EC708 Discussion 8
Numerical Optimization

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[1]Parts of the materials are from Train (2009), Kochenderfer and Wheeler (2019), and teaching slides of Shuowen Chen and Jean-Jacques Forneron.

Outline

Optimization Problem: MLE

Consider maximizing the (average) log-likelihood function

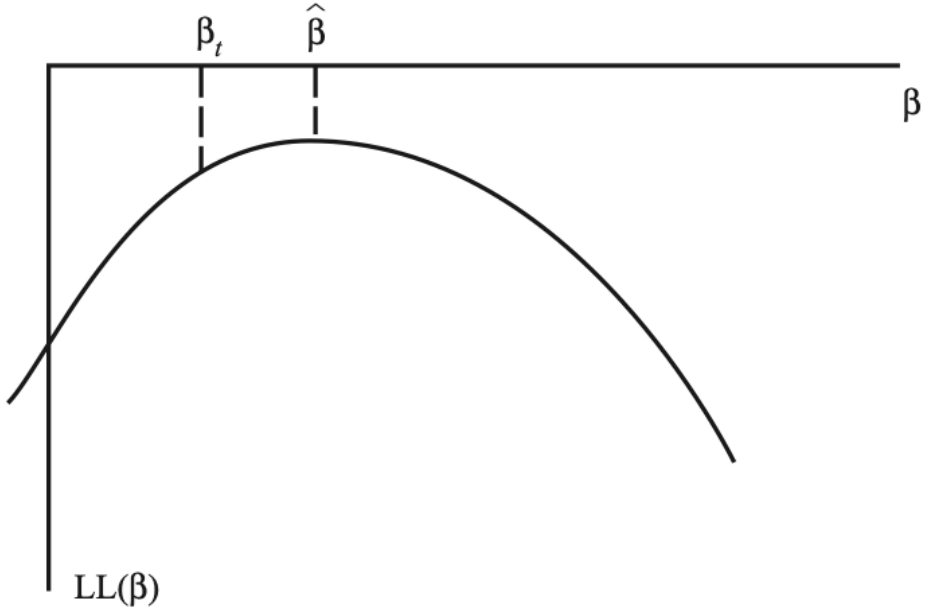
$$LL(\beta) = \frac{1}{N} \sum_{n=1}^{N} \ln P_n(\beta),$$

- $P_n(\beta)$: probability of the observed outcome for decision maker n
- N: sample size
- β: $K \times 1$ vector of parameters.

Goal: find $\hat{\beta} = \arg\max_{\beta} LL(\beta)$.

- To utilize minimization packages in practice, we usually work with $-LL(\beta)$.

Graphical Illustration of MLE



Finding $\hat{\beta}$ is a hill-climbing process:

1. Specify a starting value β_0. Decide in which direction and how far to climb.
2. Each step t moves to a new value β_{t+1} at which $LL(\beta)$ is higher than at the current value β_t.
3. Keep climbing until no further increase can be found.

Gradient and Hessian

Gradient in step t:

$$g_t = \left(\frac{\partial LL(\beta)}{\partial \beta} \right)_{\beta_t}.$$

Hessian in step t:

$$H_t = \left(\frac{\partial g_t}{\partial \beta'} \right)_{\beta_t} = \left(\frac{\partial^2 LL(\beta)}{\partial \beta \partial \beta'} \right)_{\beta_t}.$$

The gradient tells use in what direction to climb, and the Hessian can help us to know how far to climb.

Numerical Evaluation of Derivatives

Recall the definition of first-order partial derivative of function f at β:

$$\frac{\partial f(\beta)}{\partial \beta_j} = \lim_{h \to 0} \frac{f(\beta_1, \ldots, \beta_j + h, \ldots, \beta_K) - f(\beta_1, \ldots, \beta_j, \ldots, \beta_K)}{h}.$$

Numerically, we can approximate it by calculating

$$f_j(\beta) = \frac{f(\beta + hd_j) - f(\beta)}{h}, \quad j = 1, \ldots, K$$

where $d_j = (0, \ldots, 0, 1, 0, \ldots, 0)$ is the unit vector with 1 in position j and h is the step size. In practice, a more accurate approximation is

$$f_j(\beta) = \frac{f(\beta + hd_j) - f(\beta - hd_j)}{2h}.$$

Newton-Raphson Method: Algorithm

Take a second-order Taylor's approximation of $LL(\beta_{t+1})$ around $LL(\beta_t)$:

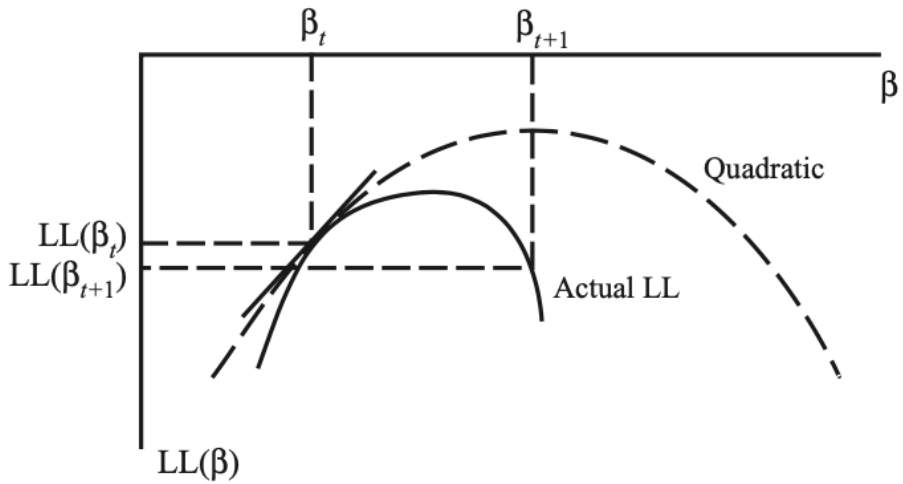
$$LL(\beta_{t+1}) = LL(\beta_t) + (\beta_{t+1} - \beta_t)' g_t + \frac{1}{2}(\beta_{t+1} - \beta_t)' H_t (\beta_{t+1} - \beta_t).$$

Find β_{t+1} that maximizes this approximation:

$$g_t + H_t(\beta_{t+1} - \beta_t) = 0 \;\Rightarrow\; \beta_{t+1} = \beta_t - \underbrace{H_t^{-1}}_{\text{step size}} \cdot \underbrace{g_t}_{\text{direction}}.$$

- Iterate until convergence, which can be defined in many ways:
  - $LL(\beta_{t+1})$ close to $LL(\beta_t)$
  - β_{t+1} close to β_t
  - g_{t+1} close to g_t
- If $LL(\beta)$ were exactly quadratic, then Newton-Raphson reaches the maximum in one step from any starting value.

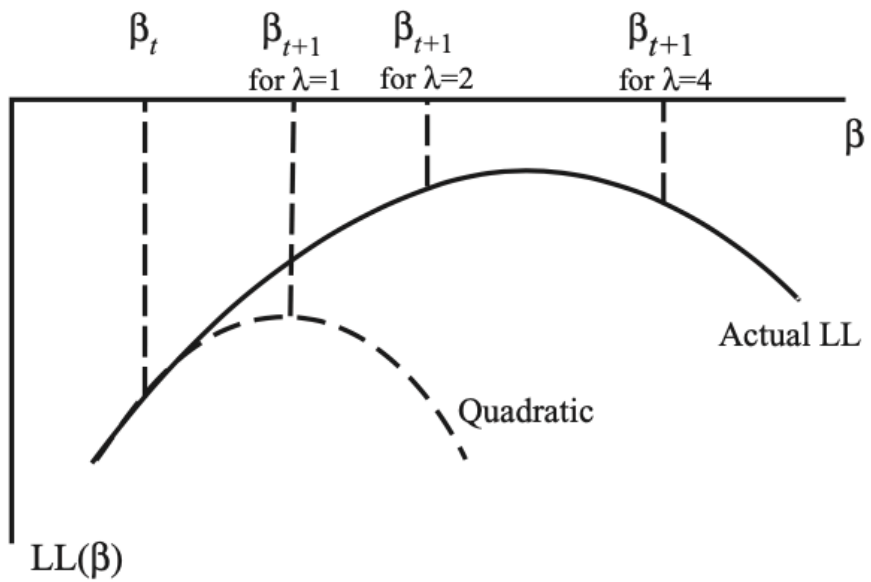
Newton-Raphson Method: Step Size



- It is possible for Newton-Raphson to step past the maximum and move to a lower $LL(\beta)$.
- To ensure each step provides an increase in $LL(\beta)$, we introduce a scalar step size λ_t:

$$\beta_{t+1} = \beta_t - \lambda_t H_t^{-1} g_t.$$

Newton-Raphson Method: Step Size



Perform step-size adjustment in each step. Start with $\lambda_t = 1$.

- If $LL(\beta_{t+1}) < LL(\beta_t)$, then set $\lambda_t = \frac{1}{2}$ and try again. Continue halving λ_t until a λ_t is found for which $LL(\beta_{t+1}) > LL(\beta_t)$.
  - A tiny λ_t is a signal that a different iteration procedure is needed.
- If $LL(\beta_{t+1}) > LL(\beta_t)$, then try $\lambda_t = 2$. Double λ_t as long as doing so further raises $LL(\beta_{t+1})$.
  - Raising λ_t reduces # of iterations needed to reach the maximum.

Newton-Raphson Method: Drawbacks

- Calculations of the Hessian is usually computation-intensive.
  - $\frac{K(K+1)}{2}$ functions to evaluate in each step
  - Numerically calculated Hessian might be ill-behaved (singular).
- Does not guarantee an increase in each step if the log-likelihood function is not globally concave.
  - Hessian may not be negative definite.
  - Remedy: regularization. Instead of using H_t^{-1} directly, use

$$(H_t + \mu_t I_K)^{-1}$$

where $\mu_t < 0$ guarantees negative definiteness.

Gauss-Newton Method

Consider the following general nonlinear model:

$$y_n = f(x_n; \beta) + u_n, \quad n = 1, \ldots, N$$

- $u_n \sim$ i.i.d.$N(0, \sigma^2)$. Assume σ^2 is known here.
- x_n: $M \times 1$ exogenous regressors.
- β: $K \times 1$ vector of parameters.
- $f(\cdot)$: some function satisfying some regularity conditions.

Gauss-Newton Method

Due to the normality assumption, we have the log-likelihood function

$$LL(\beta) = -\frac{N}{2}\ln 2\pi - \frac{N}{2}\ln\sigma^2 - \frac{1}{2\sigma^2}S(\beta)$$

where $S(\beta) = \sum_{n=1}^{N}[y_n - f(x_n;\beta)]^2 = \sum_{n=1}^{N} u_n^2$. It suffices to work with $S(\beta)$. Its first and second derivatives w.r.t. β are

$$g(\beta) = 2\sum_{n=1}^{N}\frac{\partial u_n}{\partial \beta}u_n, \quad H(\beta) = 2\sum_{n=1}^{N}\left[\frac{\partial u_n}{\partial \beta}\frac{\partial u_n}{\partial \beta'} + \frac{\partial^2 u_n}{\partial \beta \partial \beta'}u_n\right].$$

In $H(\beta)$, the blue term is usually small relative to the red term, so we **neglect** it and use the following:

$$\beta_{t+1} = \beta_t - \left[\sum_{n=1}^{N}\frac{\partial u_n}{\partial \beta}\frac{\partial u_n}{\partial \beta'}\right]^{-1}\Bigg|_{\beta=\beta_t}\sum_{n=1}^{N}\frac{\partial u_n}{\partial \beta}u_n\Bigg|_{\beta=\beta_t}.$$

Gauss-Newton Method

Remarks:

- This method doesn't compute Hessian.
- Has an OLS interpretation. Let $z_n = -\partial u_n / \partial \beta$, then

$$\beta_{t+1} = \beta_t - \left(\sum_{n=1}^{N} z_n z_n' \right)^{-1} \Bigg|_{\beta=\beta_t} \sum_{n=1}^{N} z_n u_n \Bigg|_{\beta=\beta_t}.$$

- Similar regularization can be incorporated as in Newton-Raphson: Marquart quadratic hill climbing

$$\beta_{t+1} = \beta_t - \left(\sum_{n=1}^{N} z_n z_n' + \mu_t I_K \right)^{-1} \Bigg|_{\beta=\beta_t} \sum_{n=1}^{N} z_n u_n \Bigg|_{\beta=\beta_t}.$$

Quasi-Newton Methods

- Newton-Raphson method does not utilize the fact that the objective function is the sum of log likelihoods.
- Quasi-Newton methods do so by using the approximate Hessian instead of the actual one.

Quasi-Newton Methods: BHHH

Berndt, Hall, Hall, and Hausman (1974) propose to use scores to approximate Hessian.

- Score of observation n:

$$s_n(\beta_t) = \frac{\partial \ln P_n(\beta)}{\partial \beta}\Big|_{\beta=\beta_t}.$$

- Gradient is the average score:

$$g_t = \frac{1}{N}\sum_{n=1}^{N} s_n(\beta_t).$$

Quasi-Newton Methods: BHHH

- Outer product of observation n's score is the $K \times K$ matrix

$$s_n(\beta_t)s_n(\beta_t)' = \begin{pmatrix} s_n^1 s_n^1 & s_n^1 s_n^2 & \cdots & s_n^1 s_n^K \\ s_n^2 s_n^1 & s_n^2 s_n^2 & \cdots & s_n^2 s_n^K \\ \vdots & \vdots & & \vdots \\ s_n^K s_n^1 & s_n^K s_n^2 & \cdots & s_n^K s_n^K \end{pmatrix}$$

  where s_n^j is the j-th element of $s_n(\beta_t)$.

- Average outer product of scores:

$$B_t = \frac{1}{N} \sum_{n=1}^{N} s_n(\beta_t)s_n(\beta_t)'.$$

BHHH procedure:

$$\beta_{t+1} = \beta_t + \lambda_t B_t^{-1} g_t.$$

Quasi-Newton Methods: BHHH

Why does BHHH work?

- At maximum, B_t is the sample variance of scores and thus provides a measure of the log-likelihood functions' curvature, similar to H_t.
- These ideas are formalized in the information matrix equality.
- B_t is far faster to calculate than H_t and necessarily positive definite.

Drawbacks: BHHH can give small steps when far from the maximum

- either because B_t is not a good approximation to $-H_t$,
- or because $LL(\beta)$ is highly nonquadratic since BHHH is an approximation to NR.

Quasi-Newton Methods: BFGS and DFP

- BHHH uses only information at β_t to determine each step.
- In contrast, BFGS and DFP use information at several points to obtain a sense of the curvature of the log-likelihood function.
- BFGS is the algorithm behind Matlab's fminunc.

BFGS and DFP updates have the form

$$\beta_{t+1} = \beta_t + \lambda_t Q_t g_t.$$

Quasi-Newton Methods: BFGS and DFP

DFP sets Q_0 to identity matrix and updates Q_{t+1} from Q_t using

$$Q_{t+1} = Q_t + \frac{Q_t \gamma_t \gamma_t' Q_t}{\gamma_t' Q_t \gamma_t} + \frac{\delta_t \delta_t'}{\delta_t' \gamma_t}$$

where $\delta_t = \beta_{t+1} - \beta_t$ and $\gamma_t = g_{t+1} - g_t$. BFGS further subtracts $v_t d_t d_t'$ from the DFP update, where

$$v_t = \gamma_t' Q_t \gamma_t, \quad d_t = \frac{\delta_t}{\delta_t' \gamma_t} - \frac{Q_t \gamma_t}{\gamma_t' Q_t \gamma_t}.$$

There is some evidence that BFGS is more efficient than DFP.

Steepest Ascent

The greatest possible increase in $LL(\beta)$ for the (small enough) distance between β_t and β_{t+1} is provided by

$$\beta_{t+1} = \beta_t + \lambda_t g_t.$$

Motivated by the Lagrangian:

$$L = \underbrace{LL(\beta_t) + (\beta_{t+1} - \beta_t) g_t}_{\text{1st-order Taylor expansion of } LL(\beta_{t+1})} - \frac{1}{2\lambda_t} \underbrace{[(\beta_{t+1} - \beta_t)'(\beta_{t+1} - \beta_t) - k]}_{\text{distance from } \beta_t \text{ to } \beta_{t+1} \text{ being } \sqrt{k}}$$

Can pick λ_t that maximizes $LL(\beta_t + \lambda_t g_t)$ (line search).

- "Steepest ascent" is only attained in a neighborhood of β_t. Usually converges more slowly than BHHH.
- For minimization problems, this is called the gradient descent.

Stochastic Gradient Descent

- Historically gradient descent is not popular in nonlinear or nonconvex optimization problems because it gets stuck at local minima.
- For deep learning, local minima are close to global minima in terms of prediction, so not problematic.
- Computing the gradient can be very demanding. One way to be more efficient is the stochastic gradient descent (SGD).
- Instead of evaluating the gradient of full sample, we subsample $m \ll N$ observations with replacement and compute

$$\beta_{t+1} = \beta_t - \lambda_t g_t^\star.$$

  where $g_t^\star$ denotes the gradient of the subsample evaluated at β_t.
- Practitioners prefer m small ($m = 1$): cheaper to compute and avoids overfitting (Goodfellow, Bengio, and Courville, 2016).

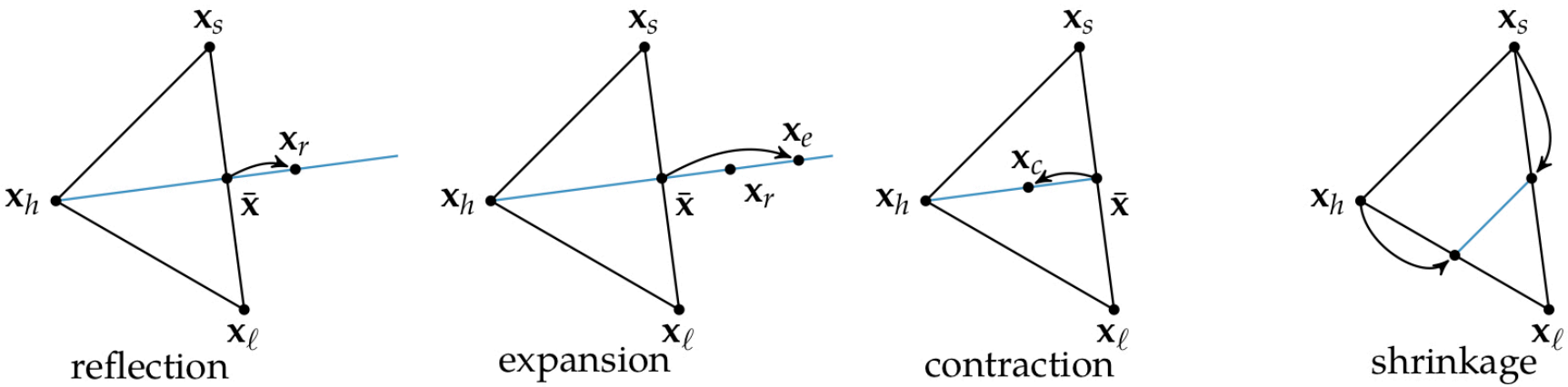
Comparison Methods

- Gradient-based methods are susceptible to converge at a local maximum. Can use a variety of starting values to investigate the issue.
- An alternative is comparison-based methods: compute objective function at several points and pick the one yielding the optimum value.
- Comparison methods better behave with non-smooth objective functions. Stochastic comparison methods are more likely to find global optimum (in theory).

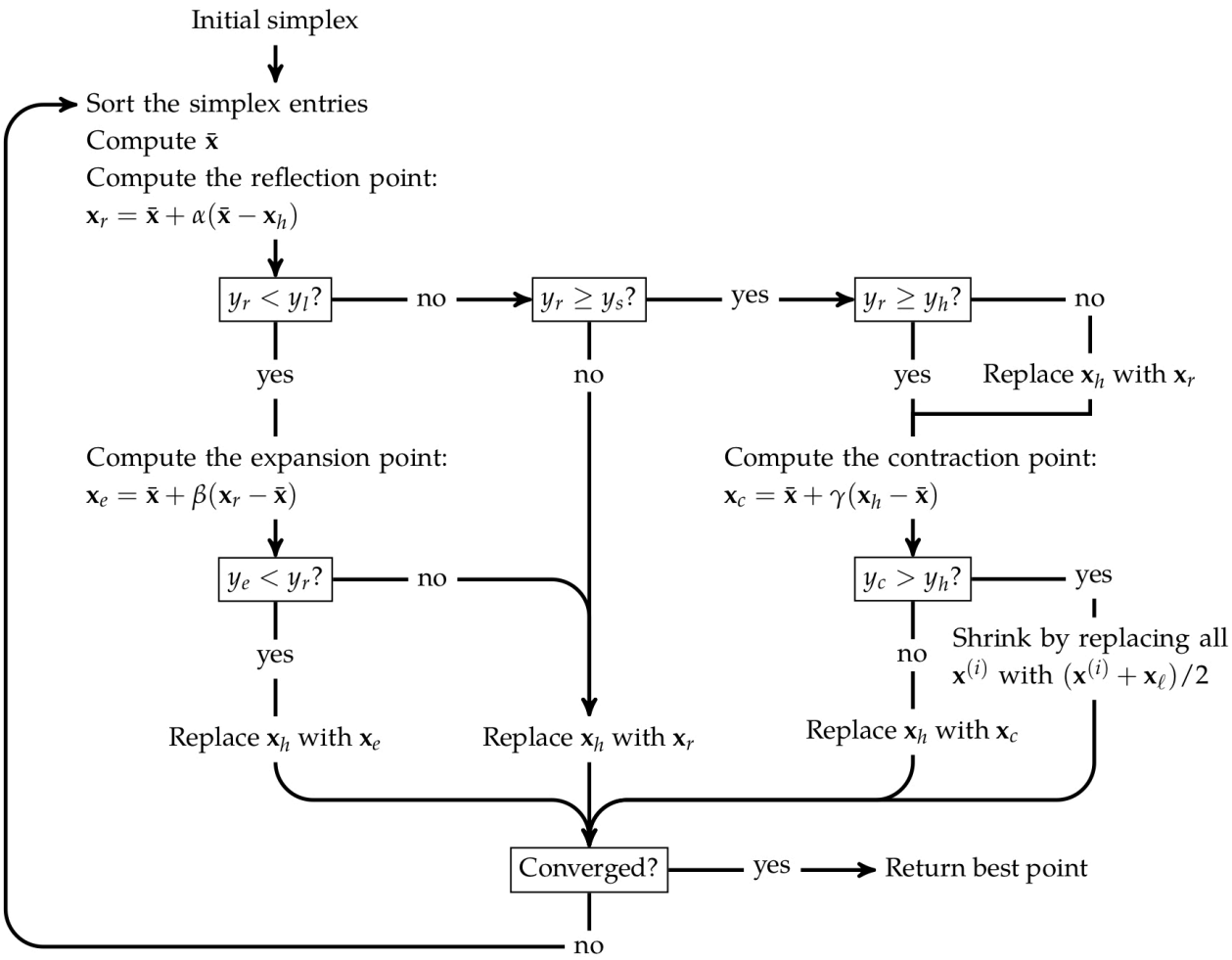
Nelder-Mead Algorithm

This is fminsearch in Matlab. Consider minimizing a generic criterion function $f(x)$ with $x \in \mathbb{R}^K$.

1. Choose initial simplex $\{x_1, x_2, \ldots, x_{n+1}\}$. Think of it as an n-dimensional version of a triangle.
2. Sort simplex vertices in descending order: $f(x_h) > f(x_s) > \cdots > f(x_l)$ (h: highest; s: second highest; l: lowest).



Nelder-Mead Algorithm



Intuition: Nelder-Mead starts with a simplex and modifies it at each iteration using one of the simplex operations.

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