# 1.204 Lecture 22

**Unconstrained nonlinear optimization:**
**Amoeba**
**BFGS**
**Linear programming: Glpk**

## Multiple optimum values

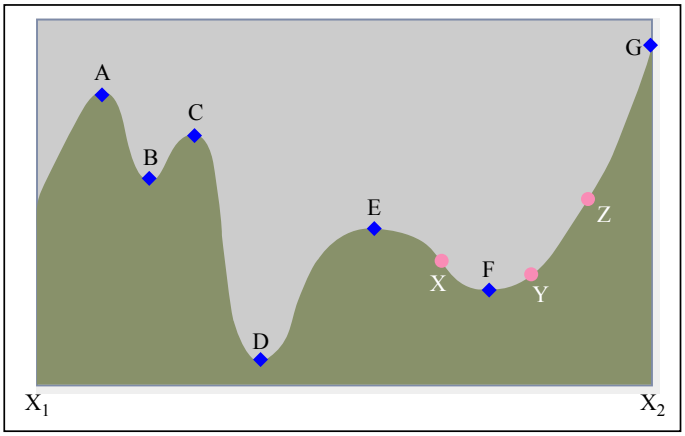



Figure by MIT OpenCourseWare.

**Heuristics to deal with multiple optima:**
- **Start at many initial points. Choose best of optima found.**
- **Find local optimum. Take a step away from it and search again.**
- **Simulated annealing takes 'random' steps repeatedly**

**From Press**

## Nonlinear optimization

- Unconstrained nonlinear optimization algorithms generally use the same strategy as unconstrained
  - Select a descent direction
  - Use a one dimensional line search to set step size
  - Step, and iterate until convergence
- Constrained optimization used the constraints to limit the maximum step size
  - Unconstrained optimization must select maximum step size
  - Step size is problem-specific and must be tuned
- Memory requirements are rarely a problem
  - Convergence, accuracy and speed are the issues

## Family of nonlinear algorithms

- Amoeba (Nelder-Mead) method
  - Solves nonlinear optimization problem directly
  - Requires no derivatives or line search
  - Adapts its step size based on change in function value
- Conjugate gradient and quasi-Newton methods
  - Require function, first derivatives* and line search
  - Line search step size adapts as algorithm proceeds
- Newton-Raphson method (last lecture)
  - Used to solve nonlinear optimization problems by solving set of first order conditions
  - Uses step size dx that makes f(x+dx)= 0. Little control.
    - 'Globally convergent' Newton variant has smaller step size
  - Needs first and second derivatives (and function)

## Choosing among the algorithms

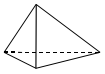
- **Amoeba is simplest, most robust, slowest**
  - **"Crawls downhill with no assumptions about function"**
  - **No derivatives required**
- **Conjugate gradient (Polak-Ribiere) (not covered)**
  - **Need first derivatives**
  - **Less storage than quasi-Newton but less accuracy**
- **Quasi-Newton (Davidon-Fletcher-Powell or Broyden-Fletcher-Goldfarb-Shanno)**
  - **Standard version uses first derivatives**
  - **Variation computes first derivatives numerically**
  - **Better than conjugate gradient for most problems**
- **Newton-Raphson**
  - **Needs function, first and second derivatives**
  - **Simplest code but not robust or flexible**
  - **Use amoeba if you want a simple approach**

## Amoeba algorithm

- **The easiest algorithm for unconstrained nonlinear optimization is known as Nelder-Mead or "the amoeba"**
- **It is very different**
  - **It requires only function evaluations**
    - **No derivatives are required**
  - **It is less efficient than the line search algorithms**
    - **But it tends to be robust (line methods are temperamental)**
  - **It is short (~150 lines) and relatively easy to implement**
  - **Works in problems where derivatives are difficult:**
    - **Fingerprint matching**
    - **Models of brain function**
  - **We'll use logit demand model estimation as test case for all the algorithms today**

# Amoeba steps

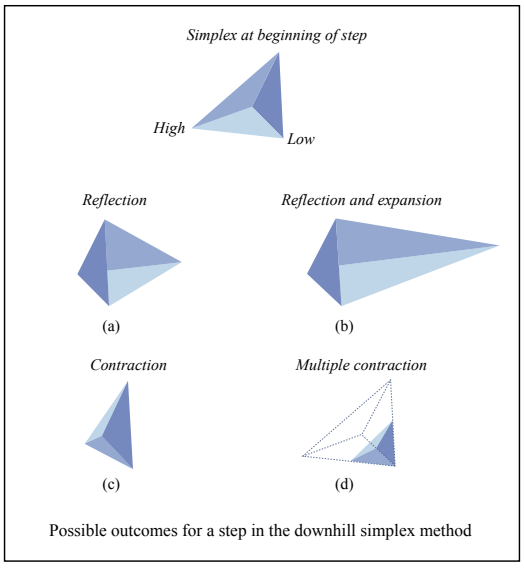
- Simplex is volume defined by n+1 points in n dimensions
  - In 3-D, it is a tetrahedron or pyramid
- Select a starting guess at point $P_0$
  - Set other points of simplex as $P_i = P_0 + \Delta e_i$



- Take a series of steps
  - Most steps move point of simplex where function is highest ("highest point"): "reflection"
    - Conserve volume of simplex -> avoid degeneracy
  - Where function is flat, method expands simplex to take larger steps: "expansion and reflection"
  - When it reaches a "valley floor", simplex "contracts" itself in transverse direction and tries to ooze down the valley
  - If trying to pass through "eye of needle" it "contracts itself in all directions" around its lowest (best) point

From Press et al

# Amoeba steps




Possible outcomes for a step in the downhill simplex method

Figure by MIT OpenCourseWare.

From Press et al

## Amoeba pseudocode: minimization

- Start at initial guess
  - Determine which point is highest by looping over simplex points and evaluating function at each
  - If difference between highest and lowest is small, return
- Otherwise ooze (iterate):
  - Reflect by factor= -1 through face of simplex from high point
    - If this is better than low point, reflect/expand by factor of 2
    - If this is worse than second highest, contract by 2 in this direction
    - If this is worst point, contract in all directions around lowest point
  - Select new face based on new high point and reflect again
  - Terminate if difference between highest and lowest points is small
    - Or terminate at maximum iterations allowed

## Amoeba termination criteria

- All nonlinear optimization algorithm termination criteria are difficult
  - Terminate when step size is small (~$10^{-8}$ with doubles)
  - Change in function value is small (~$10^{-14}$ with doubles)
- Termination can occur at a local minimum
  - Restart amoeba at a minimum it found
    - Reset initial simplex using $P_i = P_0 + \Delta e_i$ ,
    - Don't use simplex that existed at termination
- Code is in download:

```
public Amoeba(double ftol)

public double[] minimize(double[] point, double del,
MathFunction3 mf3)
// And other optional methods
```

  - This is very easy; code ran first time on demand model
    - Experiment with starting point and del, but it's usually easy

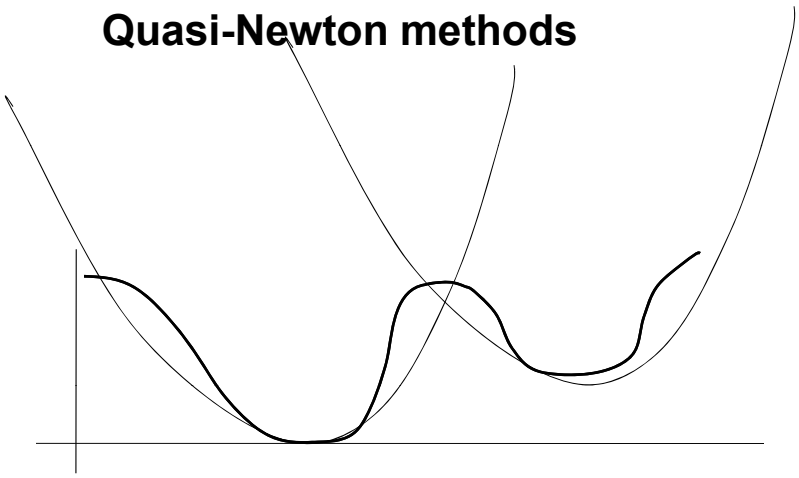
## AmoebaTest

```
public class AmoebaDemandTest {
   public static void main(String[] args) {
        double[][] x= { {1, 52.9 - 4.4},
                        {1, 4.1 - 28.5},  // Etc. };
        double[] y= {0, 0, 1, 0, 0, 1, 1, 0, 0, 0, 0, 1, 1, 0,
                1, 1, 0, 1, 1, 0, 1};
        // Almost identical to DemandModel from last lecture
        // Implements MathFunction3, which has method func2()
        // func2() returns -logLikelihood()
        DemandModelAmoeba d= new DemandModelAmoeba(x, y);
        double[] beta= {0, 0};               // Initial guess
        double log0= d.func2(beta);
        double[] initialPoint= {0.0, 0.0};
        double initialDelta= 0.1;
        double ftol= 1E-14;
        Amoeba a= new Amoeba(ftol);
        beta= a.minimize(initialPoint, initialDelta, d);
        double logB= d.func2(beta);
        double[][] jacobian= d.jacobian(beta);
        d.print(log0, logB, beta, jacobian);
}  }    // Output identical to last lecture example. 116 evals
```

## Quasi-Newton methods (DFP, BFGS)

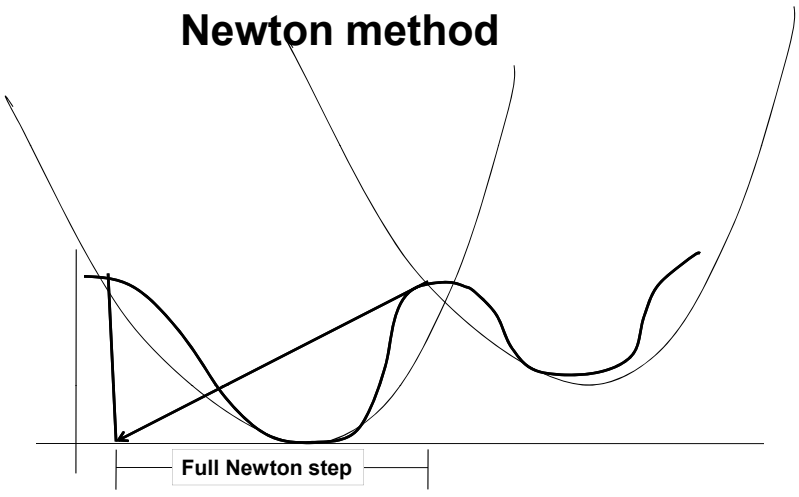
- We used a similar method to BFGS in constrained optimization:
  - Find derivatives
  - Find direction that yields maximum estimated objective function change
  - Use line search to find optimal step size
  - Move, and repeat
- DFP and BFGS are essentially the same
  - One additional ‘correction term’ in BFGS
  - Treatment of roundoff errors, tolerances is different
  - Empirically, it seems BFGS is better than DFP

## Quasi-Newton methods



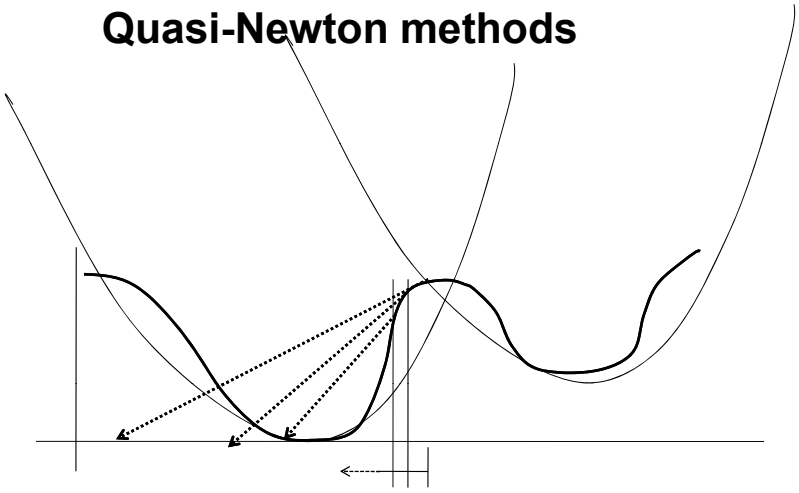
**Split problem into two minimization problems, each with a "quadratic envelope"**
**You must understand your problem well enough to do this**

## Newton method




**If the minimum region is narrow or twisty, it is hard to get down into it.**
**Full Newton steps give little control. (Amoeba just munches along)**

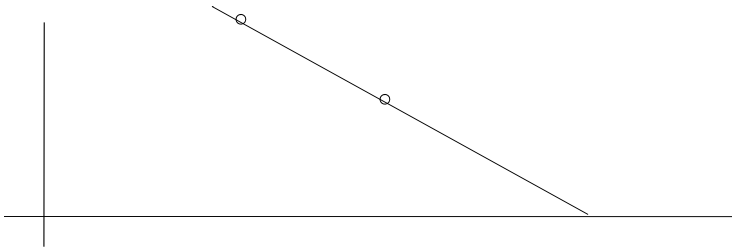
# Quasi-Newton methods



Quasi Newton steps

BFGS takes a fraction of the Newton step, so that f(x) decreases at some minimum rate proportional to the average decrease

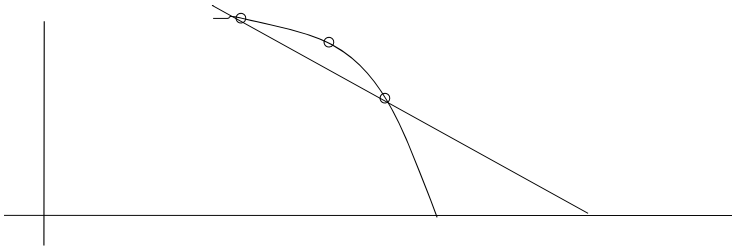
# High order derivatives



We may be tempted to use higher derivatives to fit our nonlinear functions. More terms in the Taylor series expansion mean a higher degree polynomial fit, but using higher order derivatives is difficult because they are "stiff"

This is the challenge of nonlinear methods: use only low order derivatives to explore complex surfaces. There aren't many general ways to do this. Solutions are problem-specific but use BFGS or other general algorithm: Understand problem regions; have good starting point; understand surface

# High order derivatives



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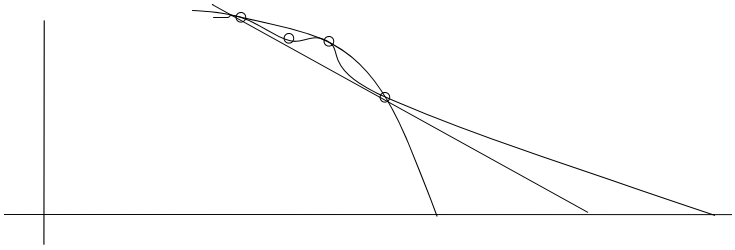
# High order derivatives



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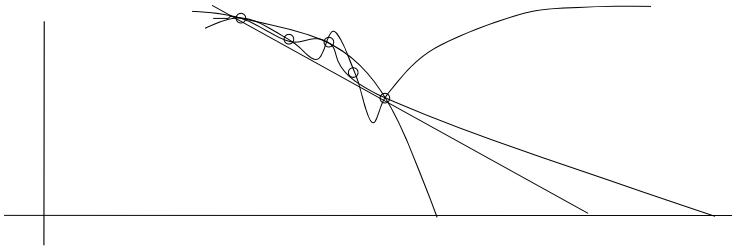
## High order derivatives



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## BFGS

Take a point P as origin. Approximate f using Taylor series:

$$f(x) = f(P) + \sum_i \frac{\partial f}{\partial x_i} x_i + \frac{1}{2} \sum_{i,j} \frac{\partial^2 f}{\partial x_i x_j} x_i x_j$$

$$\approx c - b \cdot x + \frac{1}{2} x \cdot A \cdot x$$

*where*

$$c = f(P)$$

$$b = -\nabla f \,|_P$$

$$[A]_{ij} = \frac{\partial^2 f}{\partial x_i x_j} |_P$$

A is the Hessian matrix. Gradient of f is:

$$\nabla f = A \cdot x - b$$

## BFGS, p.2

BFGS constructs a sequence of matrices $H_i$ such that:

$\lim_{i->\infty} H_i = A^{-1}$

At point $x_i$, using a Taylor series again

$$f(x) = f(x_i) + (x - x_i) \cdot \nabla f(x_i) + \frac{1}{2}(x - x_i) \cdot A \cdot (x - x_i)$$

To find a minimum, find a zero of the gradient of f(x):

$$\nabla f(x) = \nabla f(x_i) + A \cdot (x - x_i)$$

Newton's method sets $\nabla f(x) = 0$ to find the next point:

$$(x - x_i) = -A^{-1} \cdot \nabla f(x_i)$$

## BFGS, p.3

- **Newton's method, far from the minimum, can project us to points x where f(x) is greater than the current value**
  - **Large steps based on a quadratic approximation will not necessarily lead to improvements in ill-behaved function**
  - **BFGS does a line search along the Newton direction**
  - **It finds a point at which the objective has decreased**
  - **This point is used to update the Hessian (which is a matrix of second derivatives)**
  - **The Hessian is based on the previous Hessian and a set of correction terms based on ▼f , x and $x_i$**
  - **See Numerical Recipes for BFGS updating formula**
    - **Proofs are difficult**

## BFGS, p.4

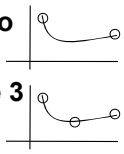
- The series of $H_i$ converge to $A^{-1}$ while guaranteeing movement downhill
  - Convergence takes N steps if f is quadratic
- The algorithm is sensitive to variable scaling:
  - Step length must be tuned
  - Scale variables to stay in "low" range of double values
- The algorithm is not too sensitive to the accuracy of the line search

## BFGS dfpmin() pseudocode

- Compute function, gradient at start point P
- Initialize inverse Hessian to identity matrix
- Find initial descent direction along gradient
- Loop until convergence
  - Line search along direction to find decrease (not min)
  - Update gradient and line direction
  - Check if change in x is small enough to converge
  - Check if gradient is close enough to 0 to converge
  - Compute difference in gradients, x for BFGS update
  - Calculate next direction
- If iteration limit reached, terminate

## BFGS lnsrch() pseudocode

- Takes point, function and gradient value at point, and direction (line) to search along as input
- Finds new point with lower function value
  - Finding minimum along line requires too much computation
  - Finding any point whose f is less than current isn't good enough either; we may take too many steps
  - We find a point where the average decrease from the current point is a fraction of the gradient projection
  - We require a minimum step size so we don't stall
  - We use a quadratic interpolation of f along the line to choose the first new point
  - We then use a cubic interpolation, now that we have 3 points ( f(0), f(1) and f(m)) for remaining points



## BFGS code

- First code set
  - BFGS: constructor, dfpmin(), lnsrch()
  - MathFunction4: interface with func(), df() [gradient]
  - DemandModelBFGS: Almost same as in Newton
  - DemandModelBFGSTest: Almost same as in Newton
- Second code set
  - Same BFGS, MathFunction4, DemandModelBFGSTest
  - DemandModelBFGS df() method computes gradient numerically, without analytic expressions for derivatives
- Both BFGS implementations converge quickly on same logit model coefficients as Newton
  - Code is subtle, especially interaction between dfpmin() and lnsrch().

## BFGSTest

```
public class DemandModelBFGSTest {
   public static void main(String[] args) {
        double[][] x= { {1, 52.9 - 4.4},
                        {1, 4.1 - 28.5},  // Etc. };
        double[] y= {0, 0, 1, 0, 0, 1, 1, 0, 0, 0, 0, 1, 1, 0,
                1, 1, 0, 1, 1, 0, 1};
        // Almost identical to DemandModel from last lecture
        // Implements MathFunction4, with func() and df()
        DemandModelBFGS d= new DemandModelBFGS(x, y);
        double[] beta= {0, 0};                // Initial guess
        double log0= d.func2(beta);
        double gtol= 1E-14;
        BFGS b= new BFGS(d, gtol);
        double logB= b.dfpmin(beta);
        double[][] jacobian= d.jacobian(beta);
        d.print(log0, logB, beta, jacobian);
}  } // Output identical to last lecture example. 10 iterations
```

## Nonlinear method performance

| Method | Iterations | Function evaluations |
|---|---|---|
| Newton | 6 | $6n^2 = 24$ |
| BFGS | 10 or 11 | 10n= 20 |
| Amoeba | 116 | 116 |

**This example is illustrative only, based on our logit test case.**
**n is the number of variables (coefficients in our test case).**
**As n increases, amoeba performance is relatively more competitive**

**Amoeba and BFGS have better convergence and precision than Newton**

## Summary: nonlinear continuous methods

- Note the similarities in solving discrete and continuous problems
  - Starting solution is null or {0, 0, 0, …}
    - Or a good guess or greedy if we need a good first guess
  - Choose initial decision or initial direction/gradient
  - Find initial solution at stage/branch or Newton/other step
  - Look for better solution locally through greedy/branching/stages or new gradient
  - Or globally through branch-and-bound/dynamic programming or with advanced continuous methods
    - Simulated annealing, multiple restarts
  - Terminate when:
    - Local or global optimum found, or
    - Upper and lower bound close enough, or
    - Maximum iterations reached

## Linear programming

- Linear programming has a linear objective function and linear constraints
- Used as a subproblem several times already:
  - Convex combinations (lecture 18)
  - Homework 8 transit network optimization
  - Network equilibrium used shortest path algorithm as a special case of linear programming
  - Often used as subproblem in branch and bound algorithms
    - We used shortest paths in our warehouse branch and bound as a special case of linear programming
    - See any integer programming text for a list of problems that use linear programming as a subproblem

## Linear programming

maximize

$$Z = 10x_1 + 6x_2 + 4x_3$$

subject to

$$\begin{aligned} x_1 + x_2 + x_3 &\leq 100 \\ 10x_1 + 4x_2 + 5x_3 &\leq 600 \\ 2x_1 + 2x_2 + 6x_3 &\leq 300 \end{aligned}$$

where all variables are non-negative

$$x_1 \geq 0,\ x_2 \geq 0,\ x_3 \geq 0$$

**From GLPK manual**



## Linear programming standard form

maximize

$$Z = 10x_1 + 6x_2 + 4x_3$$

subject to

$$\begin{aligned} p &= x_1 + x_2 + x_3 \\ q &= 10x_1 + 4x_2 + 5x_3 \\ r &= 2x_1 + 2x_2 + 6x_3 \end{aligned}$$

and bounds of variables

$$\begin{aligned} -\infty < p \leq 100 \quad & 0 \leq x_1 < +\infty \\ -\infty < q \leq 600 \quad & 0 \leq x_2 < +\infty \\ -\infty < r \leq 300 \quad & 0 \leq x_3 < +\infty \end{aligned}$$

**Formulate constraints as a set of equations and a set of bounded variables. This is easy to translate to the simplex tableau used for the computations.**

## LP program, p.1

```
import org.gnu.glpk.*;      // Glpk starts numbering at 1, not 0
public class LP {
   public static void main(String[] args) {
        int[] ia= new int[1+1000];    // Row index of coefficient
        int[] ja= new int[1+1000];    // Col index of coefficient
        double[] ar= new double[1+1000];      // Coefficient
        double z, x1, x2, x3;         // Obj value, unknowns
        GlpkSolver solver = new GlpkSolver();
        solver.setProbName("sample");
        solver.setObjDir(GlpkSolver.LPX_MAX); // Maximization
        solver.addRows(3);
        solver.setRowName(1, "p");
        solver.setRowBnds(1, GlpkSolver.LPX_UP, 0.0, 100.0);
        solver.setRowName(2, "q");
        solver.setRowBnds(2, GlpkSolver.LPX_UP, 0.0, 600.0);
        solver.setRowName(3, "r");
        solver.setRowBnds(3, GlpkSolver.LPX_UP, 0.0, 300.0);
```

## LP program, p.2

```
        solver.addCols(3);
        solver.setColName(1, "x1");
        solver.setColBnds(1, GlpkSolver.LPX_LO, 0.0, 0.0);
        solver.setObjCoef(1, 10.0);
        solver.setColName(2, "x2");
        solver.setColBnds(2, GlpkSolver.LPX_LO, 0.0, 0.0);
        solver.setObjCoef(2, 6.0);
        solver.setColName(3, "x3");
        solver.setColBnds(3, GlpkSolver.LPX_LO, 0.0, 0.0);
        solver.setObjCoef(3, 4.0);
        ia[1] = 1; ja[1] = 1; ar[1] = 1.0; /* a[1,1] = 1 */
        ia[2] = 1; ja[2] = 2; ar[2] = 1.0; /* a[1,2] = 1 */
        ia[3] = 1; ja[3] = 3; ar[3] = 1.0; /* a[1,3] = 1 */
        ia[4] = 2; ja[4] = 1; ar[4] = 10.0; /* a[2,1] = 10 */
        ia[5] = 2; ja[5] = 2; ar[5] = 4.0; /* a[2,2] = 4 */
        ia[6] = 2; ja[6] = 3; ar[6] = 5.0; /* a[2,3] = 5 */
        ia[7] = 3; ja[7] = 1; ar[7] = 2.0; /* a[3,1] = 2 */
        ia[8] = 3; ja[8] = 2; ar[8] = 2.0; /* a[3,2] = 2 */
        ia[9] = 3; ja[9] = 3; ar[9] = 6.0; /* a[3,3] = 6 */
```

## LP program, p.3

```
        solver.loadMatrix(9, ia, ja, ar);
        solver.simplex();
        z = solver.getObjVal();
        x1 = solver.getColPrim(1);
        x2 = solver.getColPrim(2);
        x3 = solver.getColPrim(3);
        System.out.printf("\nz = %g; x1 = %g; x2 = %g; x3 = %g\n",
                z, x1, x2, x3);
    }

// Output:
// z = 733.333; x1 = 33.3333; x2 = 66.6667; x3 = 0.00000
```

## Using GLPK under WindowsXP

- Download files, documentation from http://bjoern.dapnet.de/glpk/
- Copy glpk.jar to C:\Program Files\Java\jdk1.6.0_05\jre\lib
- Copy glpk_jni.dll to the directory of project in Eclipse
- Eclipse: Project->Properties->Java Build Path. Add external JAR: glpk.jar
- Create Eclipse project, write class as usual
- See GLKP documentation (pdf). Java method names are based on C names: lpx_set_obj_dir() becomes setObjDir()
- glpk.jar uses the Java Native Interface (JNI) to create Java stubs for the C native functions in the glpk library
- You now have a callable library of linear programming routines that you can use from Java
- GLPK also has:
  - Mixed integer programming method, using branch and bound
    - Use this instead of your own B&B unless you have problem-specific pruning
  - Interior point linear programming method

# 1.204 Computer Algorithms in Systems Engineering

Spring 2010