Introduction to Numerical Optimization

Biostatistics 615/815

Lecture 15

Course is More Than Half Done!

- If you have comments…
- … they are very welcome
  - Lectures
  - Lecture notes
  - Weekly Homework
  - Midterm
  - Content

Last Lecture

- Computer generated "random" numbers
- Linear congruential generators
  - Improvements through shuffling, summing
- Importance of using validated generators
  - Beware of problems with the default `rand()` function

Today ...

- Root finding
- Minimization for functions of one variable
- Ideas:
  - Limits on accuracy
  - Local approximations

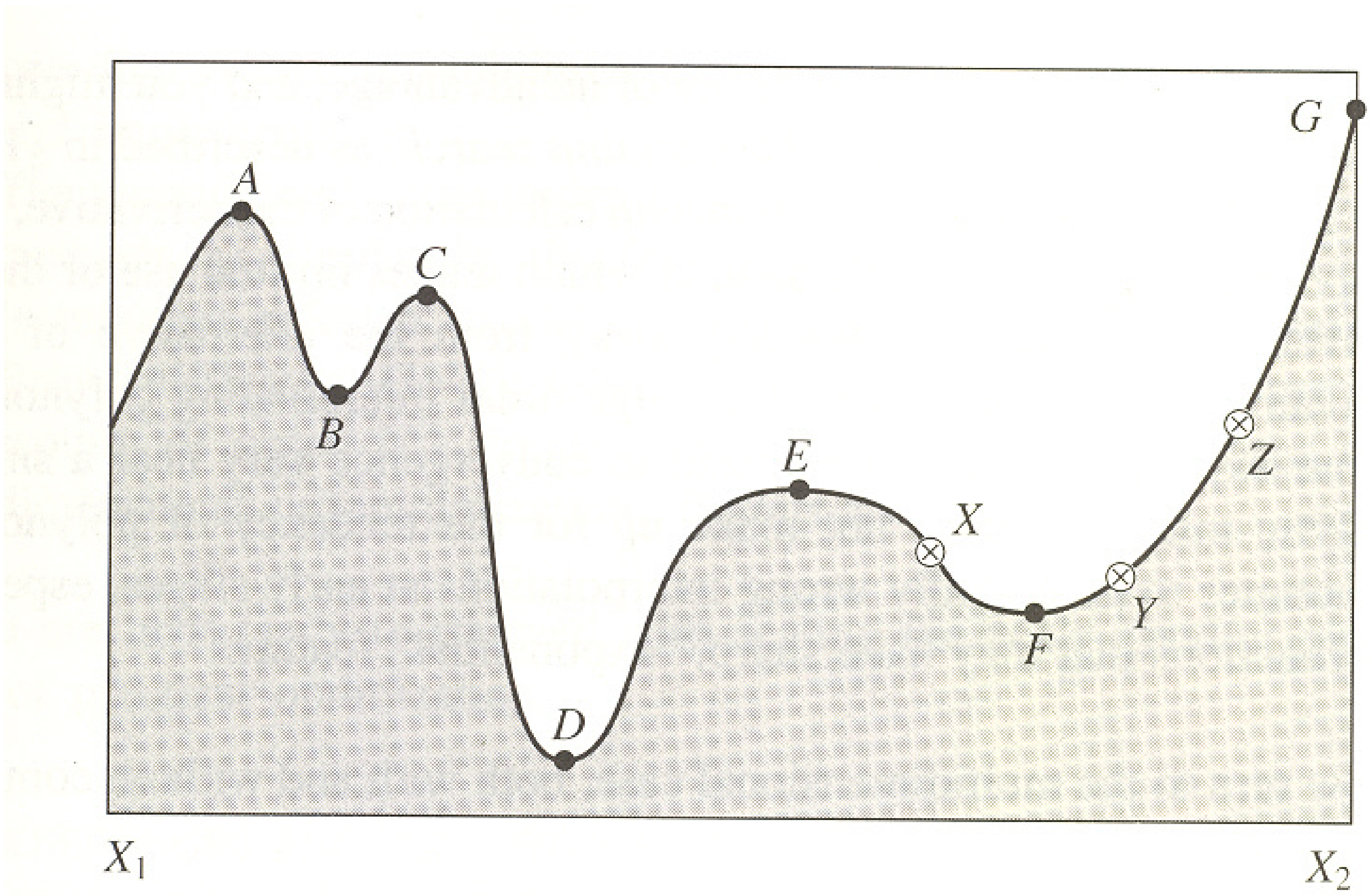
Numerical Optimization

- Consider some function *f(x)*
  - e.g. Likelihood for some model …
- Find the value of *x* for which *f* takes a maximum or minimum value
- Maximization and minimization are equivalent
  - Replace *f(x)* with *–f(x)*

Algorithmic Objectives

- Solve problem…
  - Conserve CPU time
  - Conserve memory
- Most often, the CPU time is dominated by the cost of evaluating *f(x)*
  - Minimize the number of evaluations

The Minimization Problem



Specific Objectives

- Finding global minimum
  - *The* lowest possible value of the function
  - Extremely hard problem
- Finding local minimum
  - Smallest value within finite neighborhood

Typical Quality Checks

- When solving an optimization problem it is good practice to check the quality of the solution
- Try different starting values …
- Perturb solution and repeat …

A Quick Detour

- 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?

Root Finding in C

```
double zero(double (*func)(double), double lo, double hi, double e)
   {
   while (1)
        {
        double d = hi - lo;
        double point = lo + d * 0.5;
        double fpoint = (*func)(point);

        if (fpoint < 0.0)
           { d = lo - point; lo = point; }
        else
           { d = point - hi; hi = point; }

        if (fabs(d) < e || fpoint == 0.0)
           return point;
        }
   }
```

Improvements to Root Finding

- Consider the following approximation:

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

- Select new trial point such that $f^*(x)$ is zero.

Improved Root Finding in C

```
double zero (double (*func)(double), double lo, double hi, double e)
   {
   double flo = (*func)(lo);
   double fhi = (*func)(hi);
   while (1)
        {
        double d = hi - lo;
        double point = lo + d * flo / (flo - fhi);
        double fpoint = (*func)(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)
           return point;
        }
   }
```

Performance Comparison

- Find the zero for sin(x)
  - In the interval $-\pi/4$ to $\pi/2$
  - Accuracy parameter set to 10^{-5}
- Bisection method used 17 calls to sin(x)
- Approximation used 5 calls to sin(x)

Program That Uses Root Finding

```
double zero (double (*func)(double), double lo, double hi, double e);

double function(double x)
    {
    return (4*x – 3);
    }

int main(int argc, char ** argv)
    {
    double min = zero(my_function, -5, +5, 1e-5);

    printf("Minimum for my function is %.3f at %.3f\n",
           my_function(min), min);
    }
```

Notes on Root Finding

- The 2nd method we implemented is the False Position Method
- In the bisection method, the bracketing interval is halved at each step
- For well-behaved functions, the False Position Method will converge faster, but there is no performance guarantee

Questions on Root Finding

- What care is required in setting precision?

- How to set starting brackets for minimum?
  - If the function was monotonic?
  - If there is a specific target interval?

- What would happen for a function such as $f(x) = 1 / (x - c)$

Back to Numerical Optimization

- Consider some function $f(x)$
  - e.g. Likelihood for some model …

- Find the value of x for which f takes a maximum or minimum value

- Maximization and minimization are equivalent
  - Replace $f(x)$ with $-f(x)$

Notes from Root Finding

- Introduces two useful ideas
  - Which can be applied to function minimization
- Bracketing
  - Keep track of interval containing solution
- Accuracy
  - Recognize that solution has limited precision

Note on Accuracy

- 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 $\text{sqrt}(\varepsilon)$

Note on Accuracy II

- The error results from the second term in the Taylor approximation:

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

- 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 $\varepsilon^{1/4}$

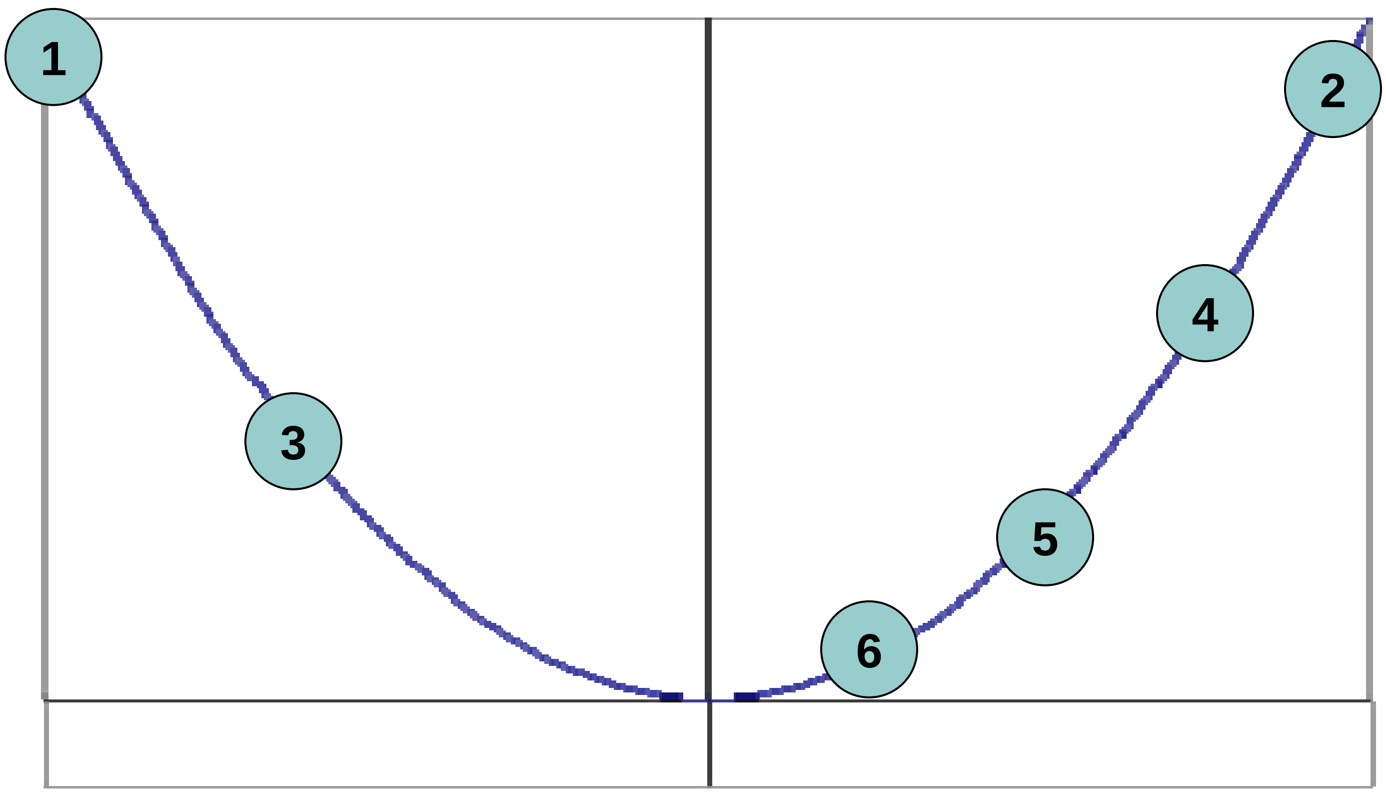
Outline of Minimization Strategy

- Part I
  - Bracket minimum
- Part II
  - Successively tighten bracketing interval

Detailed Minimization Strategy

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

Minimization after Bracketing



Part I:
Finding a Bracketing Interval

- Consider two points
  - a, b
  - $f(a) > f(b)$
- Take successively larger steps beyond b until function starts increasing

Bracketing in C

```
#define SCALE   1.618

void bracket (double (*f)(double), double* a, double* b, double* c)
   {
   double fa = (*f)( *a);
   double fb = (*f)( *b);
   double fc = (*f)( *c = *b + SCALE * (*b - *a) );

   while (fb > fc)
        {
        *a = *b; fa = fb;
        *b = *c; fb = fc;
        *c = *b + SCALE * (*b - *a);
        fc = (*f) (*c);
        }
   }
```

Bracketing in C++

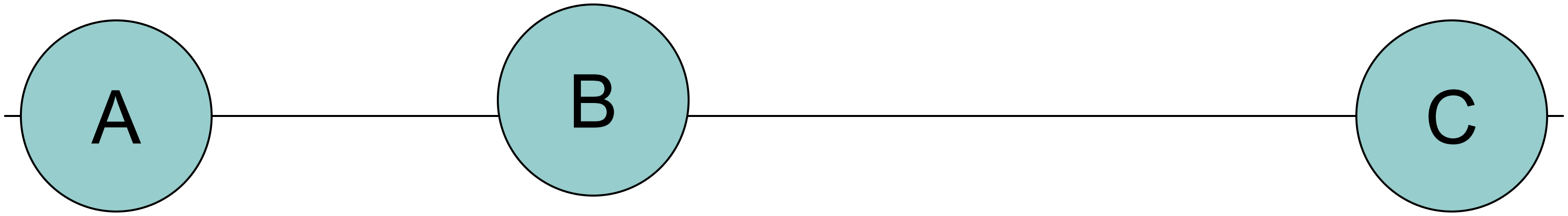
```
#define SCALE   1.618

void bracket (double (*f)(double), double & a, double & b, double & c)
   {
   double fa = (*f)(a);
   double fb = (*f)(b);
   double fc = (*f)(c = b + SCALE * (b - a) );

   while (fb > fc)
        {
        a = b; fa = fb;
        b = c; fb = fc;
        c = b + SCALE * (b - a);
        fc = (*f) (c);
        }
   }
```

Part II: Finding Minimum after Bracketing

- Given 3 points such that
  - $a < b < c$
  - $f(b) < f(a)$ and $f(b) < f(c)$

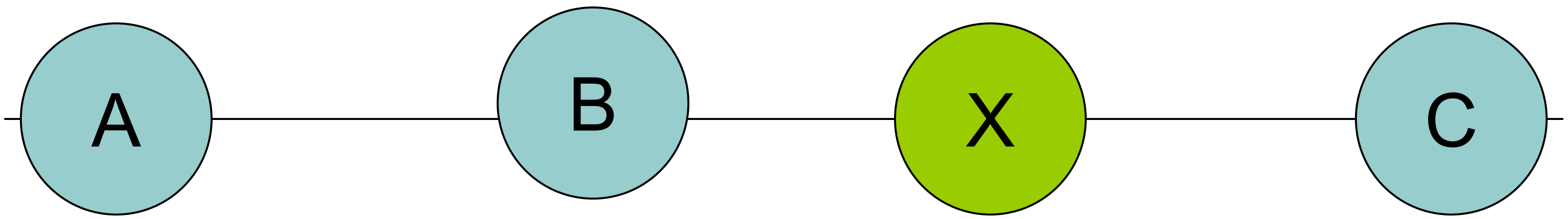
- How do we select new trial point?

Consider ...



What is the best location for a new point X?

Consider …



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

Formulae ...

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

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

Segments will have length

$1-w$ or $w+z$

We want to minimize worst case possibility so...

Effectively …

The optimal case is

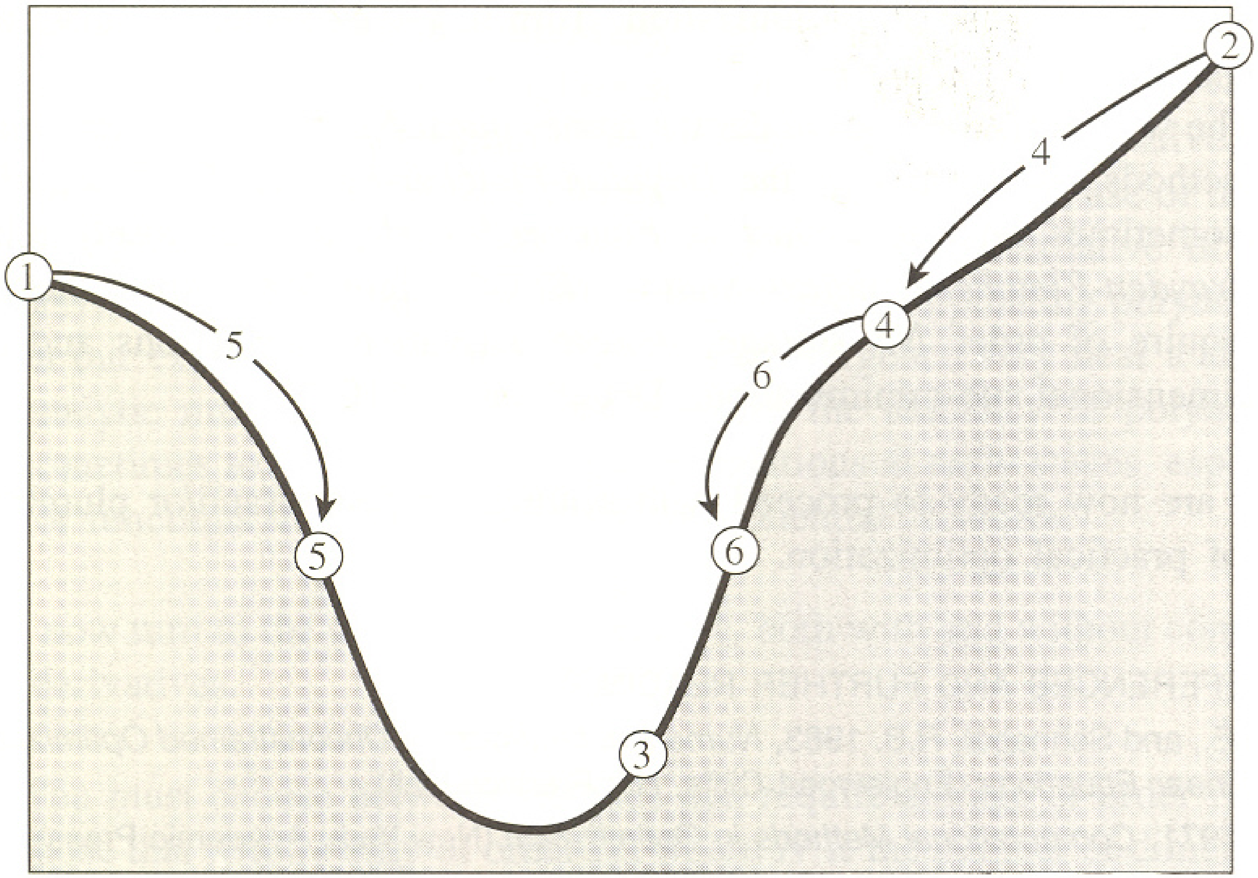
$$z = 1 - 2w$$

$$\frac{z}{1-w} = w$$

This gives

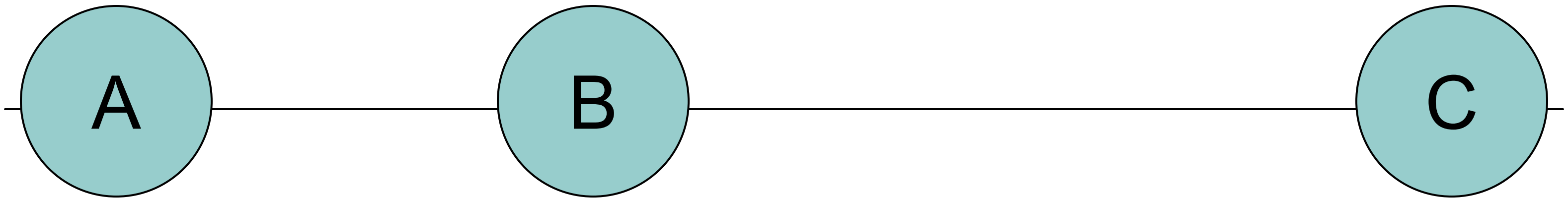
$$\mathrm{w} = \frac{3 - \sqrt{5}}{2} = 0.38197$$

Golden Search

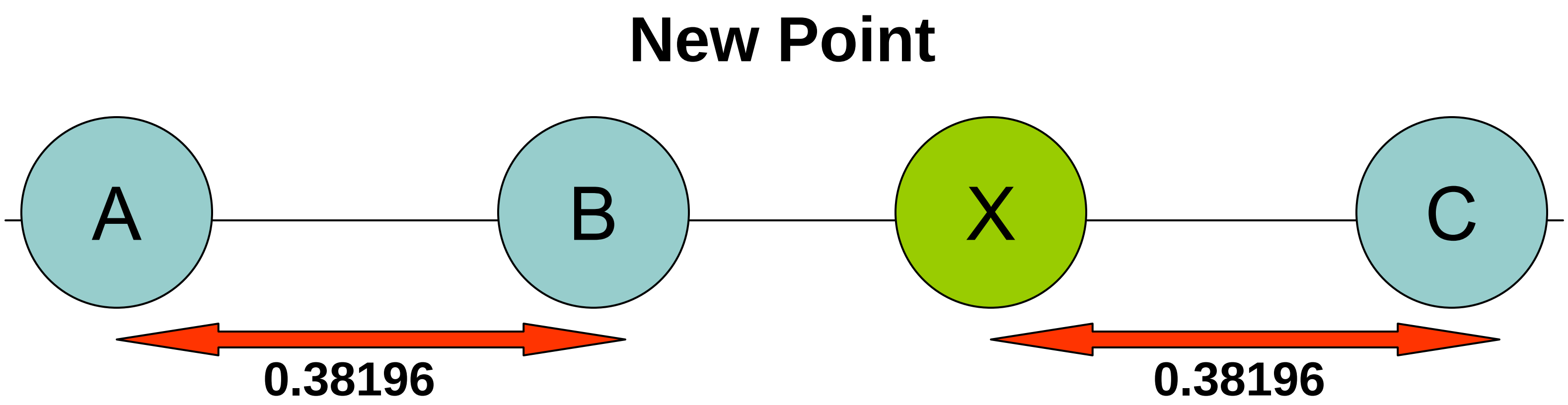


The Golden Ratio

Bracketing Triplet



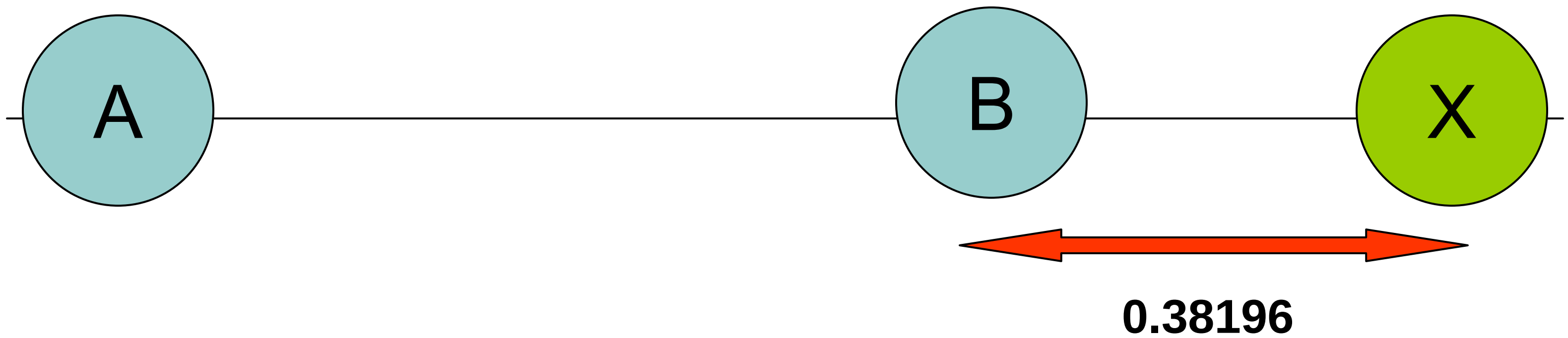
The Golden Ratio



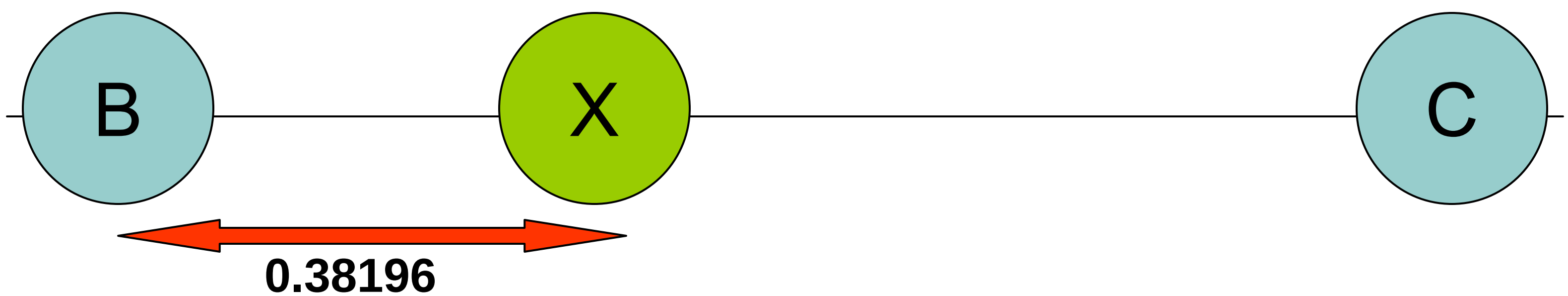
The number 0.38196 is related to the *golden mean* studied by Pythagoras

The Golden Ratio

New Bracketing Triplet



Alternative New Bracketing Triplet



Golden Search

- Reduces bracketing by ~40% after each function evaluation
- Performance is independent of the function that is being minimized
- Potentially, better schemes are possible

Golden Step

```
#define GOLD   0.38196
#define ZEPS   1e-10

double golden_step (double a, double b, double c)
   {
   double mid = (a + c) * 0.5;

   if (b > mid)
      return GOLD * (a - b);
   else
      return GOLD * (c - b);
   }
```

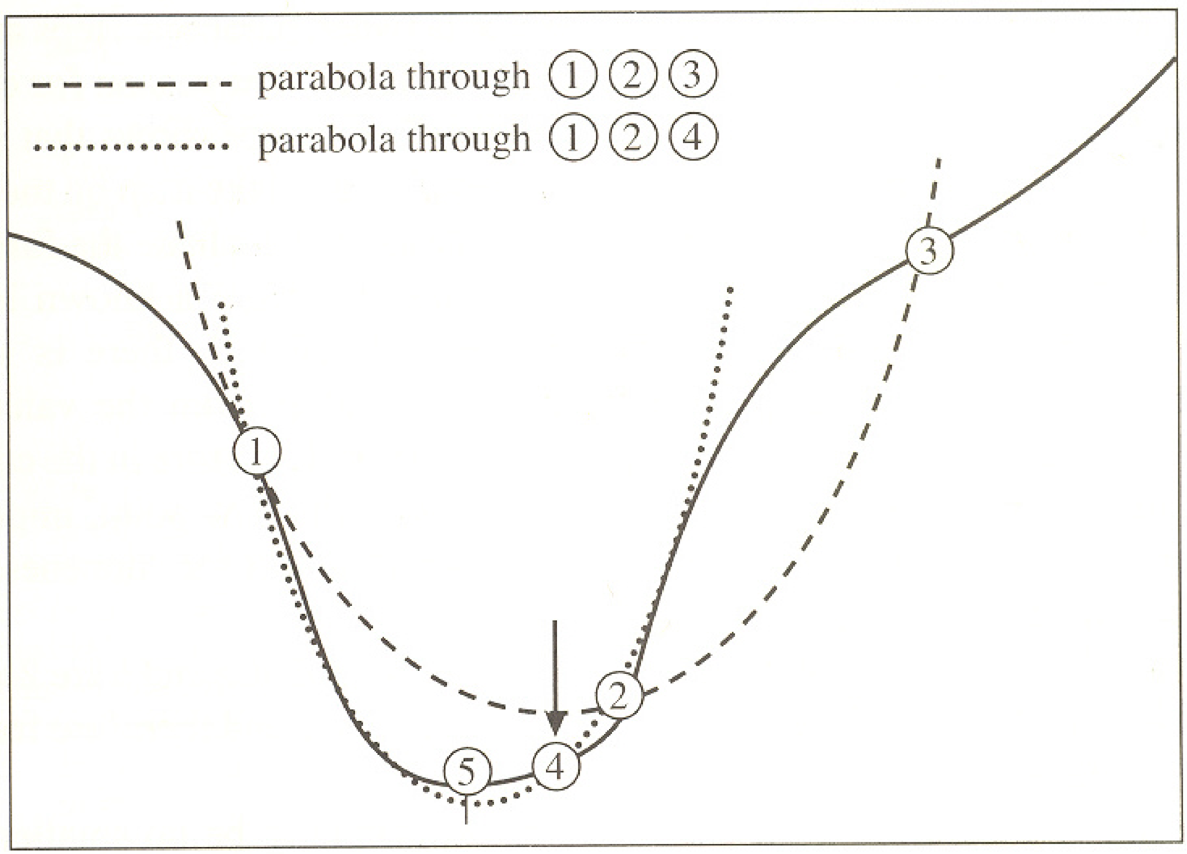
Golden Search

```
double golden_search(double (*func)(double),
                     double a, double b, double c, double e)
   {
   double fb = (*func)(b);

   while ( fabs(c - a) > fabs(b * e) + ZEPS)
      {
      double x = b + golden_step(a, b, c);
      double fx = (*func)(x);

      if (fx < fb)
         {
         if (x > b) { a = b; } else { c = b; }
         b = x; fb = fx;
         }
      else
         if (x < b) { a = x; } else { c = x; }
      }
   return b;
   }
```

Further Improvements

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

Approximating The Function



Recommended Reading

- Numerical Recipes in C (or C++)
  - Press, Teukolsky, Vetterling, Flannery
  - Chapters 10.0 – 10.2
- Excellent resource for scientific computing
- Online at
  - http://www.numerical-recipes.com/
  - http://www.library.cornell.edu/nr/