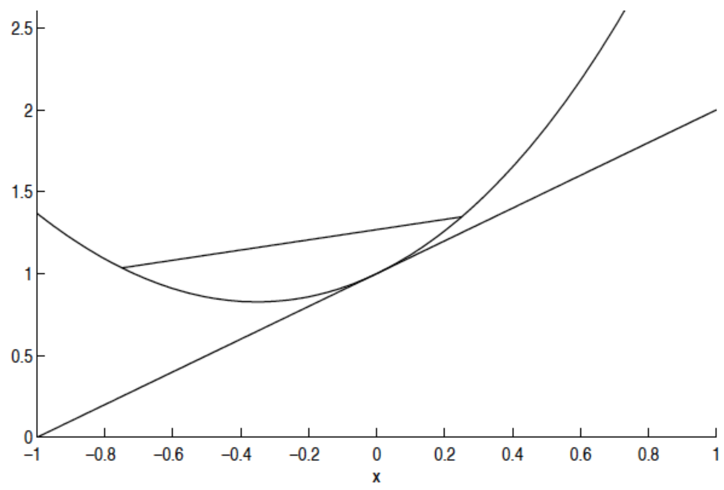
- **Jensen's Inequality:** For a convex function $\kappa(x)$ and any random variable X,

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

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

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

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



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

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

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

Proof by Jensen's inequality:

Because negative logarithm is convex, we have

$$-\log\left(\frac{1}{m}\sum_{i=1}^{m} x_i\right) \leq \frac{1}{m}\sum_{i=1}^{m} -\log x_i = -\sum_{i=1}^{m} \log x_i^{1/m} = -\log\left(\prod_{i=1}^{m} x_i\right)^{1/m}$$

The monotonicity of $-\log$ leads to the result. $\square$

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

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

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

- **Quadratic upper bound:** Suppose a convex function $\kappa(\theta)$ is twice differentiable and have bounded curvature, 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.,

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

Note: flipping the above results, we can find a **quadratic lower bound** for a *concave* function, when M is *negative* definite and $\nabla^2\kappa(\theta) - M$ is nonnegative definite.

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

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

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

$$\mathrm{E}[\log a(Y)] \leq \mathrm{E}[\log b(Y)],$$

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**

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

- By the **information inequality**,

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

Note: here within the expectation operation, $Y_{\rm mis}|Y_{\rm obs}, \theta^{(k)}$ is a random variable, with density function $c(Y_{\rm mis}|Y_{\rm obs}, \theta^{(k)})$.

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

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

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

Example 2: Finding a Sample Median

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

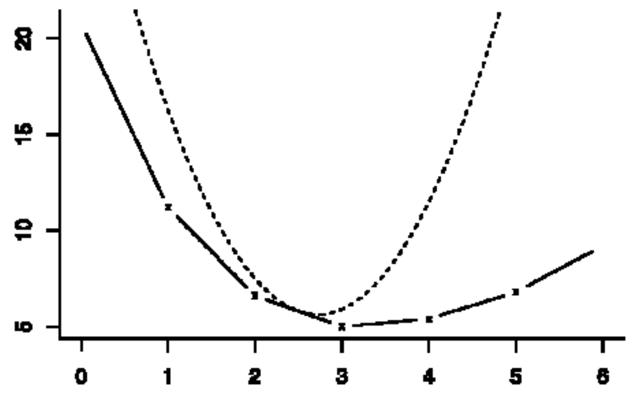
$$f(\theta) = \sum_{i=1}^{n} |y_i - \theta|.$$

- 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 $\theta^{(k)}$ (Arithmetic-Geometric Mean Inequality).

- Hence, $g(\theta|\theta^{(k)}) = \sum_{i=1}^{n} h_i(\theta|\theta^{(k)})$ majorizes $f(\theta)$.



- We have following weighted sum of squares:

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

- The **minimum** of $g(\theta|\theta^{(k)})$ occurs at

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

- 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. 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

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

  We estimate $\boldsymbol{\theta}$ by **maximizing** $f(\boldsymbol{\theta}) = \ln L(\boldsymbol{\theta})$ and then rank the teams on the basis of the estimates.

- The log-likelihood is: $f(\boldsymbol{\theta}) = \sum_{i \neq j} b_{ij} \left[\ln \theta_i - \ln(\theta_i + \theta_j) \right]$.

- We need to **linearize** the term $-\ln(\theta_i + \theta_j)$ to **separate parameters**.

- By the **supporting hyperplane property** ($\kappa(\theta) \geq \kappa(\theta^{(k)}) + \left[\nabla\kappa(\theta^{(k)})\right]' (\theta - \theta^{(k)})$ when κ is convex) and the convexity of $-\ln(.)$, we have

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

- The inequality indicates that

$$-\ln(\theta_i + \theta_j) \geq -\ln(\theta_i^{(k)} + \theta_j^{(k)}) - \frac{\theta_i + \theta_j}{\theta_i^{(k)} + \theta_j^{(k)}} + 1$$

- Thus, the **minorizing** function is:

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

- The parameters are now **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** $v_j(\theta) \geq 0$ 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 $-v_j(\theta)$,

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

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

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

- By (2) and (3),

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

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 $f(\theta)$,

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

- **Note:**
  - **Majorization gets rid of the inequality constraints.**
  - The presence of $\ln v_j(\theta)$ ensures $v_j(\theta) \geq 0$.

- 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 $v_j(\theta) \geq 0$, 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:

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

- Remember the definition of **quadratic lower bound**:

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

  where $\kappa(\theta)$ is concave and twice differentiable, and M is a negative definite matrix.

- 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 $l(\theta)$ (note: $l(\theta)$ is concave).

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

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

- Computational advantage of the MM algorithm over Newton-Raphson
  - **MM**: invert $X'X$ **only once**.
  - **NR**: invert the Hessian (4) **for every iteration**.

Comparing MM & Newton Raphson

- **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 and numerical stability.

- 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)