Biostatistics 615/815 Lecture 18: Single Dimensional and Multidimensional Optimizations

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Annoucements

Homework and Grading

- Homework #5 annouced
- Homework grading is still pending

Thursday March 24th

- Mary Kate Trost will introduce us a very useful C++ library

Recap : Root Finding with C++

```
double binaryZero(myFunc foo, double lo, double hi, double e) {
  for (int i=0;; ++i) {
    double d = hi - lo;  // f(lo) < 0, f(hi) > 0, d can be positive or negative
    double point = lo + d * 0.5;   // d is + for increasing func, - for decreasing
    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 accruate)
    if (fabs(d) < e || fpoint == 0.0) {
      std::cout << "Iteration " << i << ", point = " << point
                << ", d = " << d << std::endl;
      return point;
    }
  }
}
```

Recap : Improvements to Root Finding

Approximation using linear interpolation

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

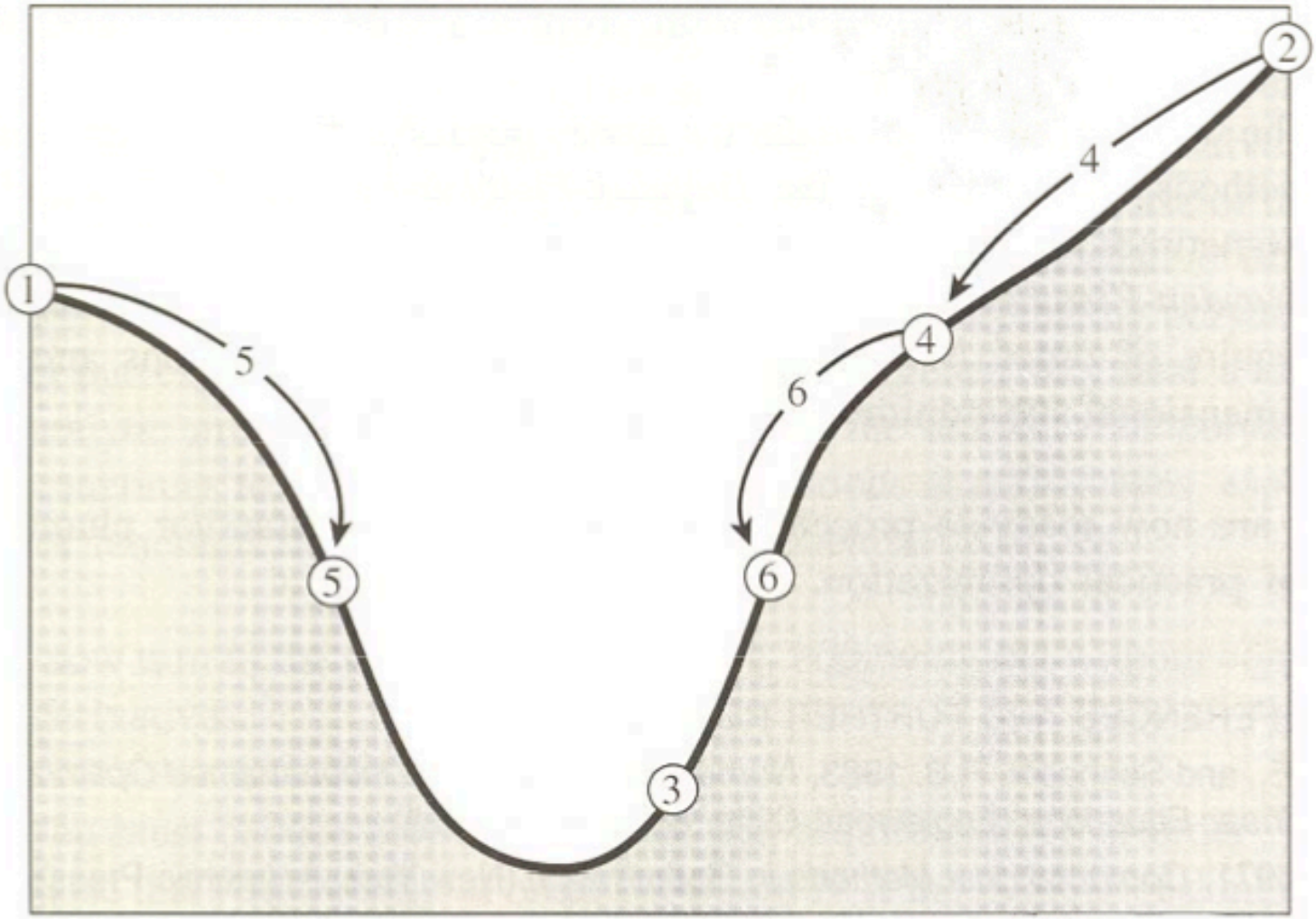
Root Finding Strategy

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

Recap : 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

Recap : The Golden Search



Recap : 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;
}
```

Today

A better single-dimensional optimization

- Parabolic interpolation
- Adaptive method

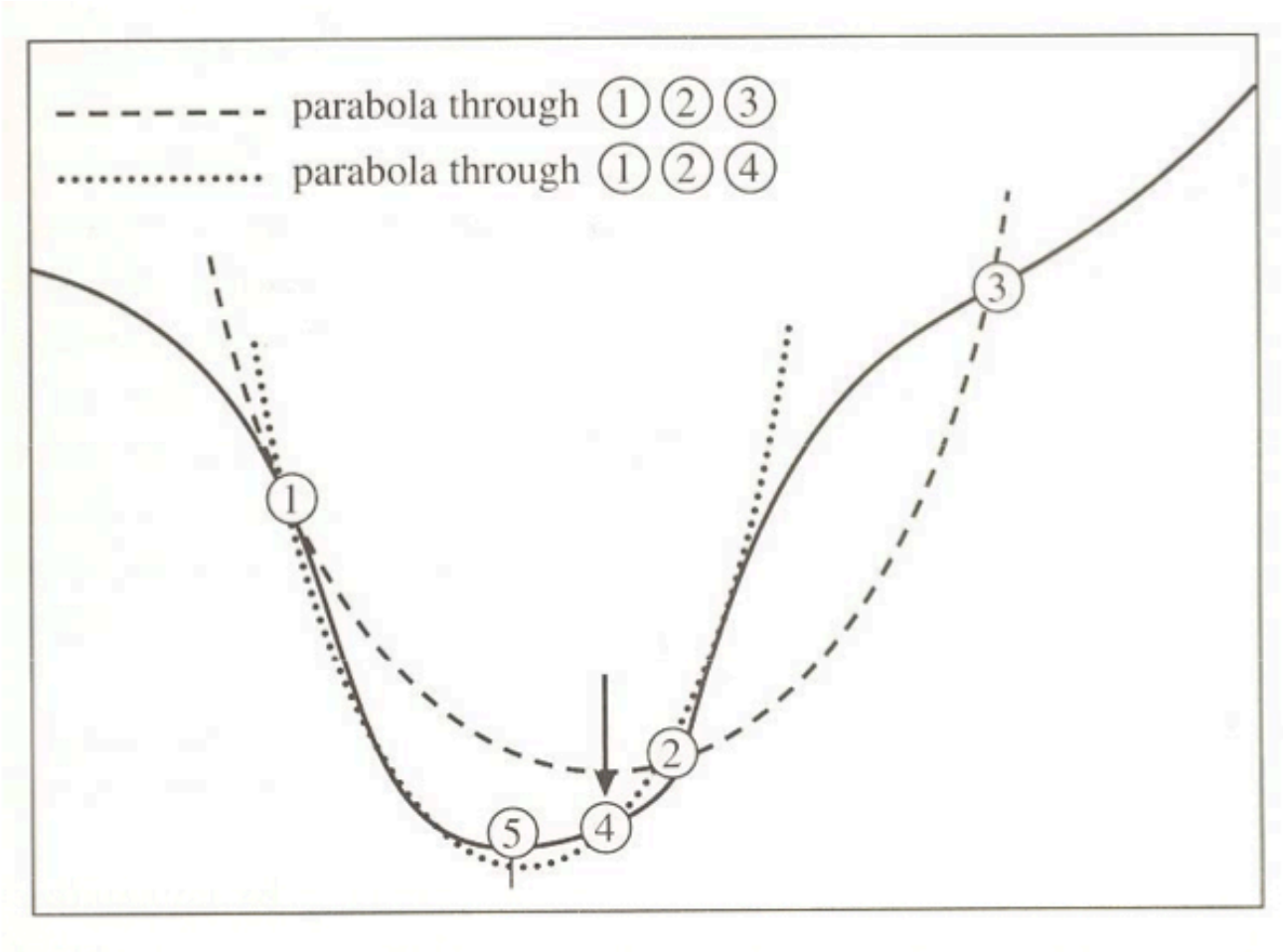
Multi-dimensional optimization

- Simplex algorithm

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

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

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

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

Fitting a Parabola

```
// Returns the distance between b and the abscissa for the
// fitted minimum using parabolic interpolation
double parabola_step (double a, double fa, double b, double fb, double c, double f
  // 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 q is not zero
  if (fabs(y) < ZEPS)
    return golden_step (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 adjust_step(double a, double b, double c, double step, double e) {
  double min_step = fabs(e * b) + ZEPS;
  if (fabs(step) < min_step)
    return step > 0 ? min_step : 0-min_step;
    // 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 calculate_step(double a, double fa, double b, double fb,
                      double c, double fc, double last_step, double e) {
  double step = parabola_step(a, fa, b, fb, c, fc);
  step = adjust_step(a, b, c, step, e);
  if (fabs(step) > fabs(0.5 * last_step) || step == 0.0)
     step = golden_step(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

```
double find_minimum(myFunc 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 = calculate_step (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

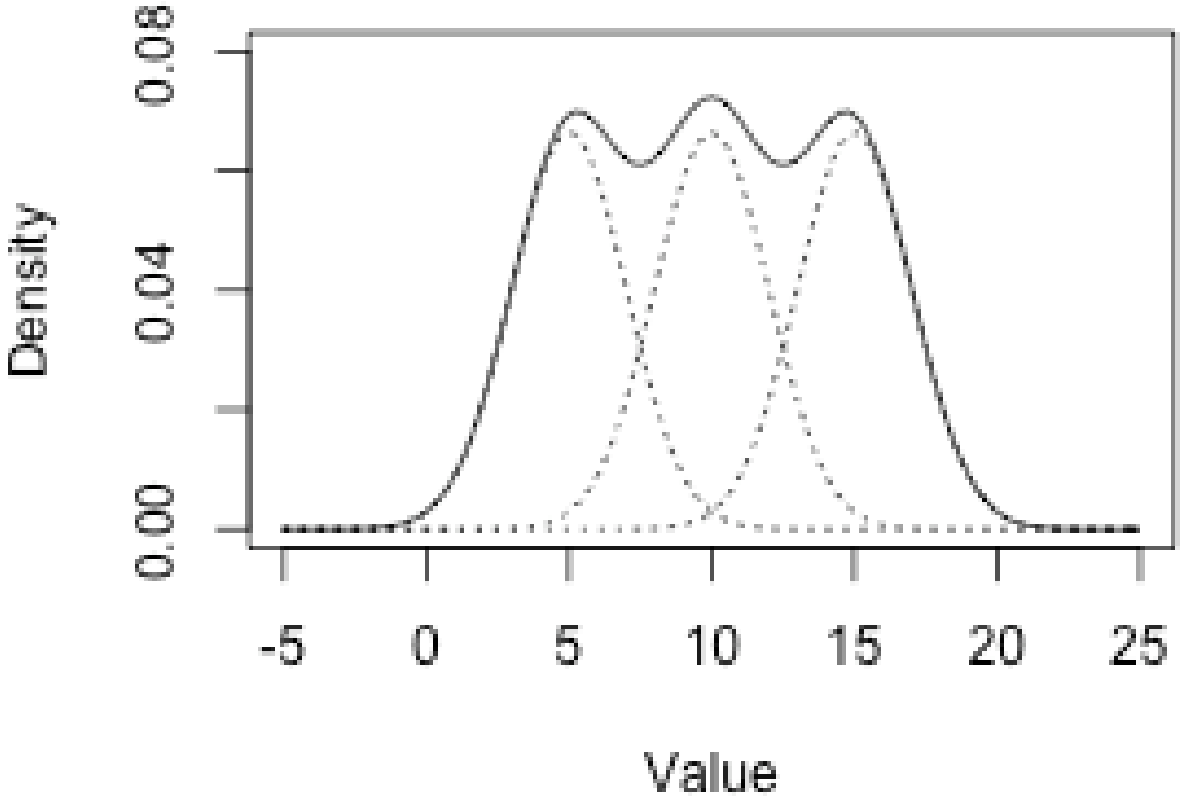
More advanced strategy : Brent's algorithm

- 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

Multidimensional Optimization : A mixture distribution



A general mixture distribution

$$p(x; \pi, \phi, \eta) = \sum_{i=1}^{k} \pi_i f(x; \phi_i, \eta)$$

- x observed data
- π mixture proportion of each component
- f the probability density function
- ϕ parameters specific to each component
- η parameters shared among components
- k numer of mixture components

Problem : Maximum Likelihood Estimation

Finding Maximum-likelihood

Find parameters that maximizes the likelihood of the entire sample

$$L = \prod_i p(x_i|\pi, \phi, \eta)$$

Calculating in log-space

Or equivalently, consider log-likelihood to avoid underflow

$$l = \sum_i \log p(x_i|\pi, \phi, \eta)$$

Gaussian MLE in single-dimensional space

$$p(x; \mu, \sigma^2) = \mathcal{N}(x; \mu, \sigma^2)$$

Given x, what is the MLE parameters of μ and σ^2?

Gaussian MLE in single-dimensional space

$$p(x; \mu, \sigma^2) = \mathcal{N}(x; \mu, \sigma^2)$$

Given x, what is the MLE parameters of μ and σ^2?

- Analytical solution does exist
- $\hat{\mu} = \sum_{i=1}^{n} x_i / n$
- $\hat{\sigma}^2 = \sum_{i=1}^{n} (x_i - \hat{\mu})^2 / n$

MLE in Gaussian mixture

Parameter estimation in Gaussian mixture

- No analytical solution
- Numerical optimization required
- Multi-dimensional optimization problem
  - $\mu_1, \mu_2, \cdots, \mu_k$
  - $\sigma_1^2, \sigma_2^2, \cdots, \sigma_k^2$

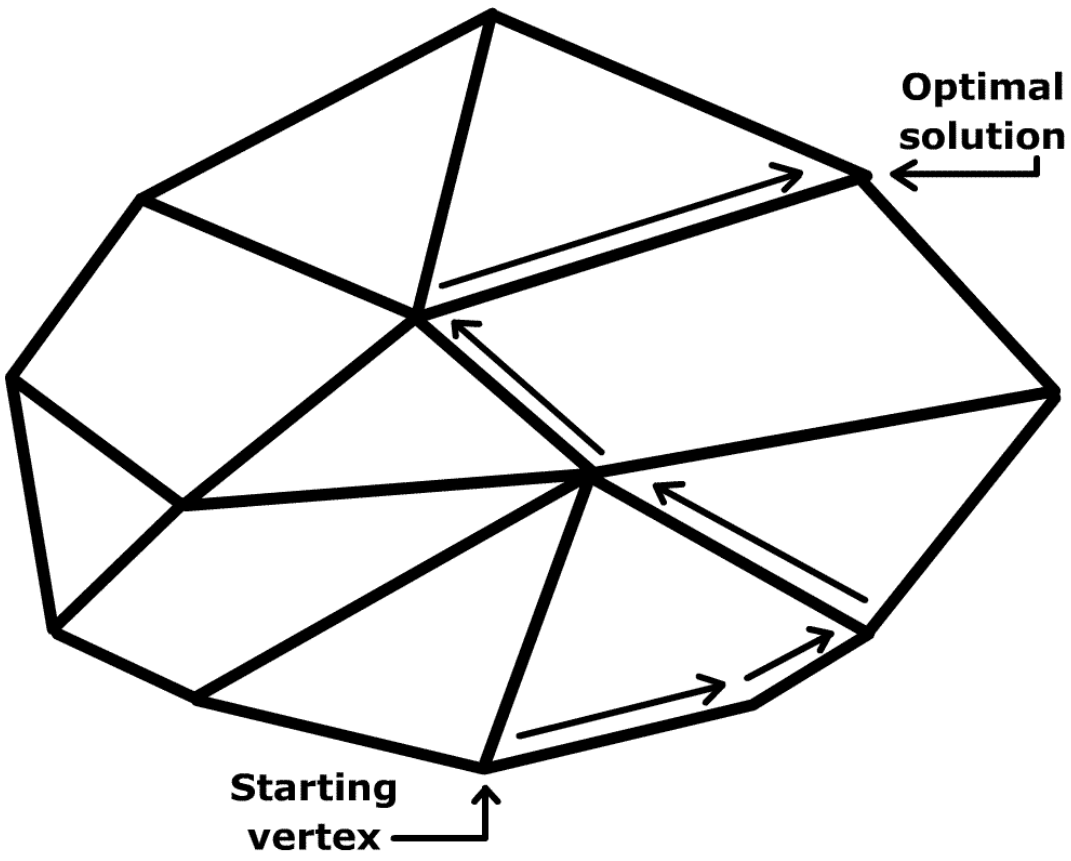
Possible approaches

- Simplex Method
- Expectation Maximization
- Markov-Chain Monte Carlo

The Simplex Method

- Calculate likelihoods at simplex vetices
  - Geomtric shape with $k+1$ corners
  - A triangle in $k=2$ dimensions
- Simplex *crawls*
  - Towards minimum
  - Away from maximum
- Probably the most widely used optimization method

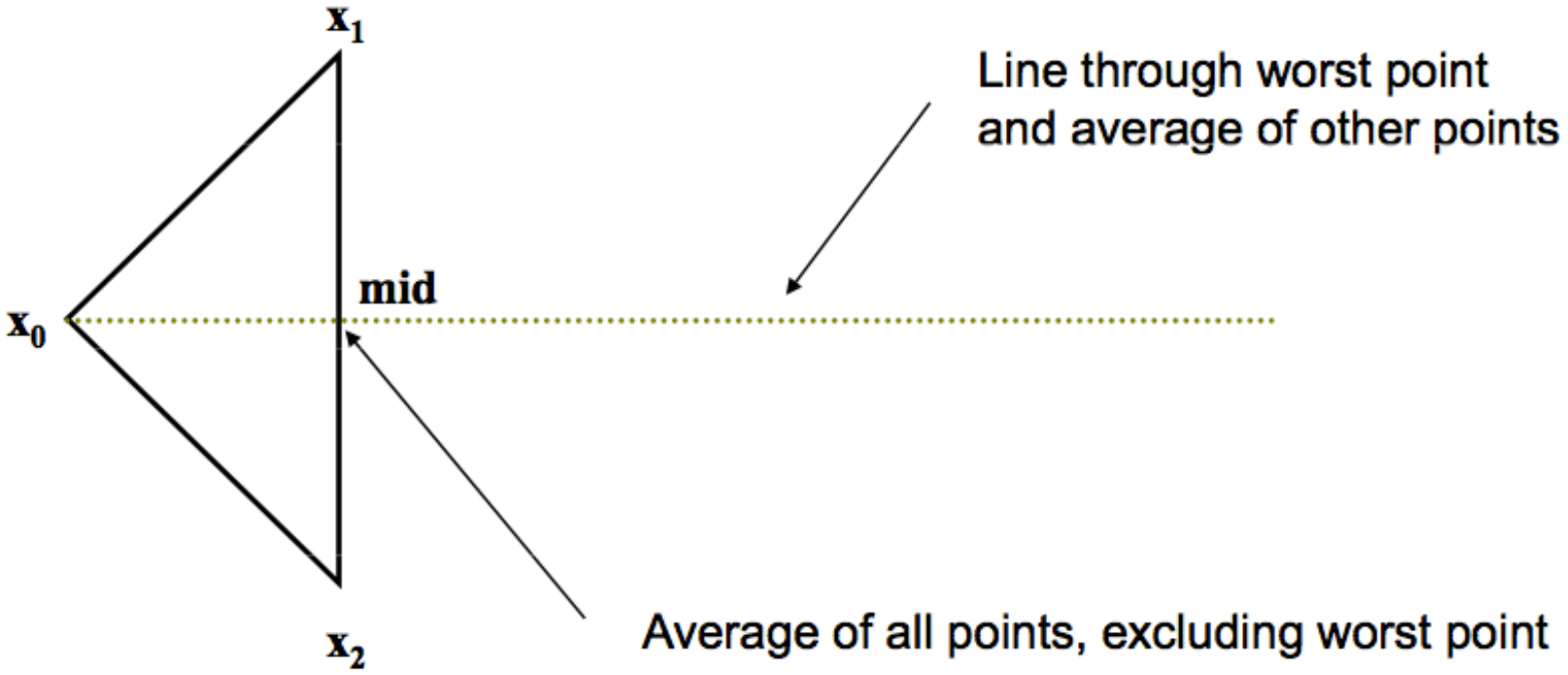
How the Simplex Method Works



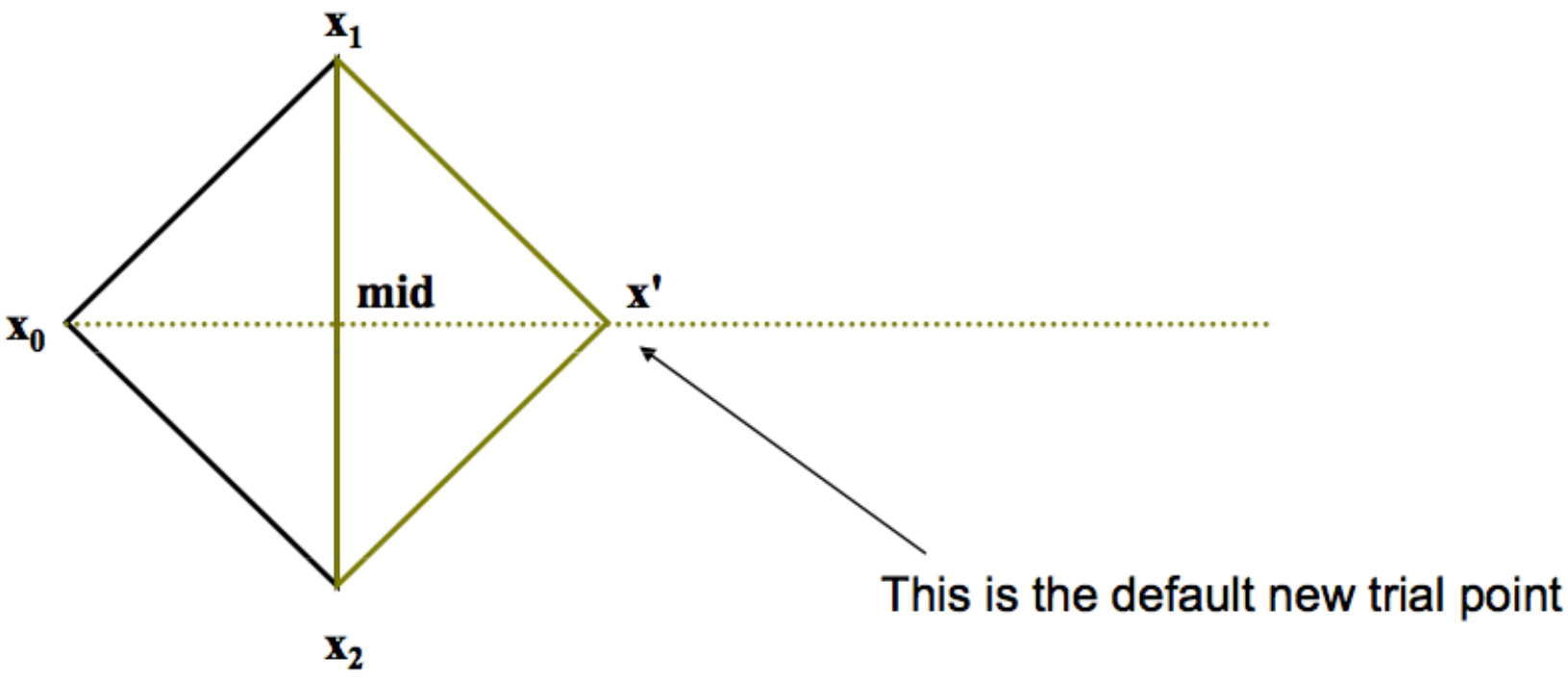
Simplex Method in Two Dimensions

- Evaluate functions at three vertices
  - The highest (worst) point
  - The next highest point
  - The lowest (best) point
- Intuition
  - Move away from high point, towards low point

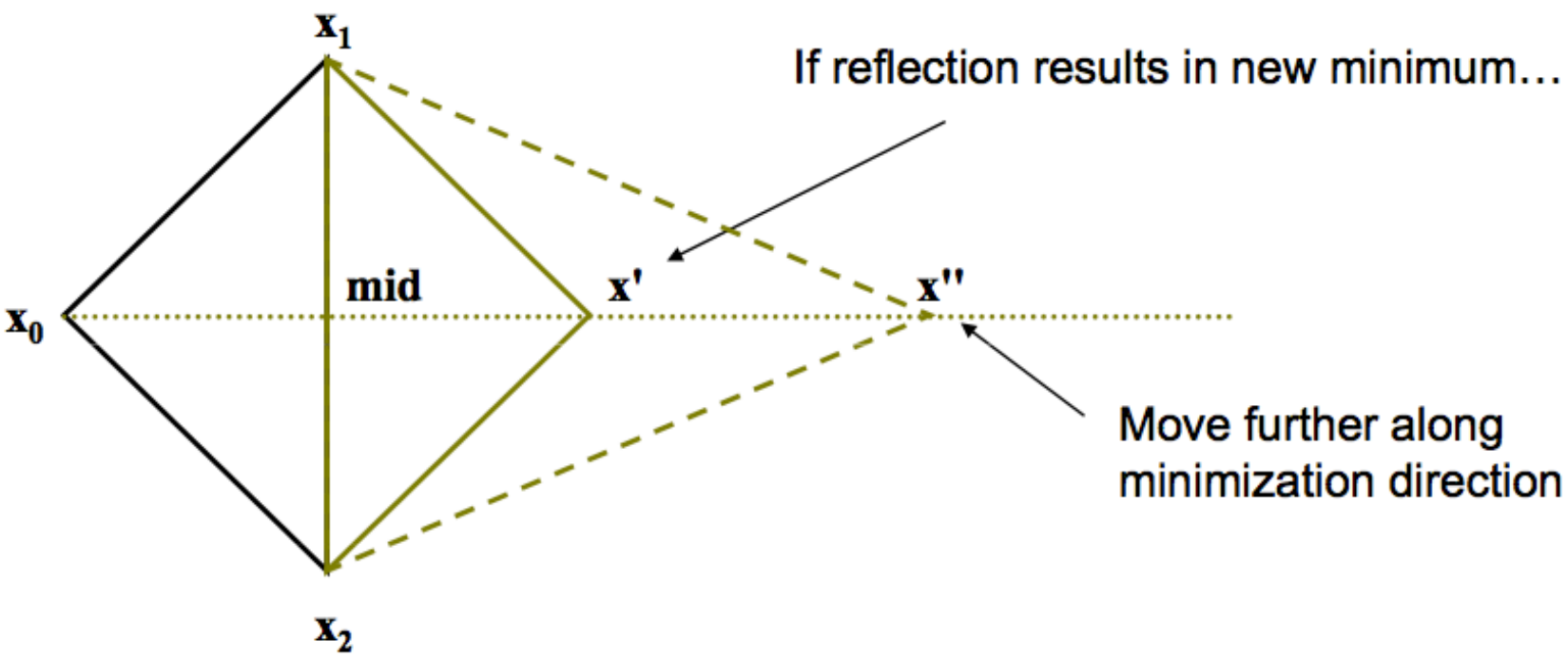
Direction for Optimization



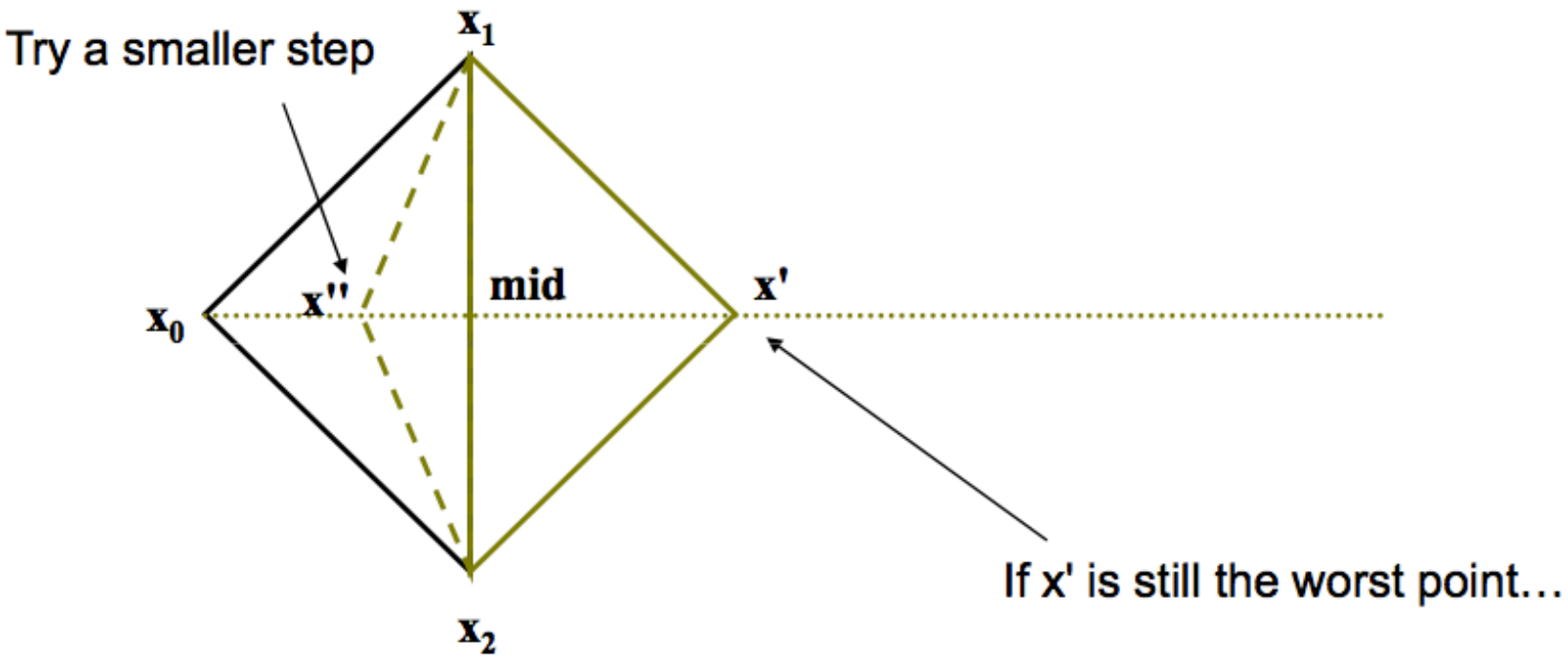
Reflection



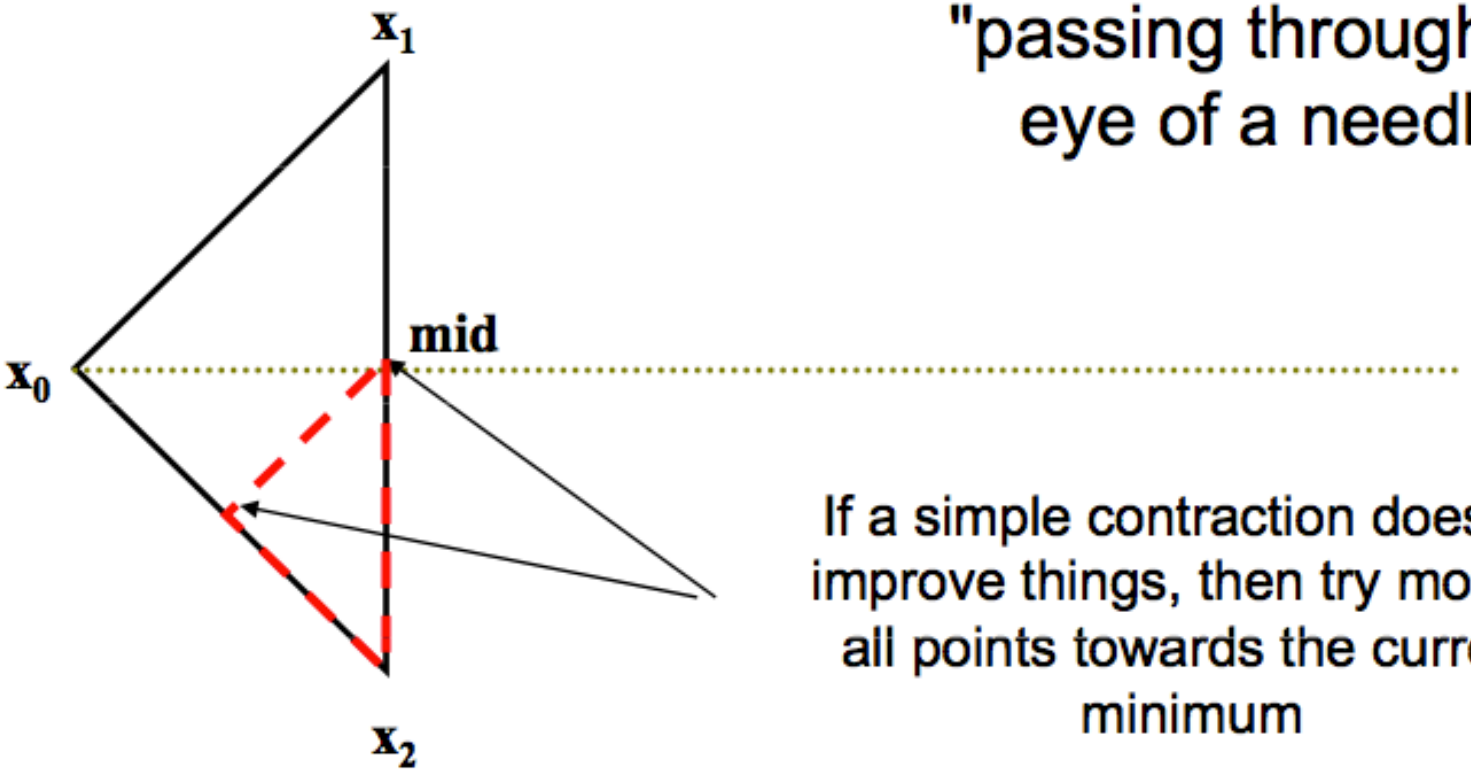
Reflection and Expansion



Contaction (1-dimension)



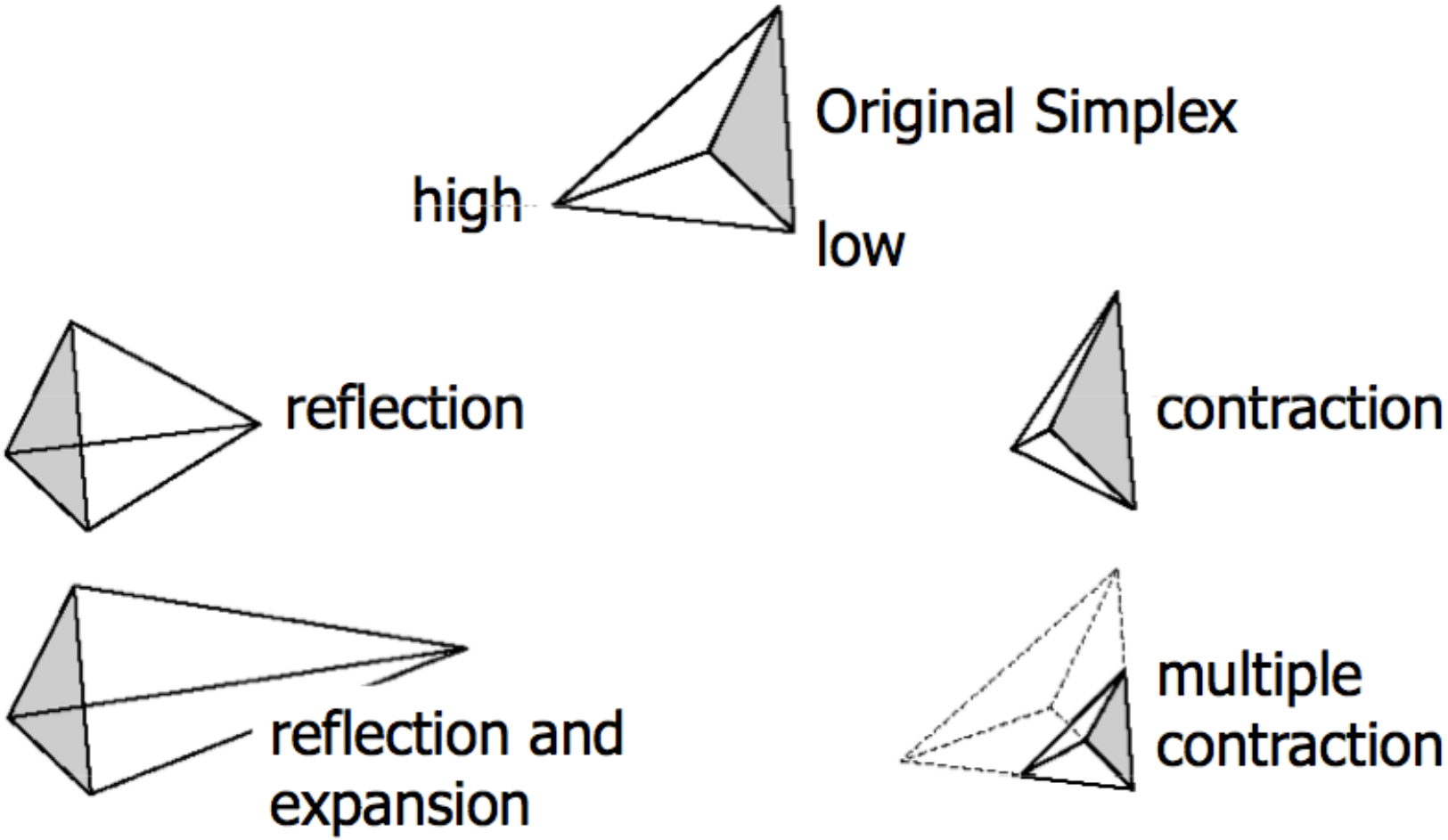
Contaction



"passing through the eye of a needle"

If a simple contraction doesn't improve things, then try moving all points towards the current minimum

Summary : The Simplex Method



Today

- Single-dimensional minimization
  - Minimization using Parabola
  - Adaptive minimization using parabola and golden search
  - A taste of Brent's method
- Multi-dimensional optimization
  - Gaussian mixture example
  - Simplex algorithm

Upcoming lectures

Next Lecture

- Special lecturer : Mary Kate Trost
- Practical lessons in C++

Next week

- Details of simplex algorithm
- Expectation-Maximization algorithm