Biostatistics 615/815 Lecture 16: Importance sampling Single dimensional optimization

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November 1st, 2012

The crude Monte-Carlo Methods

An example problem

Calculating

$$\theta = \int_0^1 f(x)\,dx$$

where $f(x)$ is a complex function with $0 \leq f(x) \leq 1$

The problem is equivalent to computing $E[f(u)]$ where $u \sim U(0,1)$.

Algorithm

- Generate $u_1, u_2, \cdots, u_B$ uniformly from $U(0,1)$.
- Take their average to estimate θ

$$\hat{\theta} = \frac{1}{B}\sum_{i=1}^{B} f(u_i)$$

Accept-reject (or hit-and-miss) Monte Carlo method

Algorithm

1. Define a rectangle R between $(0,0)$ and $(1,1)$
   - Or more generally, between (x_m, x_M) and (y_m, y_M).
2. Set $h = 0$ (hit), $m = 0$ (miss).
3. Sample a random point $(x,y) \in R$.
4. If $y < f(x)$, then increase h. Otherwise, increase m
5. Repeat step 3 and 4 for B times
6. $\hat{\theta} = \frac{h}{h+m}$.

Which method is better?

$$\begin{aligned}
\sigma^2_{AR} - \sigma^2_{crude} &= \frac{\theta(1-\theta)}{B} - \frac{1}{B}E[f(u)^2] + \frac{\theta^2}{B} \\
&= \frac{\theta - E[f(u)]^2}{B} \\
&= \frac{1}{B}\int_0^1 f(u)(1-f(u))\,du \geq 0
\end{aligned}$$

The crude Monte-Carlo method has less variance then accept-rejection method

Revisiting The Crude Monte Carlo

$$\theta = E[f(u)] = \int_0^1 f(u)\,du$$
$$\hat{\theta} = \frac{1}{B}\sum_{i=1}^{B} f(u_i)$$

More generally, when x has pdf $p(x)$, if x_i is random variable following $p(x)$,

$$\theta_p = E_p[f(x)] = \int f(x)p(x)\,dx$$
$$\hat{\theta}_p = \frac{1}{B}\sum_{i=1}^{B} f(x_i)$$

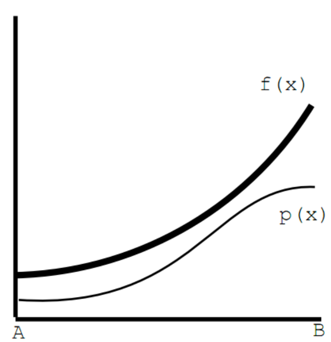
Importance sampling

Let x_i be random variable, and let $p(x)$ be an arbitrary probability density function.

$$\theta = E_u[f(x)] = \int f(x)\,dx = \int \frac{f(x)}{p(x)}p(x)\,dx = E_p\left[\frac{f(x)}{p(x)}\right]$$
$$\hat{\theta} = \frac{1}{B}\sum_{i=1}^{B} \frac{f(x_i)}{p(x_i)}$$

where x_i is sampled from distribution represented by pdf $p(x)$

Key Idea



- When $f(x)$ is not uniform, variance of $\hat{\theta}$ may be large.
- The idea is to pretend sampling from (almost) uniform distribution.

Analysis of Importance Sampling

Bias

$$E[\hat{\theta}] = \frac{1}{B}\sum_{i=1}^{B} E_p\left[\frac{f(x_i)}{p(x_i)}\right] = \frac{1}{B}\sum_{i=1}^{B}\theta = \theta$$

Variance

$$\mathrm{Var}[\hat{\theta}] = \frac{1}{B}\int\left(\frac{f(x)}{p(x)} - \theta\right)^2 p(x)\,dx$$
$$= \frac{1}{B}E_p\left[\left(\frac{f(x)}{p(x)}\right)^2\right] - \frac{\theta^2}{B}$$

The variance may or may not increase. Roughly speaking, if $p(x)$ is similar to $f(x)$, $f(x)/p(x)$ becomes flattened and will have smaller variance.

Simulation of rare events

Problem

- Consider a random variable $X \sim N(0,1)$
- What is $\Pr[X \geq 10]$?

Possible Solutions

- Let $f(x)$ and $F(x)$ be pdf and CDF of standard normal distribution.
- Then $\Pr[X \geq 10] = 1 - F(10) = 7.62 \times 10^{-24}$, and we're all set.
- But what if we don't have $F(x)$ but only $f(x)$?
  - In many cases, CDF is not easy to obtain compared to pdf or random draws.

If we don't have CDF: ways to calculate $\Pr[X \geq 10]$

Accept-reject sampling

Sample random variables from $N(0,1)$, and count how many of them are greater than 10

- How many random variables should be sampled to observe at least one $X \geq 10$?
- $1/\Pr[X \geq 10] = 1.3 \times 10^{23}$

Monte-Carlo Integration

- If we have pdf $f(x)$, $\Pr[X \geq 10] = \int_{10}^{\infty} f(x)\,dx$
- Use Monte-Carlo integration to compute this quantity
  1. Sample B values uniformly from $[10, 10+W]$ for a large value of W (e.g. 50).
  2. Estimate $\hat{\theta} = \frac{1}{B}\sum_{i=1}^{B} f(u_i)$.

An Importance Sampling Solution

1. Transform the problem into an unbounded integration problem (to make it simple)

$$\Pr[X \geq 10] = \int_{10}^{\infty} f(x)\,dx = \int I(x \geq 10) f(x)\,dx$$

2. Sample B random values from $N(\mu, 1)$ where μ is a large value nearby 10, and let $f_\mu(x)$ be the pdf.
3. Estimate the probability as an weighted average

$$\hat{\theta} = \frac{1}{B}\left[I(x_i \geq 10) \frac{f(x)}{f_\mu(x)} \right]$$

An Example R code

```
## pnormUpper() function to calculate Pr[x>t] using n random samples
pnormUpper <- function(n, t) {
  lo <- t
  hi <- t + 50    ## hi is a reasonably large number

  ## accept-reject sampling
  r <- rnorm(n)       ## random sampling from N(0,1)
  v1 <- sum(r > t)/n  ## count how many meets the condition

  ## Monte-Carlo integration
  u <- runif(n,lo,hi)           ## uniform sampling [t,t+50]
  v2 <- mean(dnorm(u))*(hi-lo)  ## Monte-Carlo integration

  ## importance sampling using N(t,1)
  g <- rnorm(n,t,1)    ## sample from N(t,1)
  v3 <- sum( (g > t) * dnorm(g)/dnorm(g,t,1)) / n;  ## take a weighted average

  return (c(v1,v2,v3))  ## return three values
}
```

Evaluating different methods

```
## test pnormUpperTest(n,t) function using r times of repetition
pnormUpperTest <- function(r, n, t) {
  gold <- pnorm(t,lower.tail=FALSE)  ## gold standard answer
  emp <- matrix(nrow=r,ncol=3)  ## matrix containing empirical answers
  for(i in 1:r) { emp[i,] <- pnormUpper(n,t) }  ## repeat r times
  m <- colMeans(emp)        ## obtain mean of the estimates
  s <- apply(emp,2,sd)      ## obtain stdev of the estimates
  print("GOLD :")
  print(gold);              ## print gold standard answer
  print("BIAS (ABSOLUTE) :")
  print(m-gold)             ## print bias
  print("STDEV (ABSOLUTE) :")
  print(s)                  ## print stdev
  print("BIAS (RELATIVE) :")
  print((m-gold)/gold)      ## print relative bias
  print("STDEV (RELATIVE) :")
  print(s/gold)             ## print relative stdev
}
```


An example output

```
> pnormUpperTest(100,1000,10)
[1] "GOLD :"
[1] 7.619853e-24
[1] "BIAS (ABSOLUTE) :"
[1] -7.619853e-24 -5.596279e-26  4.806933e-26
[1] "STDEV (ABSOLUTE) :"
[1] 0.000000e+00 3.917905e-24 7.559024e-25
[1] "BIAS (RELATIVE) :"
[1] -1.000000000 -0.007344339  0.006308433
[1] "STDEV (RELATIVE) :"
[1] 0.0000000 0.5141707 0.0992017
```


Another example output

```
> pnormUpperTest(100,10000,10)
[1] "GOLD :"
[1] 7.619853e-24
[1] "BIAS (ABSOLUTE) :"
[1] -7.619853e-24  2.202168e-26  1.972362e-26
[1] "STDEV (ABSOLUTE) :"
[1] 0.000000e+00 1.186711e-24 2.935474e-25
[1] "BIAS (RELATIVE) :"
[1] -1.000000000  0.002890040  0.002588451
[1] "STDEV (RELATIVE) :"
[1] 0.00000000 0.15573932 0.03852402
```

1,000 importance sampling gives smaller variance than Monte-Carlo integration with 10,000 random samples.

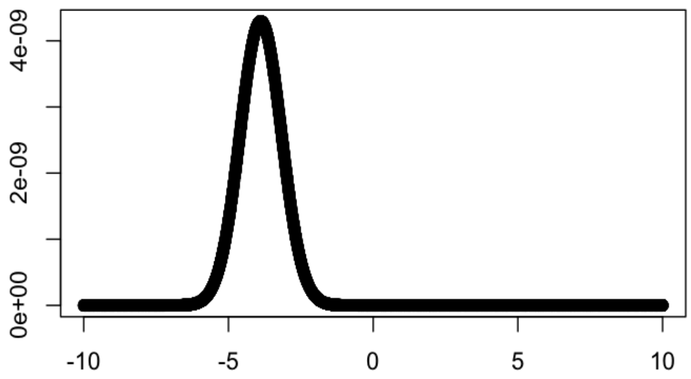
Integral of probit normal distribution

- Disease risk score of an individual follows $x \sim N(\mu, \sigma^2)$.
- Probability of disease $\Pr(y = 1) = \Phi(x)$, where $\Phi(x)$ is CDF of standard normal distribution.
- Want to compute the disease prevalence across the population.

$$\theta = \int_{-\infty}^{\infty} \Phi(x)\mathcal{N}(x; \mu, \sigma^2)\,dx$$

where $\mathcal{N}(\cdot; \mu, \sigma^2)$ is pdf of normal distribution.

Plot of $\Phi(x)\mathcal{N}(x; -8, 1^2)$



Monte-Carlo integration using uniform samples

1. Sample x uniformly from a sufficiently large interval (e.g. $[-50, 50]$).
2. Evaluate integrals using

$$\hat{\theta} = \frac{1}{B}\sum_{i=1}^{B}\Phi(x_i)\mathcal{N}(x_i; \mu, \sigma^2)$$

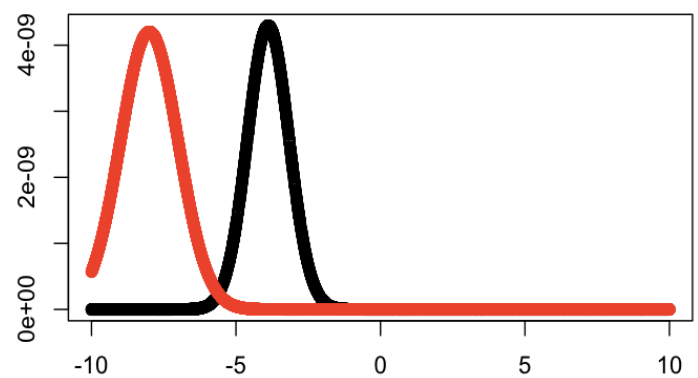
Note that, for some μ and σ^2, $[-50, 50]$ may not be a sufficiently large interval.

Monte-Carlo integration using normal distribution

1. Sample x from $N(\mu, \sigma^2)$
2. Evaluate integrals by

$$\hat{\theta} = \frac{1}{B}\sum_{i=1}^{B}\Phi(x_i)$$

$\mathcal{N}(x; -8, 1^2)$ (red) and $\Phi(x)\mathcal{N}(x; -8, 1^2)$ (black)



Two distributions are quite different – $\mathcal{N}(x; -8, 1^2)$ may not be an ideal distribution for Monte-Carlo integration

Monte-Carlo integration by importance sampling

1. Sample x from a new distribution
   - For example, $N(\mu', \sigma'^2)$
   - $\mu' = \frac{\mu}{\sigma^2+1}$
   - $\sigma' = \sigma$.
2. Evaluate integrals by weighting importance samples

$$\hat{\theta} = \frac{1}{B}\sum_{i=1}^{B}\left[\Phi(x_i)\frac{\mathcal{N}(x;\mu,\sigma^2)}{\mathcal{N}(x;\mu',\sigma'^2)}\right]$$

An Example R code

```
probitNormIntegral <- function(n,mu,sigma) {
  ## integration across uniform distribution
  lo <- -50
  hi <- 50
  u <- runif(n,lo,hi)
  v1 <- mean(dnorm(u,mu,sigma)*pnorm(u))*(hi-lo)

  ## integration using random samples from N(mu,sigma^2)
  g <- rnorm(n,mu,sigma)
  v2 <- mean(pnorm(g))

  ## importance sampling using N(mu',sigma^2)
  adjm <- mu/(sigma^2+1)
  r <- rnorm(n,adjm,sigma)
  v3 <- mean(pnorm(r)*dnorm(r,mu,sigma)/dnorm(r,adjm,sigma))
  return (c(v1,v2,v3))
}
```


Testing different methods

```
probitNormTest <- function(r, n, mu,sigma) {
  emp <- matrix(nrow=r,ncol=3)
  for(i in 1:r) {
    emp[i,] <- probitNormIntegral(n,mu,sigma)
  }
  m <- colMeans(emp)
  s <- apply(emp,2,sd)
  print("MEAN :")
  print(m)
  print("STDEV :")
  print(s)
  print("STDEV (RELATIVE) :")
  print(s/m)
}
```


Example Output

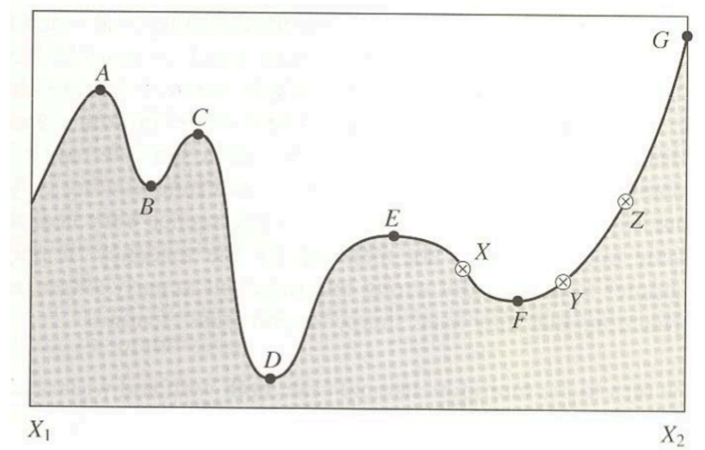
```
> probitNormTest(100,1000,-8,1)
[1] "MEAN :"
[1] 7.643951e-09 6.205931e-09 7.701978e-09
[1] "STDEV :"
[1] 1.579951e-09 1.239459e-08 1.019870e-10
[1] "STDEV (RELATIVE) :"
[1] 0.20669298 1.99721608 0.01324166
```

Importance sampling shows smallest variance.

Summary

- Crude Monte Carlo method
  - Use uniform distribution (or other original generative model) to calculate the integration
  - Every random sample is equally weighted.
  - Straightforward to understand
- Rejection sampling
  - Estimation from discrete count of random variables
  - Larger variance than crude Monte-Carlo method
  - Typically easy to implement
- Importance sampling
  - Reweight the probability distribution
  - Possible to reduce the variance in the estimation
  - Effective for inference involving rare events
  - Challenge is how to find the good sampling distribution.

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); //
    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

```
> uniroot( sin, c(0-pi/4,pi/2) )
$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 $\epsilon^{1/4}$.

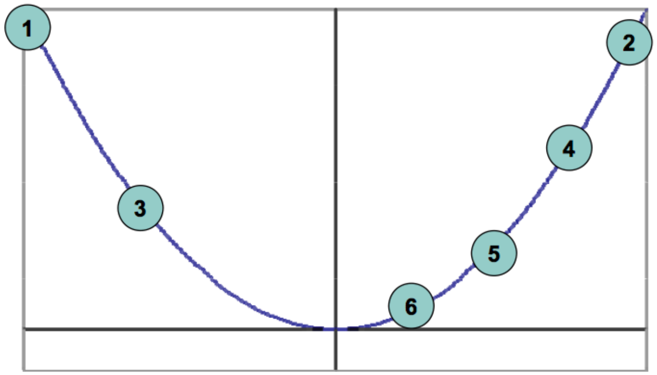
Outline of Minimization Strategy

1. Bracket minimum
2. Successively tighten bracket interval

Detailed 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

Minimization after Bracketing



Part I : Finding a Bracketing Interval

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

Bracketing in C++

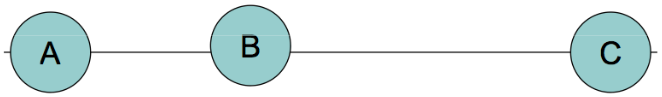
```
#define SCALE 1.618

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);
  }
}
```

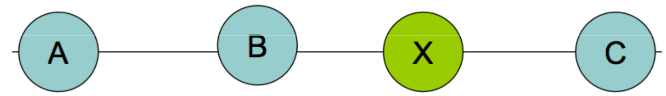

Part II : Finding Minimum After Bracketing

- 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

Minimizing worst case possibility

- Formulae

$$w = \frac{b-a}{c-a}$$
$$z = \frac{x-b}{c-a}$$

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

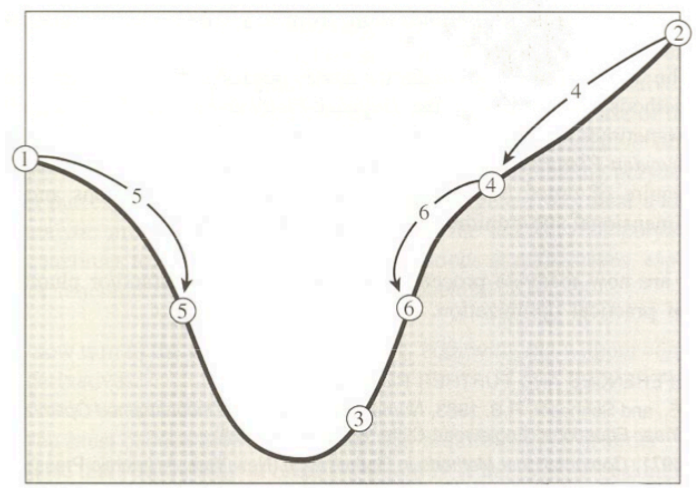
- Optimal case

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

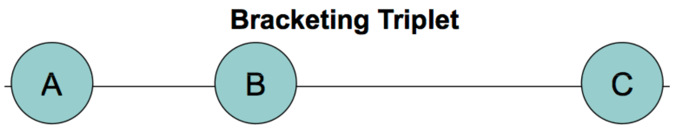
- Solve It

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

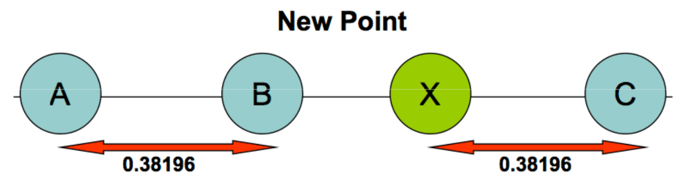
The Golden Search



The Golden Ratio

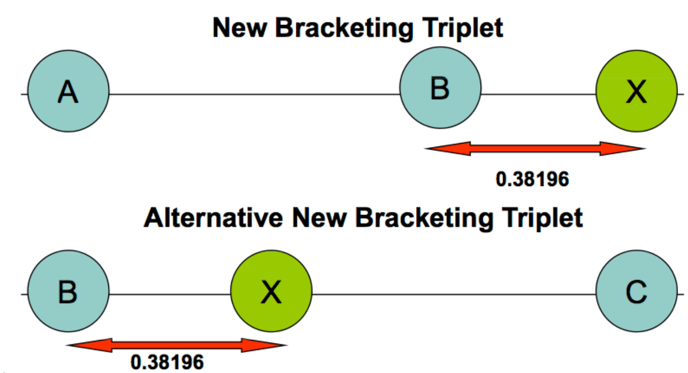


The Golden Ratio



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

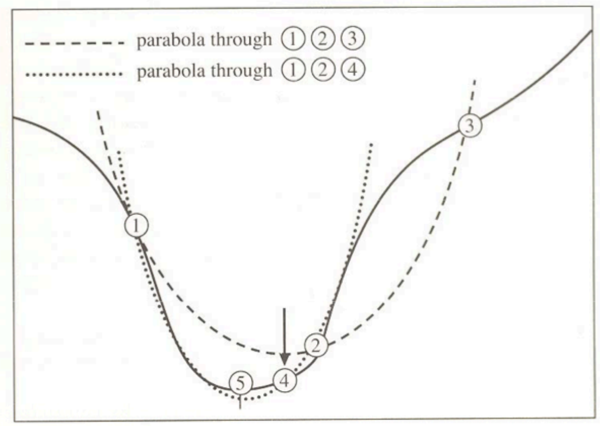
```
> optimize(cos,interval=c(0-pi/4,pi/2),maximum=TRUE)
$maximum
[1] -8.648147e-07

$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



Summary

Today

- 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

Next Lecture

- More Single-dimensional minimization
  - Brent's method
- Multidimensional optimization
  - Simplex method