Biostatistics 615/815 Lecture 17: Single dimensional optimization

Hyun Min Kang

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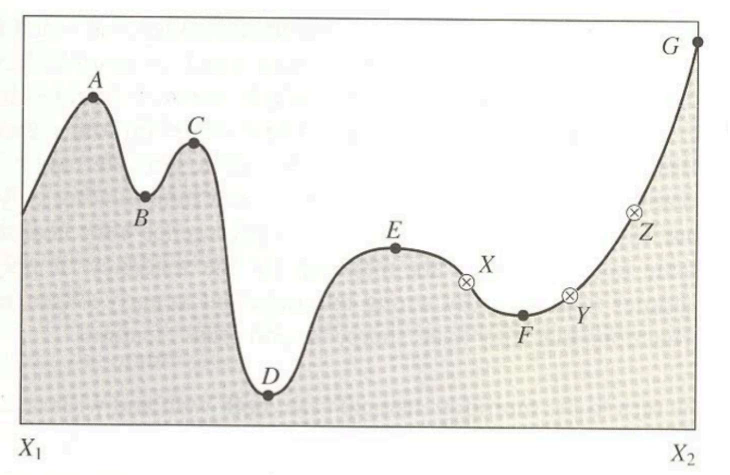
The Minimization Problem



Specific Objectives

Finding global minimum

- The lowest possible value of the function
- Very hard problem to solve generally

Finding local minimum

- Smallest value within finite neighborhood
- Relatively easier problem

A quick detour - The root finding problem

- Consider the problem of finding zeros for $f(x)$
- Assume that you know
  - Point a where $f(a)$ is positive
  - Point b where $f(b)$ is negative
  - $f(x)$ is continuous between a and b
- How would you proceed to find x such that $f(x) = 0$?

A C++ Example : defining a function object

```
#include <iostream>

class myFunc {   // a typical way to define a function object
public:
  double operator() (double x) const {
    return (x*x-1);
  }
};

int main(int argc, char** argv) {
  myFunc foo;
  std::cout << "foo(0) = " << foo(0) << std::endl;
  std::cout << "foo(2) = " << foo(2) << std::endl;
}
```

Root Finding with C++

```
// binary-search-like root finding algorithm
double binaryZero(myFunc foo, double lo, double hi, double e) {
  for (int i=0;; ++i) {
    double d = hi - lo;
    double point = lo + d * 0.5;   // find midpoint between lo and hi
    double fpoint = foo(point);    // evaluate the value of the function
    if (fpoint < 0.0) {
      d = lo - point;  lo = point;
    }
    else {
      d = point - hi;  hi = point;
    }
    // e is tolerance level (higher e makes it faster but less accurate)
    if (fabs(d) < e || fpoint == 0.0) {
      std::cout << "Iteration " << i << ", point = " << point
                << ", d = " << d << std::endl;
      return point;
    }
  }
}
```

Improvements to Root Finding

Approximation using linear interpolation

$$f^*(x) = f(a) + (x-a)\frac{f(b)-f(a)}{b-a}$$

Root Finding Strategy

- Select a new trial point such that $f^*(x) = 0$

Root Finding Using Linear Interpolation

```
double linearZero (myFunc foo, double lo, double hi, double e) {
  double flo = foo(lo);   // evaluate the function at the end points
  double fhi = foo(hi);
  for(int i=0;;++i) {
    double d = hi - lo;
    double point = lo + d * flo / (flo - fhi); // use linear interpolation
    double fpoint = foo(point);
    if (fpoint < 0.0) {
      d = lo - point;
      lo = point;
      flo = fpoint;
    }
    else {
      d = point - hi;
      hi = point;
      fhi = fpoint;
    }
    if (fabs(d) < e || fpoint == 0.0) {
      std::cout << "Iteration " << i << ", point = " << point << ", d = " << d << std::endl;
      return point;
    }
  }
}
```

Performance Comparison

Finding `sin(x) = 0` between $-\pi/4$ and $\pi/2$

```
#include <cmath>
class myFunc {
public:
  double operator() (double x) const {  return sin(x); }
};
...
int main(int argc, char** argv) {
  myFunc foo;
  binaryZero(foo,0-M_PI/4,M_PI/2,1e-5);
  linearZero(foo,0-M_PI/4,M_PI/2,1e-5);
  return 0;
}
```

Experimental results

```
binaryZero() : Iteration 17, point = -2.99606e-06, d = -8.98817e-06
linearZero() : Iteration 5, point = 0, d = -4.47489e-18
```

R example of root finding

```
# use uniroot() function for root finding
> uniroot( sin, c(0-pi/4,pi/2) )  ## function and interval as arguments
$root
[1] -3.531885e-09

$f.root
[1] -3.531885e-09

$iter
[1] 4

$estim.prec
[1] 8.719466e-05
```

Summary on root finding

- Implemented two methods for root finding
  - Bisection Method : `binaryZero()`
  - False Position Method : `linearZero()`
- In the bisection method, the bracketing interval is halved at each step
- For well-behaved function, the False Position Method will converge faster, but there is no performance guarantee.

Back to the Minimization Problem

- Consider a complex function $f(x)$ (e.g. likelihood)
- Find x which $f(x)$ is maximum or minimum value
- Maximization and minimization are equivalent
  - Replace $f(x)$ with $-f(x)$

Notes from Root Finding

- Two approaches possibly applicable to minimization problems
- Bracketing
  - Keep track of intervals containing solution
- Accuracy
  - Recognize that solution has limited precision

Notes on Accuracy - Consider the Machine Precision

- When estimating minima and bracketing intervals, floating point accuracy must be considered
- In general, if the machine precision is ϵ, the achievable accuracy is no more than $\sqrt{\epsilon}$.
- $\sqrt{\epsilon}$ comes from the second-order Taylor approximation

$$f(x) \approx f(b) + \frac{1}{2}f''(b)(x-b)^2$$

- For functions where higher order terms are important, accuracy could be even lower.
  - For example, the minimum for $f(x) = 1 + x^4$ is only estimated to about $\epsilon^{1/4}$.

Outline of Minimization Strategy

1. Find 3 points such that
   - $a < b < c$
   - $f(b) < f(a)$ and $f(b) < f(c)$
2. Then search for minimum by
   - Selecting trial point in the interval
   - Keep minimum and flanking points

Part I : Finding a Bracketing Interval

- Consider two points
  - x-values a, b
  - y-values $f(a) > f(b)$

Bracketing in C++

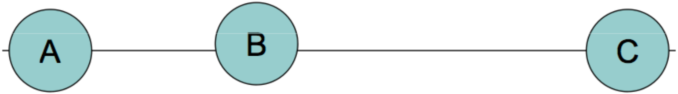
```
#define SCALE 1.618

void bracket( myFunc foo, double& a, double& b, double& c) {
  double fa = foo(a);
  double fb = foo(b);
  double fc = foo(c = b + SCALE*(b-a) );
  while( fb > fc ) {
    a = b; fa = fb;
    b = c; fb = fc;
    c = b + SCALE * (b-a);
    fc = foo(c);
  }
  // after the loop, fb < fa and fb < fc will hold.
}
```

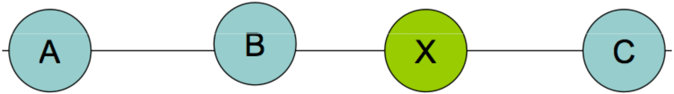
Part II : Finding Minimum After Bracketing

- Given 3 points such that
  - $a < b < c$
  - $f(b) < f(a)$ and $f(b) < f(c)$
- How do we select new trial point?

What is the best location for a new point X?



What we want



We want to minimize the size of next search interval, which will be either from A to X or from B to C

- If $f(X) < f(B)$, the next search interval will be (B, C)
- If $f(X) > f(B)$, the next search interval will be (A, X)

Minimizing worst case possibility

- Formulae

$$\begin{aligned} w &= \frac{b-a}{c-a} \\ z &= \frac{x-b}{c-a} \end{aligned}$$

Segments will have length either $1-w$ or $w+z$.

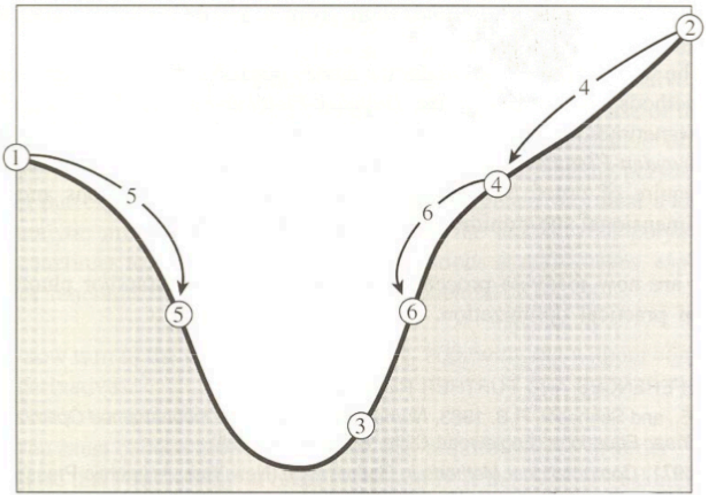
- Optimal case

$$\begin{cases} 1-w = w+z \\ \frac{z}{1-w} = w \end{cases}$$

- Solve It

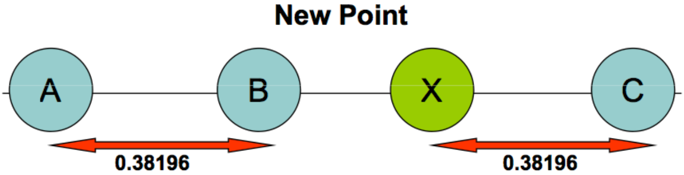
$$w = \frac{3-\sqrt{5}}{2} = 0.38197$$

The Golden Search



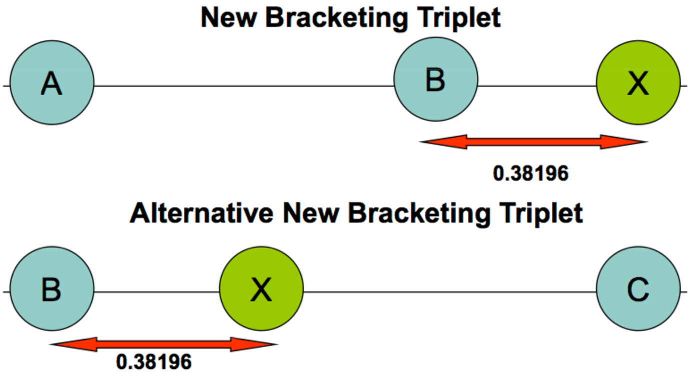
The Golden Ratio

The Golden Ratio



The number 0.38196 is related to the *golden mean* studied by Pythagoras

The Golden Ratio



Golden Search

- Reduces bracketing by $\sim 40\%$ after function evaluation
- Performance is independent of the function that is being minimized
- In many cases, better schemes are available

Golden Step

```
#define GOLD 0.38196
#define ZEPS 1e-10    // precision tolerance
double goldenStep (double a, double b, double c) {
  double mid = ( a + c ) * .5;
  if ( b > mid )
    return GOLD * (a-b);
  else
    return GOLD * (c-b);
}
```

Golden Search

```
double goldenSearch(myFunc foo, double a, double b, double c, double e) {
  int i = 0;
  double fb = foo(b);
  while ( fabs(c-a) > fabs(b*e) ) {
    double x = b + goldenStep(a, b, c);
    double fx = foo(x);
    if ( fx < fb ) {
      (x > b) ? ( a = b ) : ( c = b);
      b = x; fb = fx;
    }
    else {
      (x < b) ? ( a = x ) : ( c = x );
    }
    ++i;
  }
  std::cout << "i = " << i << ", b = " << b << ", f(b) = " << foo(b) << std::endl;
  return b;
}
```

A running example

Finding minimum of $f(x) = -\cos(x)$

```
class myFunc {
public:
  double operator() (double x) const {
    return 0-cos(x);
  }
};
..
int main(int argc, char** argv) {
  myFunc foo;
  goldenSearch(foo,0-M_PI/4,M_PI/4,M_PI/2,1e-5);
  return 0;
}
```

Results

```
i = 66, b = -4.42163e-09, f(b) = -1
```

R example of minimization

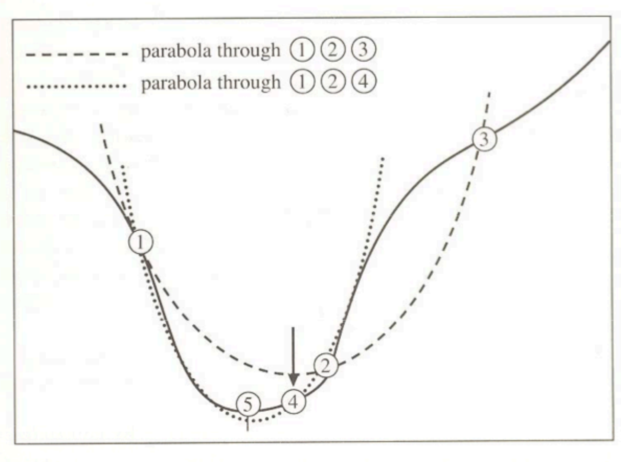
```
> optimize(cos,interval=c(0-pi/4,pi/2),maximum=TRUE)
$maximum
[1] -8.648147e-07

$objective
[1] 1
```

Further improvements

- As with root finding, performance can improve substantially when local approximation is used
- However, a linear approximation won't do in this case.

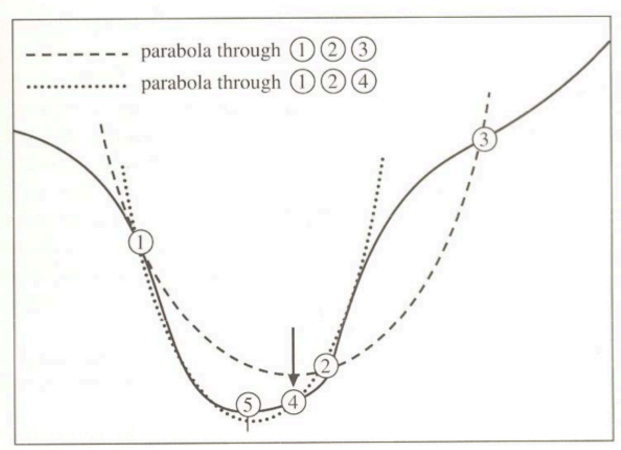
Approximation Using Parabola



Better optimization using local approximation

- Root finding example
  - Binary search reduces the search space by constant factor 1/2
  - Linear approximation may reduce the search space more rapidly for most well-defined functions
- Minimization problem
  - Golden search reduces the search space by 38%
  - Using a quadratic approximation of the function may achieve better optimization results

Approximation using parabola



Parabolic Approximation

$$f^*(x) = Ax^2 + Bx + C$$

The value minimizes $f^*(x)$ is

$$x_{min} = -\frac{B}{2A}$$

This strategy is called "inverse parabolic interpolation"

Fitting a parabola

- Can be fitted with three points
- Points must not be co-linear
- $f^*(x_1) = f(x_1), f^*(x_2) = f(x_2), f^*(x_3) = f(x_3)$.

$$
\begin{aligned}
C &= f(x_1) - Ax_1^2 - Bx_1 \\
B &= \frac{A(x_2^2 - x_1^2) + f(x_1) - f(x_2)}{x_1 - x_2} \\
A &= \frac{f(x_3) - f(x_2)}{(x_3 - x_2)(x_3 - x_1)} - \frac{f(x_1) - f(x_2)}{(x_1 - x_2)(x_3 - x_1)}
\end{aligned}
$$

Minimum for a Parabola

- General expression for finding minimum of a parabola fitted through three points

$$x_{min} = x_2 - \frac{1}{2}\frac{(x_2-x_1)^2(f(x_2)-f(x_1)) - (x_2-x_3)^2(f(x_2)-f(x_1))}{(x_2-x_1)(f(x_2)-f(x_3)) - (x_2-x_3)(f(x_2)-f(x_3))}$$

Fitting a Parabola

```
// Returns the distance between b and the abscissa for the
// fitted minimum using parabolic interpolation
double parabolaStep (double a, double fa, double b, double fb, double c,
                     double fc) {
  // Quantities for placing minimum of fitted parabola
  double p = (b - a) * (fb - fc);
  double q = (b - c) * (fb - fa);
  double x = (b - c) * q - (b - a) * p;
  double y = 2.0 * (p - q);
  // Check that y is not too close to zero
  if (fabs(y) < ZEPS)
    return goldenStep (a, b, c);
  else
    return x / y;
}
```

Avoiding degenerate case

- Fitted minimum could overlap with one of original points
- Ensure that each new point is distinct from previously examined points

Avoiding degenerate steps

```
double adjustStep(double a, double b, double c, double step, double e) {
  double minStep = fabs(e * b) + ZEPS;
  if (fabs(step) < minStep)
    return step > 0 ? minStep : 0-minStep;
    // If the step ends up to close to previous points,
    // return zero to force a golden ratio step ...
  if (fabs(b + step - a) <= e || fabs(b + step - c) <= e)
    return 0.0;
  return step;
}
```

Generating New Points

- Use parabolic interpolation by default
- Check whether improvement is slow
- If step sizes are not decreasing rapidly enough, switch to golden section

Adaptive calculation of step size

```
double calculateStep(double a, double fa, double b, double fb,
                     double c, double fc, double lastStep, double e) {
  double step = parabolaStep(a, fa, b, fb, c, fc);
  step = adjustStep(a, b, c, step, e);
  if (fabs(step) > fabs(0.5 * lastStep) || step == 0.0)
     step = goldenStep(a, b, c);
   return step;
}
```

Overall

The main function simply has to

- Generate new points using building blocks
- Update the triplet bracketing the minimum
- Check for convergence

Overall Minimization Routine

```
template<class F>
double adaptiveMinimum(F foo, double a, double b, double c, double e) {
  double fa = foo(a), fb = foo(b), fc = foo(c);
  double step1 = (c - a) * 0.5, step2 = (c - a) * 0.5;
  while ( fabs(c - a) > fabs(b * e) + ZEPS) {
     double step = calculateStep (a, fa, b, fb, c, fc, step2, e);
     double x = b + step;
     double fx = foo(x);
     if (fx < fb) {
        if (x > b) { a = b; fa = fb; }
        else { c = b; fc = fb; }
        b = x; fb = fx;
     }
     else {
        if (x < b) { a = x; fa = fx; }
        else { c = x; fc = fx; }
        step2 = step1; step1 = step;
     }
  }
  return b;
}
```

Important Characteristics

- Parabolic interpolation often converges faster
  - The preferred algorithm
- Golden search provides worst-cast performance guarantee
  - A fall-back for uncooperative functions
- Switch algorithms when convergence is slow
- Avoid testing points that are too close

More advanced strategy : Brent's algorithm

- Track 6 points (not all distinct)
  - The bracket boundaries (a, b)
  - The current minimum x
  - The second and third smallest value (w, v)
  - The new points to be examined u
- Parabolic interpolation
  - Using (x, w, v) to propose new value for u.
  - Additional care is required to ensure u falls between a and b.
- Recommended Reading
  - Numerical Recipes in C++ : Chapter 10.0 - 10.3

Using boost library for root finding / minimization

```
#include <cmath>
#include <iostream>
#include <boost/math/tools/roots.hpp>

#define EPS 1e-6

bool tol(double a, double b) { return ( fabs(b-a) <= EPS ); }

int main(int argc, char** argv) {
  double lo = 0-M_PI/4;
  double hi = M_PI/2;
  boost::uintmax_t niter;
  std::pair<double,double> rBi = boost::math::tools::bisect(sin, lo, hi, tol, niter);
  std::cout << "bisect : (" << rBi.first << ", " << rBi.second
            << ") at " << niter << " iterations" << std::endl;
  std::pair<double,double> r748 =
             boost::math::tools::toms748_solve(sin, lo, hi, tol, niter);
  std::cout << "toms748 : (" << r748.first << ", " << r748.second
            << ") at " << niter << " iterations" << std::endl;
  return 0;
}
```

Other Algorithms for Root Finding

- TOMS Algorithm 748
  - Uses a mixture of cubic, quadratic, and linear interpolation to locate the root of $f(x)$.
- Newton-Raphson algorithm
  - Uses first derivative of $f(x)$ to better approximate the root
- Halley's method
  - Uses first and second derivatives of $f(x)$ to approximate the root
- Householder's method
  - Uses up to d-th derivative of $f(x)$ to approximate the root for faster convergence

Summary

Root Finding Algorithms

- Bisection Method : Simple but likely less efficient
- False Position Method : More efficient for most well-behaved function

Single-dimensional minimization

- Golden Search : 38% reduction of interval per iteration
- Parabola Method : Likely more efficient reduction, but not always guaranteed.
- Brent's Method : Combination of above two methods. More efficient than both.