Math Camp

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Multivariate Optimization

Optimizing multivariate functions

- Parameters $\boldsymbol{\beta} = (\beta_1, \beta_2, \dots, \beta_n)$ such that $f(\boldsymbol{\beta}|\boldsymbol{X}, \boldsymbol{Y})$ is maximized
- Policy $\mathbf{x} \in \Re^n$ that maximizes $U(\mathbf{x})$
- Weights $\pi = (\pi_1, \pi_2, \dots, \pi_K)$ such that a weighted average of forecasts $\mathbf{f} = (f_1, f_2, \dots, f_k)$ have minimum loss

$$\min_{\pi} = -(\sum_{j=1}^{K} \pi_j f_j - y)^2$$

Today we'll describe analytic and computational approaches to optimization

- Analytic recipe for optimization
- Computational optimization
 - Multivariate Newton-Raphson
 - BFGS
 - Approximate Optimization: k-means



Multivariate Optimization

Definition

Let $\mathbf{x} \in \mathbb{R}^n$ and let $\delta > 0$. Define a neighborhood of \mathbf{x} , $B(\mathbf{x}, \delta)$, as the set of points such that,

$$B(\mathbf{x}, \delta) = \{\mathbf{y} \in \Re^n : ||\mathbf{x} - \mathbf{y}|| < \delta\}$$

Definition

Suppose $f: X \to \Re$ with $X \subset \Re^n$. A vector $\mathbf{x}^* \in X$ is a global maximum if , for all other $\mathbf{x} \in X$

$$f(\mathbf{x}^*) > f(\mathbf{x})$$

A vector \mathbf{x}^{local} is a local maximum if there is a neighborhood around \mathbf{x}^{local} , $Q \subset X$ such that, for all $x \in Q$,

$$f(\mathbf{x}^{local}) > f(\mathbf{x})$$



Multivariate Optimization

Definition

A set $X \subset \mathbb{R}^n$ is compact if it is closed and bounded

Theorem

Multivariate Extreme Value Theorem Suppose $f: X \to \Re$ be continuous and $X \subset \Re^n$ and X compact. Then f takes on its maximum and minimum values on X.

We're going to come up with the multivariate equivalent of the first order and second order conditions now

Gradient

Definition

Suppose $f: X \to \mathbb{R}^n$ with $X \subset \mathbb{R}^1$ is a differentiable function. Define the gradient vector of f at \mathbf{x}_0 , $\nabla f(\mathbf{x}_0)$ as,

$$\nabla f(\mathbf{x}_0) = \left(\frac{\partial f(\mathbf{x}_0)}{\partial x_1}, \frac{\partial f(\mathbf{x}_0)}{\partial x_2}, \frac{\partial f(\mathbf{x}_0)}{\partial x_3}, \dots, \frac{\partial f(\mathbf{x}_0)}{\partial x_n}\right)$$

Gradient First Order Condition

Theorem

Suppose $f: X \to \Re^1$, $X \subset \Re^n$. Suppose $\mathbf{a} \in X$ is a local extremum. Then,

$$\nabla f(\mathbf{a}) = \mathbf{0}$$
$$= (0, 0, \dots, 0)$$

- Proof (intuition): same as one dimensional case (left-hand, right hand), just do it dimension by dimension
- Critical Values:
 - 1) Maximum
 - 2) Minimum
 - 3) Saddle point
- Second Derivative Test!

Second Order Conditions: Hessian

Definition

Suppose $f: X \to \Re^1$, $X \subset \Re^n$, with f a twice differentiable function. We will define the Hessian matrix as the matrix of second derivatives at $\mathbf{x}^* \in X$,

$$\boldsymbol{H}(f)(\boldsymbol{x}^*) = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1 \partial x_1}(\boldsymbol{x}^*) & \frac{\partial^2 f}{\partial x_1 \partial x_2}(\boldsymbol{x}^*) & \dots & \frac{\partial^2 f}{\partial x_1 \partial x_n}(\boldsymbol{x}^*) \\ \frac{\partial^2 f}{\partial x_2 \partial x_1}(\boldsymbol{x}^*) & \frac{\partial^2 f}{\partial x_2 \partial x_2}(\boldsymbol{x}^*) & \dots & \frac{\partial^2 f}{\partial x_2 \partial x_n}(\boldsymbol{x}^*) \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1}(\boldsymbol{x}^*) & \frac{\partial^2 f}{\partial x_n \partial x_2}(\boldsymbol{x}^*) & \dots & \frac{\partial^2 f}{\partial x_n \partial x_n}(\boldsymbol{x}^*) \end{pmatrix}$$

General test → Two Dimensional Test → Example

Hessians

Definition

Consider $n \times n$ matrix **A**. If, for all $\mathbf{x} \in \mathbb{R}^n$ where $\mathbf{x} \neq 0$:

x'Ax > 0 A is positive definite x'Ax < 0 A is negative definite

If $\mathbf{x}' \mathbf{A} \mathbf{x} > 0$ for some \mathbf{x} and $\mathbf{x}' \mathbf{A} \mathbf{x} < 0$ for other \mathbf{x} , then we say \mathbf{A} is indefinite

Approximating functions and second order conditions

Theorem

Taylor's Theorem Suppose $f: \Re \to \Re$, f(x) is infinitely differentiable function. Then, the taylor expansion of f(x) around a is given by

$$f(x) = f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f'''(a)}{3!}(x-a)^3 + \dots$$

$$f(x) = \sum_{n=0}^{\infty} \frac{f^n(a)}{n!}(x-a)^n$$

Example Function

Suppose a = 0 and $f(x) = e^x$. Then,

$$f'(x) = e^{x}$$

$$f''(x) = e^{x}$$

$$\vdots \vdots \vdots$$

$$f^{n}(x) = e^{x}$$

This implies

$$e^{x} = 1 + x + \frac{x^{2}}{2!} + \frac{x^{3}}{3!} + \dots + \frac{x^{n}}{n!} + \dots$$

Multivariate Taylor's Theorem

Theorem

Suppose $f: \Re^n \to \Re$ is a three-times continously differentiable function, then around $\mathbf{a} \in \Re^n$,

$$f(x) = f(a) + \nabla f(a)(x - a) + \frac{1}{2}(x - a)' H(f)(a)(x - a) + R(a, x)$$

where
$$\frac{R(\pmb{x},\pmb{a})}{||\pmb{x}-\pmb{a}||^2} \to 0$$
 as $\pmb{x} \to \pmb{a}$

Intuition for Quadratic Form

Suppose x^* is some critical value,

$$f(x) = f(x^*) + \nabla f(x^*)(x - x^*) + (x - \frac{1}{2}x^*)H(f)(x^*)(x - x^*) + R(x^*, x^*)$$

$$f(x) - f(x^*) = 0(x - x^*) + (x - \frac{1}{2}x^*)H(f)(x^*)(x - x^*) + R(x^*, x)$$

For \mathbf{x} near \mathbf{x}^* , $R(\mathbf{x}^*, \mathbf{x}) \approx 0$

 $m{H}(f)(m{x}^*)$ positive definite $o f(m{x}) > f(m{x}^*) o ext{local minimum}$ $m{H}(f)(m{x}^*)$ negative definite $o f(m{x}) < f(m{x}^*) o ext{local maximum}$

Theorem

Second Derivative Test

- If H(f)(a) is positive definite then a is a local minimum
- If H(f)(a) is negative definite then a is a local maximum
- If H(f)(a) is indefinite then a is a saddle point

Second Derivative Test

Many ways to assess definiteness → use determinant

Theorem

Two Dimensional, Second Derivative Test. Suppose $f: X \to \Re$ with $X \subset \Re^2$ and f twice differentiable. Write the Hessian of f at a critical value \mathbf{a} ,

$$\mathbf{H}(f)(\mathbf{a}) = \begin{pmatrix} A & B \\ B & C \end{pmatrix}$$

Then, we can conduct the second derivative test as:

- $AC B^2 > 0$ and $A > 0 \rightsquigarrow$ positive definite \rightsquigarrow **a** is a local minimum
- $AC B^2 > 0$ and $A < 0 \rightsquigarrow$ negative definite \rightsquigarrow **a** is a local maximum
- $AC B^2 < 0 \rightsquigarrow indefinite \rightsquigarrow saddle point$
- $AC B^2 = 0$ inconclusive

Multivariate Recipe

- 1) Calculate gradient
- 2) Set equal to zero, solve system of equations
- 3) Calculate Hessian
- 4) Assess Hessian at critical values
- 5) Boundary values? (if relevant)

Example 1: A Simple Optimization Problem

Suppose $f: \Re^2 \to \Re$ with

$$f(x_1, x_2) = 3(x_1 + 2)^2 + 4(x_2 + 4)^2$$

Calculate gradient

$$\nabla f(\mathbf{x}) = (6x_1 + 12, 8x_2 + 32)$$

 $\mathbf{0} = (6x_1^* + 12, 8x_2^* + 32)$

We now solve the system of equations to yield $x_1^st=-2$ and $x_2^st=-4$

Example 1: A Simple Optimization Problem

$$\mathbf{H}(f)(\mathbf{x}^*) = \begin{pmatrix} 6 & 0 \\ 0 & 8 \end{pmatrix}$$

 $det(\mathbf{H}(f)(\mathbf{x}^*)) = 48$ and 6 > 0 so $\mathbf{H}(f)(\mathbf{x}^*)$ is positive definite. local minimum

Example 2: Two Dimensional Ideal Points

Suppose legislators are considering legislation $\mathbf{x} \in \mathbb{R}^2$. And suppose legislator i has utility function $U_i : \mathbb{R}^2 \to \mathbb{R}$,

$$U(\mathbf{x})_i = -(x_1 - \mu_1)^2 - (x_2 - \mu_2)^2$$

What is legislator i's optimal policy?

$$\nabla f(\mathbf{x}) = (-2(x_1 - \mu_1), -2(x_2 - \mu_2))$$

 $\nabla f(\mathbf{x}) = \mathbf{0}$

$$-2(x_1^* - \mu_1) = 0$$

$$-2(x_2^* - \mu_2) = 0$$

Solving yields $x_1^* = \mu_1$ and $x_2^* = \mu_2$.

Example 2: Two Dimensional Ideal Points

$$U(\mathbf{x})_i = -(x_1 - \mu_1)^2 - (x_2 - \mu_2)^2$$

Call $\mu = (\mu_1, \mu_2)$

The Hessian at the critical value is

$$\mathbf{H}(f)(\boldsymbol{\mu}) = \begin{pmatrix} \frac{\partial^2 U_i}{\partial x_1 \partial x_1}(\boldsymbol{\mu}) & \frac{\partial^2 U_i}{\partial x_1 \partial x_2}(\boldsymbol{\mu}) \\ \frac{\partial^2 U_i}{\partial x_2 \partial x_1}(\boldsymbol{\mu}) & \frac{\partial^2 U_i}{\partial x_2 \partial x_2}(\boldsymbol{\mu}) \end{pmatrix} \\
= \begin{pmatrix} -2 & 0 \\ 0 & -2 \end{pmatrix}$$

So, -2*-2-0=4>0 and $-2<0 \rightsquigarrow$ negative definite, maximum $\mu=(\mu_1,\mu_2)$ are legislator i's two dimensional ideal point.

Suppose that we draw an independent and identically distributed random sample of n observations from a normal distribution,

$$Y_i \sim \text{Normal}(\mu, \sigma^2)$$

 $\mathbf{Y} = (Y_1, Y_2, ..., Y_n)$

Our task:

- Obtain likelihood (summary estimator)
- Derive maximum likelihood estimators for μ and σ^2
- Characterize sampling distribution

$$L(\mu, \sigma^2 | \mathbf{Y}) \propto \prod_{i=1}^n f(Y_i | \mu, \sigma^2)$$

$$\propto \prod_{i=1}^N \frac{\exp[-\frac{(Y_i - \mu)^2}{2\sigma^2}]}{\sqrt{2\pi\sigma^2}}$$

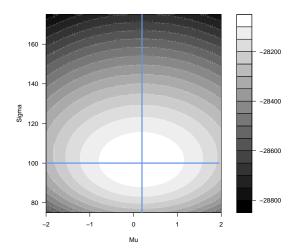
$$\propto \frac{\exp[-\sum_{i=1}^n \frac{(Y_i - \mu)^2}{2\sigma^2}]}{(2\pi)^{n/2} \sigma^{2n/2}}$$

Taking the logarithm, we have

$$I(\mu, \sigma^{2} | \mathbf{Y}) = -\sum_{i=1}^{n} \frac{(Y_{i} - \mu)^{2}}{2\sigma^{2}} - \frac{n}{2}log(2\pi) - \frac{n}{2}log(\sigma^{2}) + c$$

$$= -\sum_{i=1}^{n} \frac{(Y_{i} - \mu)^{2}}{2\sigma^{2}} - \frac{n}{2}log(\sigma^{2}) + c'$$

Example 3: Log-Likelihood Plot



Let's find $\widehat{\mu}$ and $\widehat{\sigma}^2$ that maximizes log-likelihood.

$$I(\mu, \sigma^{2} | \mathbf{Y}) = -\sum_{i=1}^{n} \frac{(Y_{i} - \mu)^{2}}{2\sigma^{2}} - \frac{n}{2} \log(\sigma^{2}) + c'$$

$$\frac{\partial I(\mu, \sigma^{2}) | \mathbf{Y})}{\partial \mu} = \sum_{i=1}^{n} \frac{2(Y_{i} - \mu)}{2\sigma^{2}}$$

$$\frac{\partial I(\mu, \sigma^{2}) | \mathbf{Y})}{\partial \sigma^{2}} = -\frac{n}{2\sigma^{2}} + \frac{1}{2\sigma^{4}} \sum_{i=1}^{n} (Y_{i} - \mu)^{2}$$

$$0 = -\sum_{i=1}^{n} \frac{2(Y_{i} - \widehat{\mu})}{2\widehat{\sigma}^{2}}$$
$$0 = -\frac{n}{2\widehat{\sigma}^{2}} + \frac{1}{2\widehat{\sigma}^{4}} \sum_{i=1}^{n} (Y_{i} - \mu^{*})^{2}$$

Solving for $\widehat{\mu}$ and $\widehat{\sigma}^2$ yields,

$$\widehat{\mu} = \frac{\sum_{i=1}^{n} Y_i}{n}$$

$$\widehat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^{n} (Y_i - \overline{Y})^2$$

$$\mathbf{H}(f)(\widehat{\mu},\widehat{\sigma}^2) = \begin{pmatrix} \frac{\partial^2 l(\mu,\sigma^2|\mathbf{Y})}{\partial \mu^2} & \frac{\partial^2 l(\mu,\sigma^2|\mathbf{Y})}{\partial \sigma^2 \partial \mu} \\ \frac{\partial^2 l(\mu,\sigma^2|\mathbf{Y})}{\partial \sigma^2 \partial \mu} & \frac{\partial^2 l(\mu,\sigma^2|\mathbf{Y})}{\partial^2 \sigma^2} \end{pmatrix}$$

Taking derivatives and evaluating at MLE's yields,

$$\mathbf{H}(f)(\widehat{\mu},\widehat{\sigma}^2) = \begin{pmatrix} \frac{-n}{\widehat{\sigma}^2} & 0\\ 0 & \frac{-n}{(\widehat{\sigma}^2)^2} \end{pmatrix}$$

 $\det(\mathbf{H}(f)(\widehat{\mu},\widehat{\sigma}^2)) = n^2/\widehat{\sigma}^5$ and $-n/\widehat{\sigma}^2 < 0 \leadsto \text{maximum}$

Computational Optimization

Analytic solutions: often hard.

Computational solutions: simplify. Trade offs

- Newton-Raphson: expensive

BFGS: less expensive

- EM-like optimization: solve intractable problems, parallelizable

Multivariate Newton Raphson

Suppose $f: \Re^n \to \Re$. Suppose we have guess \mathbf{x}_t . Then our update is:

$$\mathbf{x}_{t+1} = \mathbf{x}_t - \mathbf{H}(f)(\mathbf{x}_t)^{-1} \nabla f(\mathbf{x}_t)$$

Derivation (intuition): Approximate function with tangent plane. Find value of x_{t+1} that makes the plane equal to zero. Update again. R. Code

Multivariate Newton Raphson

- Expensive to calculate (requires inverting Hessian)
- Very sensitive to starting points
- Ideally: method that exploits Newton-like structure, but is cheaper and more robust

BFGS: Quasi-Newton method

R code

Optimization that is Both Discrete and Continuous

K-means: most commonly used clustering algorithm.

Story: Data are grouped in K clusters and each cluster has a center or mean.

- ightarrow Two types of parameters to estimate
 - 1) For each cluster j, $(j=1,\ldots,K)$

 r_{ij} =Indicator, Document i assigned to cluster j

$$\mathbf{r}_{j} = (\mathbf{r}_{1j}, \mathbf{r}_{2j}, \dots, \mathbf{r}_{Nj})$$

 $\mathbf{r} = (\mathbf{r}_{1}^{'}, \mathbf{r}_{2}^{'}, \dots, \mathbf{r}_{K}^{'}) (N \times K \text{ matrix})$

2) For each cluster j

 μ_i a cluster center for cluster j.

$$\boldsymbol{\mu}_j = (\mu_{1j}, \mu_{2j}, \dots, \mu_{Mj})$$

Notation. Representation of document *i*:

$$\mathbf{y}_i = (y_{i1}, y_{i2}, \dots, y_{iM})$$

Specifying the Method

- 1) Assume Euclidean distance between objects.
- 2) Objective function

$$f(\mathbf{r}, \boldsymbol{\mu}, \mathbf{y}) = \sum_{i=1}^{N} \sum_{j=1}^{K} r_{ij} \left(\sum_{m=1}^{M} (y_{im} - \mu_{km})^{2} \right)$$

Goal:

Choose r^* and μ^* to minimize $f(r, \mu, y)$

Two observations:

- If K = N $f(r^*, \boldsymbol{\mu}^*, \boldsymbol{y}) = 0$ (Minimum)
 - Each observation in own cluster
 - $\boldsymbol{\mu}_i = \boldsymbol{y}_i$
- If K=1, $f(r^*, \boldsymbol{\mu}^*, \boldsymbol{y}) = N \times \sigma^2$
 - Each observation in one cluster
 - Center: average of documents



Specifying the Method

- 1) Assume Euclidean distance between objects
- 2) Objective function
- 3) Algorithm for optimization

Iterative algorithm, Each Iteration t

- Conditional on μ^{t-1} (from previous iteration), choose r^t
- Conditional on ${m r}^t$, choose ${m \mu}^t$

Repeat until convergence, measured as change in f.

Change =
$$f(\boldsymbol{\mu}^t, \boldsymbol{r}^t, \boldsymbol{y}) - f(\boldsymbol{\mu}^{t-1}, \boldsymbol{r}^{t-1}, \boldsymbol{y})$$

Specifying the Method

$$f(\mathbf{r}, \boldsymbol{\mu}, \mathbf{y}) = \sum_{i=1}^{N} \sum_{j=1}^{K} r_{ij} \left(\sum_{m=1}^{M} (y_{im} - \mu_{km})^{2} \right)$$

Algorithm for estimation:

Begin: initialize $\mu_1^{t-1}, \mu_2^{t-1}, \dots, \mu_K^{t-1}$

Choose r^t

$$r_{ij}^t = \left\{ egin{array}{l} 1 ext{ if } j = rg \min_k \sum_{m=1}^M (y_{im} - \mu_{km})^2 \ 0 ext{ otherwise }, \end{array}
ight.$$

In words: Assign each document $oldsymbol{y}_i$ to the closest center $oldsymbol{\mu}_k$

$$f(\mathbf{r}, \boldsymbol{\mu}, \mathbf{y}) = \sum_{i=1}^{N} \sum_{j=1}^{K} r_{ij} \left(\sum_{m=1}^{M} (y_{im} - \mu_{km})^{2} \right)$$

Conditional on ${m r}^t$, choose ${m \mu}^t$ Let's focus on ${m \mu}_k$

$$f(\mathbf{r}, \boldsymbol{\mu}_k, \mathbf{y})_k = \sum_{i=1}^N r_{ik} \left(\sum_{m=1}^M (y_{im} - \mu_{km})^2 \right)$$

Focus on just μ_{km}

$$f(\mathbf{r}, \mu_{km}, \mathbf{y})_{km} = \sum_{i=1}^{N} r_{ik} (y_{im} - \mu_{km})^2$$

Quadratic: take derivative, set equal to zero (second derivative test works)

$$\frac{\partial f(\mathbf{r}, \mu_{km}, \mathbf{y})_{km}}{\partial \mu_{km}} = -2 \sum_{i=1}^{N} r_{ik} (y_{im} - \mu_{km})$$

$$2 \sum_{i=1}^{N} r_{ik} (y_{im} - \mu_{km}^{t}) = 0$$

$$\sum_{i=1}^{N} r_{ik} y_{im} - \mu_{km}^{t} \sum_{i=1}^{N} r_{ik} = 0$$

$$\frac{\sum_{i=1}^{N} r_{ik} y_{im}}{\sum_{i=1}^{N} r_{ik}} = \mu_{km}^{t}$$

$$\boldsymbol{\mu}_k^t = \frac{\sum_{i=1}^N r_{ik} \boldsymbol{y}_i}{\sum_{i=1}^N r_{ik}}$$

In words:

- μ_k^t is the average of documents assigned to the k^{th} cluster

Algorithm, In Words

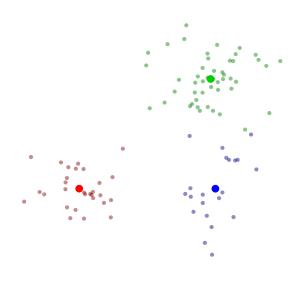
- Conditional on center estimates, assign documents to closest cluster centers
- Conditional on document assignments, cluster centers are averages of documents assigned to the cluster

Expectation-Maximization (EM) [connection guarantees convergence]

- Estimation of $r \rightsquigarrow$ Expectation step (data augmentation)
- Estimation of $\mu_k \rightsquigarrow \mathsf{Maximization}$ Step



Visual Example



Many Optimization Procedures!!!

Nelder Mead:

- Evaluate points on a simplex (triangle)
- Either Reflect, Expand, or Contract (based on values)
- Converges to local extrema

Stochastic Optimization:

- Sample a subset of data, perform optimization
- Sample a new subset, perform optimization, combine with previous sample
- Converges on local extrema (given regulatory conditions)

Genetic Optimization:

- Evaluate fitness of solutions
- Randomly select most fit, then combine
- Can converge to global maximum, but might require extensive run time

Where We Are Going

- Done with math component
- Start probability tomorrow