15-780: Grad AI
Lecture 7: Optimization

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Last time, on Grad AI

Plan graphs

- A way to do propositional planning
- How to build them
  - mutex conditions for literals, actions
- How to use them
  - conversion to SAT

Optimization & Search

- Classes of optimization problem
  - LP, CP, ILP, MILP
  - algorithms for solving, and complexity
  - constraints, objective, integrality
- How to use DFID, etc. for optimization
- Definition of convexity

Bounds

- Pruning search w/ lower bounds on objective
- Stopping early w/ upper bounds
- Getting bounds from a relaxation of an optimization problem (increase feasible region)
  - particularly the LP relaxation of an ILP

Duality

- How to find dual of an LP or ILP
- Interpretations of dual
  - linearly combine constraints to get a new constraint orthogonal to objective
  - find prices for scarce resources
  - game between primal and dual players
  - correspondence faces $\Leftrightarrow$ vertices of feasible regions (doesn't include objective)

Constrained optimization

Minimization

- Unconstrained: set $\nabla f(x) = 0$
- E.g., minimize

$$f(x, y) = x^2 + y^2 + 6x - 4y + 5$$

$$\nabla f(x, y) = (2x + 6, 2y - 4)$$

$$(x, y) = (-3, 2)$$

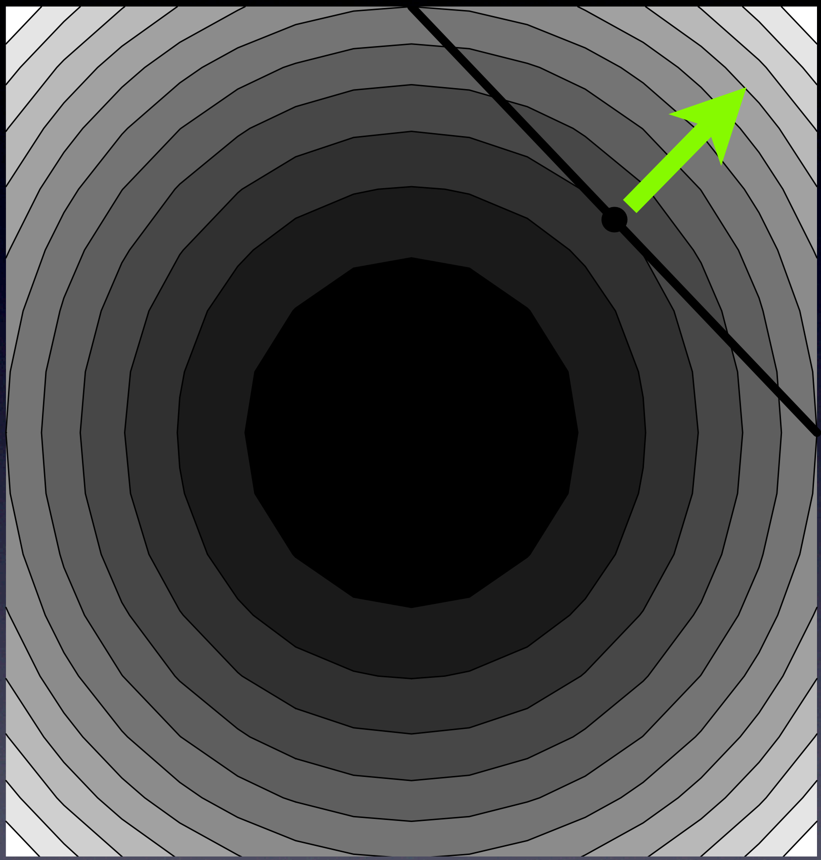
Equality constraints

- Equality constraint:

  minimize f(x) s.t. g(x) = 0

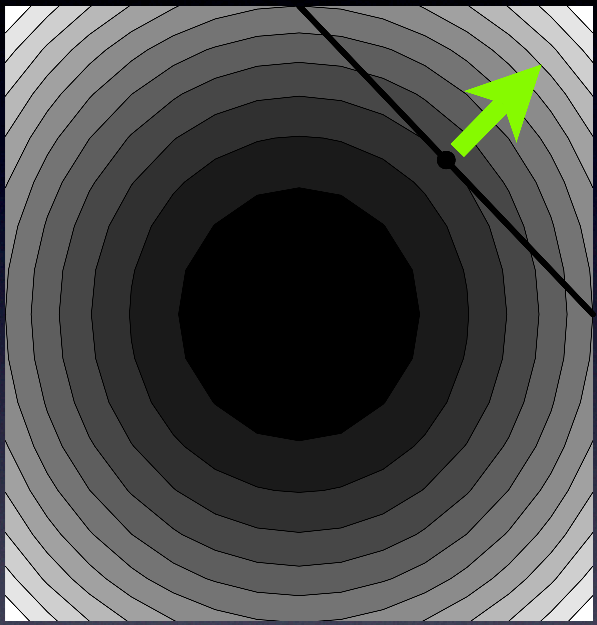
- can't just set ∇f to 0 (might violate constraint)
- Instead, want gradient along constraint's normal direction: any motion that decreases objective will violate the constraint

Example



- E.g., minimize $x^2 + y^2$ subject to $x + y = 2$

Lagrange multipliers



- Minimize f(x) s.t. g(x) = 0
- Constraint normal is ∇g
  - (1, 1) in our example
- Want ∇f parallel to ∇g
- Equivalently, want $\nabla f = \lambda \nabla g$
- λ is a **Lagrange multiplier**

More than one constraint

- With multiple constraints, use multiple multipliers:

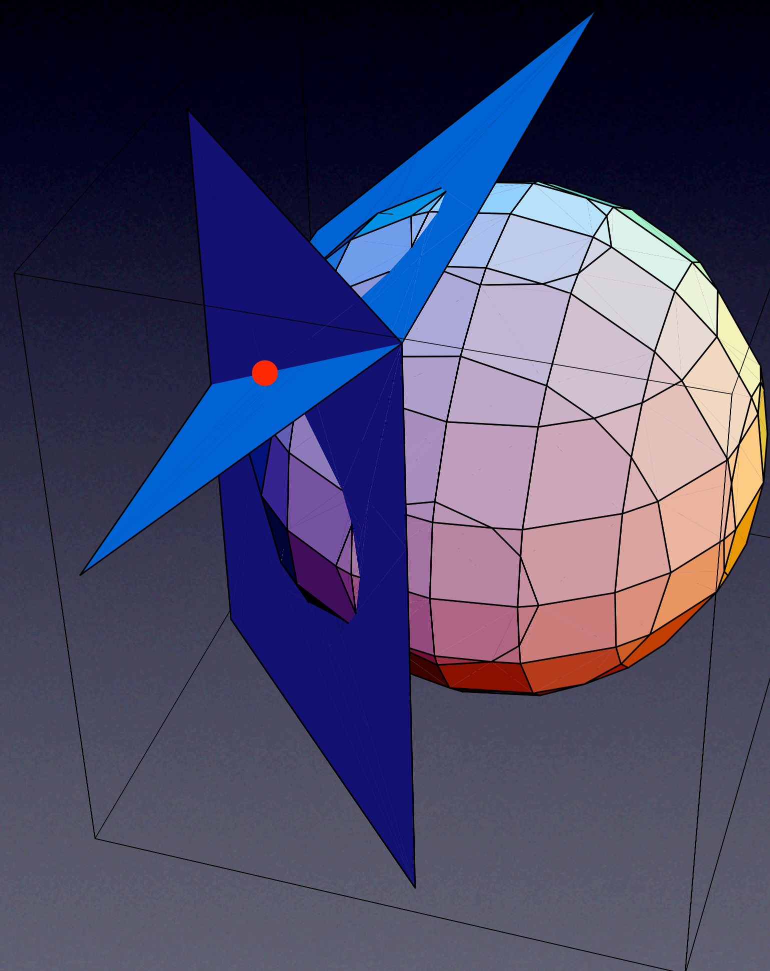
$$\min x^2 + y^2 + z^2 \text{ st}$$

$$x + y = 2$$

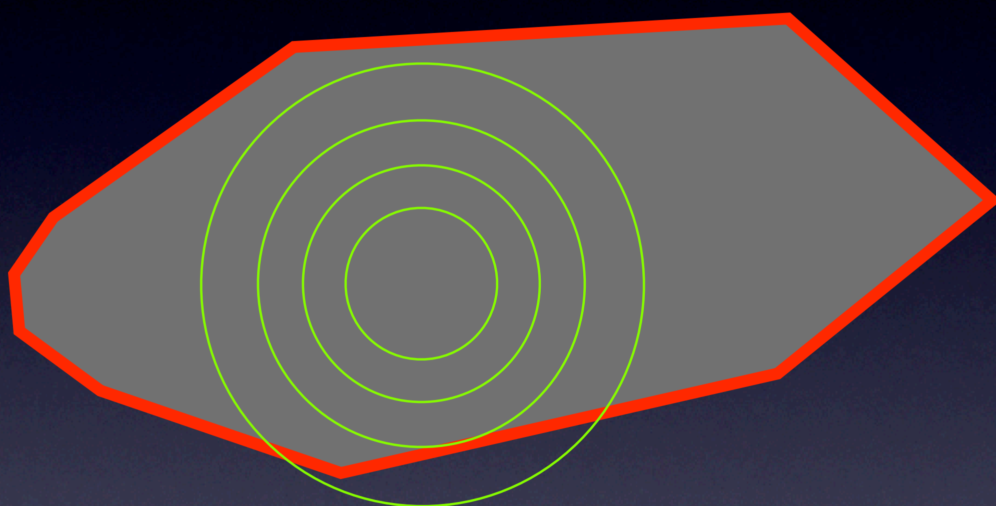
$$x + z = 2$$

$$(2x, 2y, 2z) = \lambda(1, 1, 0) + \mu(1, 0, 1)$$

Two constraints: the picture

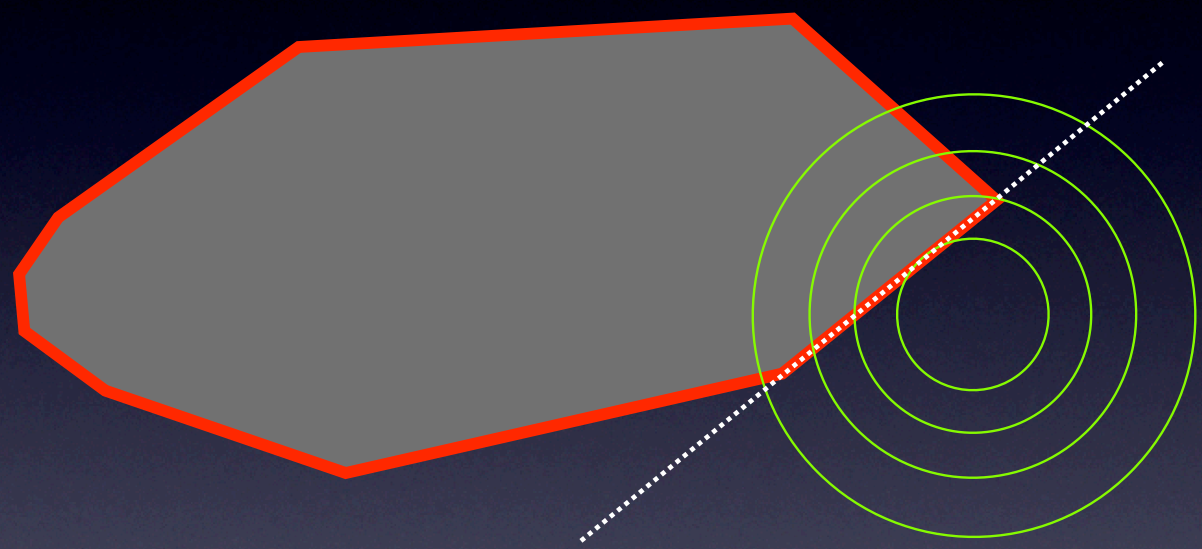


What about inequalities?



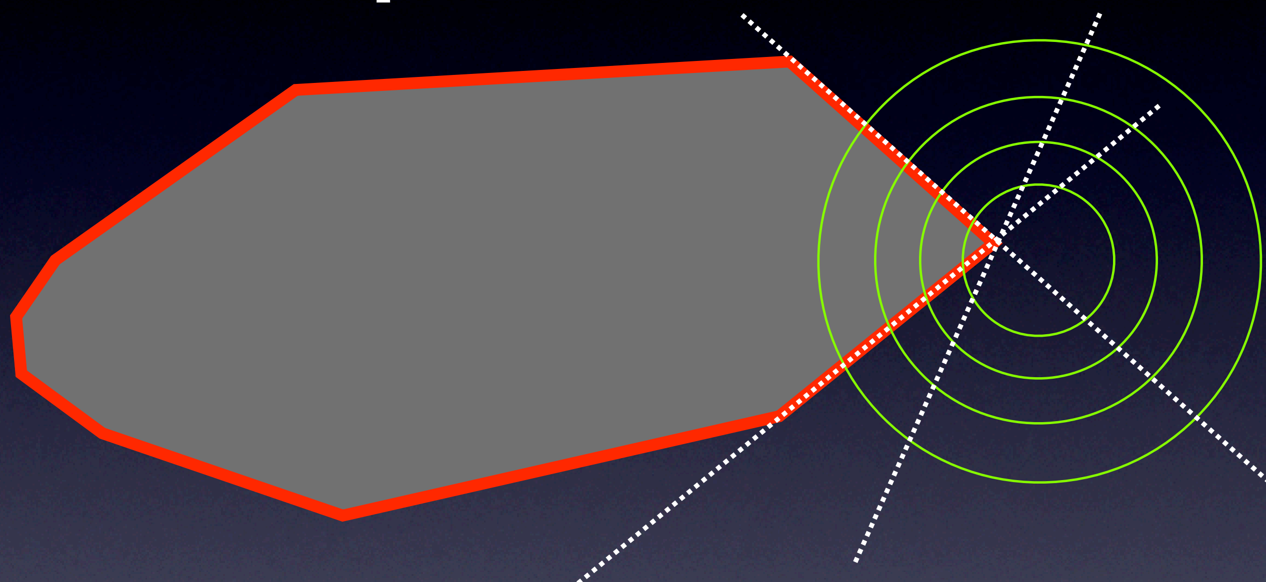
- Two cases: if minimum is in interior, can get it by setting $\nabla f = 0$

What about inequalities?



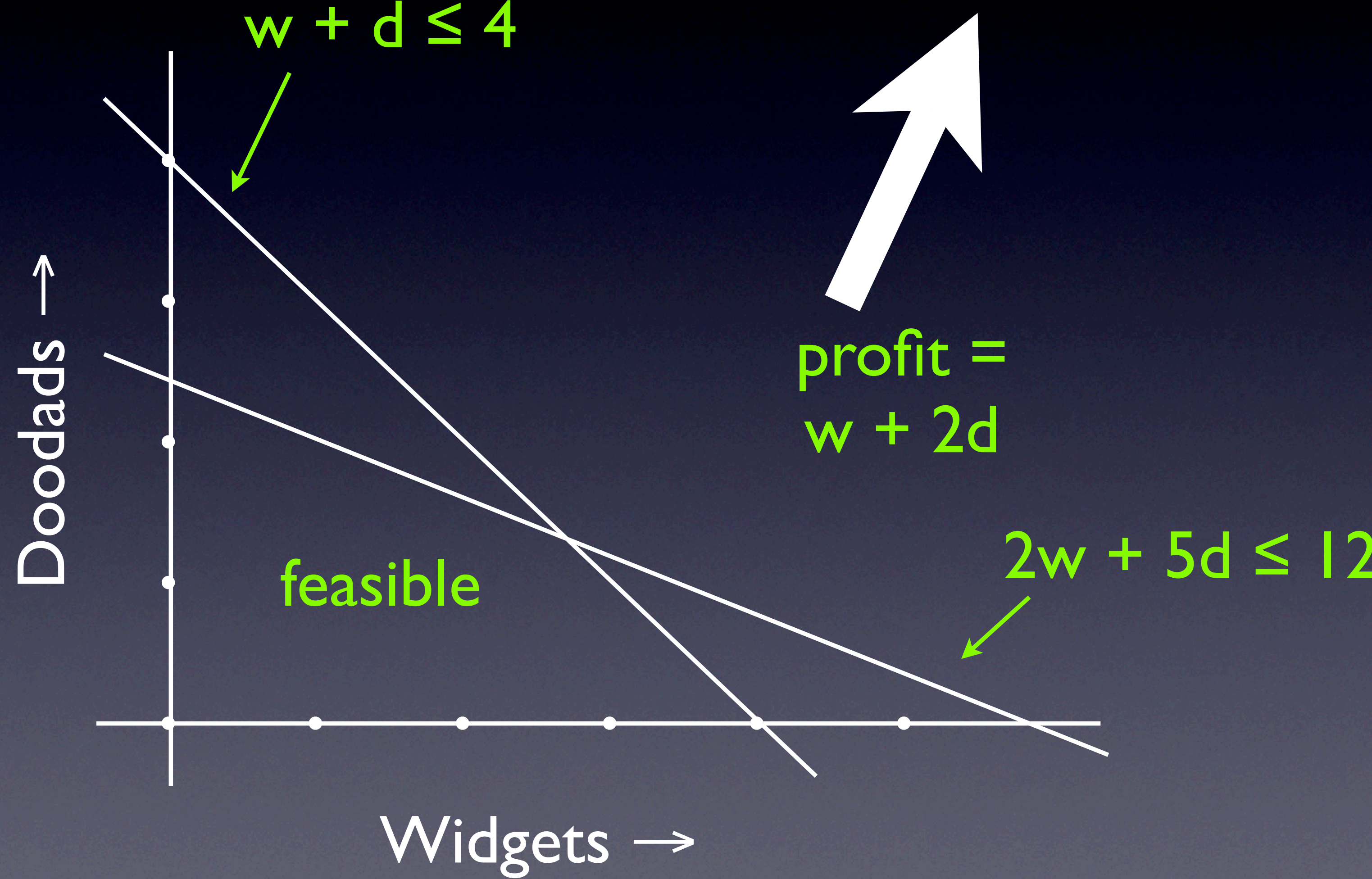
- But if minimum is on boundary, treat as if boundary were an equality constraint (use Lagrange multiplier)

What about inequalities?



- Minimum could be at a corner: two boundary constraints are active
- In n dims, up to n linear inequalities may be active (more in case of degeneracy)

Back to LP



Back to LP

$$\max\ w + 2d \text{ st}$$

$$w + d \leq 4$$

$$2w + 5d \leq 12$$

$$w, d \geq 0$$

- In LP we're minimizing linear fn subject to linear constraints
- So gradients are really easy to compute

Back to LP

- Minimum can’t* occur in interior of feasible region
- In fact we can assume it’s at a vertex
- So to find it, we must check vertices
- How many boundary vertices could there be?

Bases

- With m constraints and n variables, any subset of n constraints might be active
- So up to (m choose n) possibilities
- Given subset, easy to find corresponding vertex (solve linear system)
- Subset = **basis**

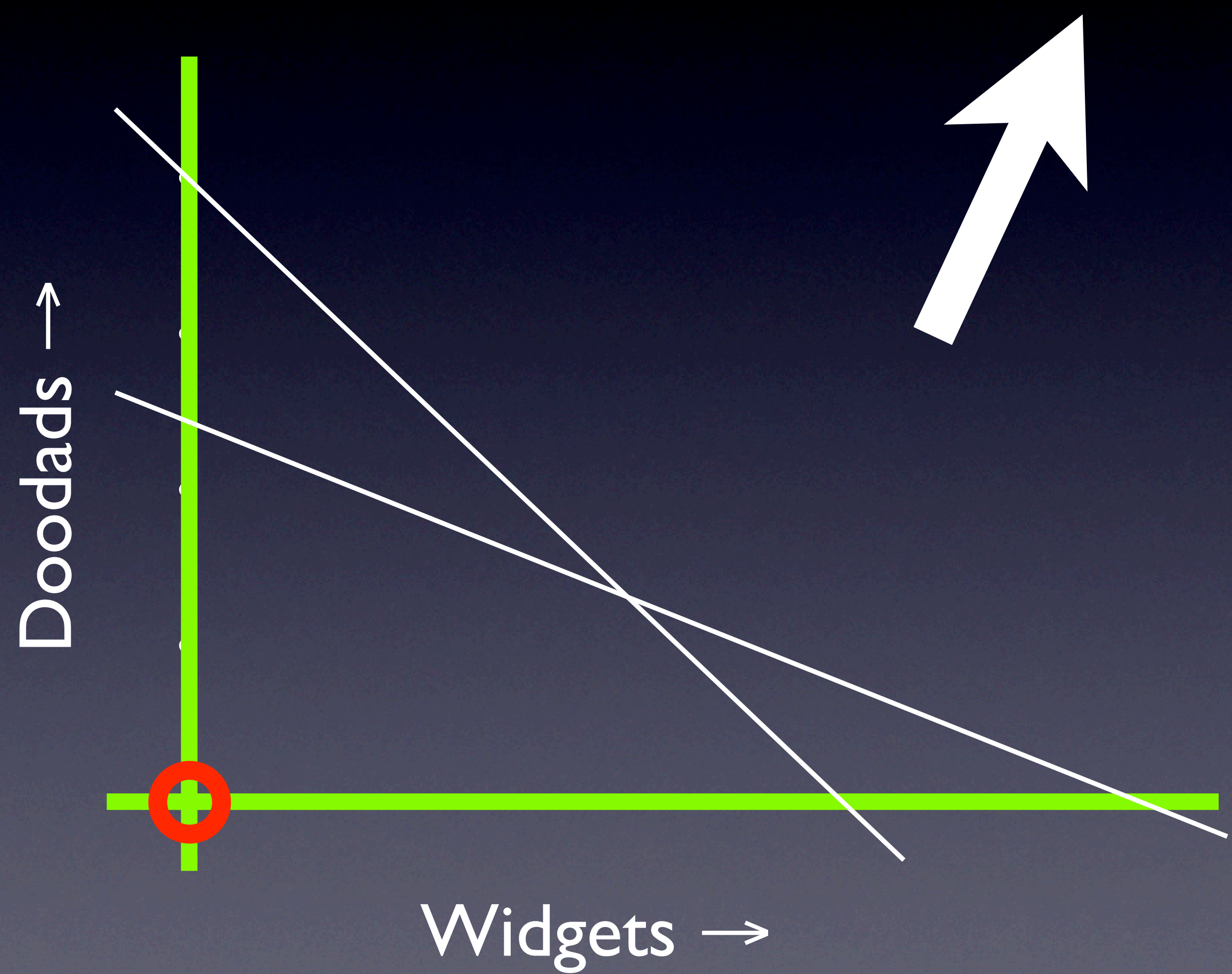
Search

- This is a combinatorial optimization problem, so could use one of our standard search algorithms
- Search space:
  - node = basis
  - objective = linear function of vertex
  - neighbor = ?

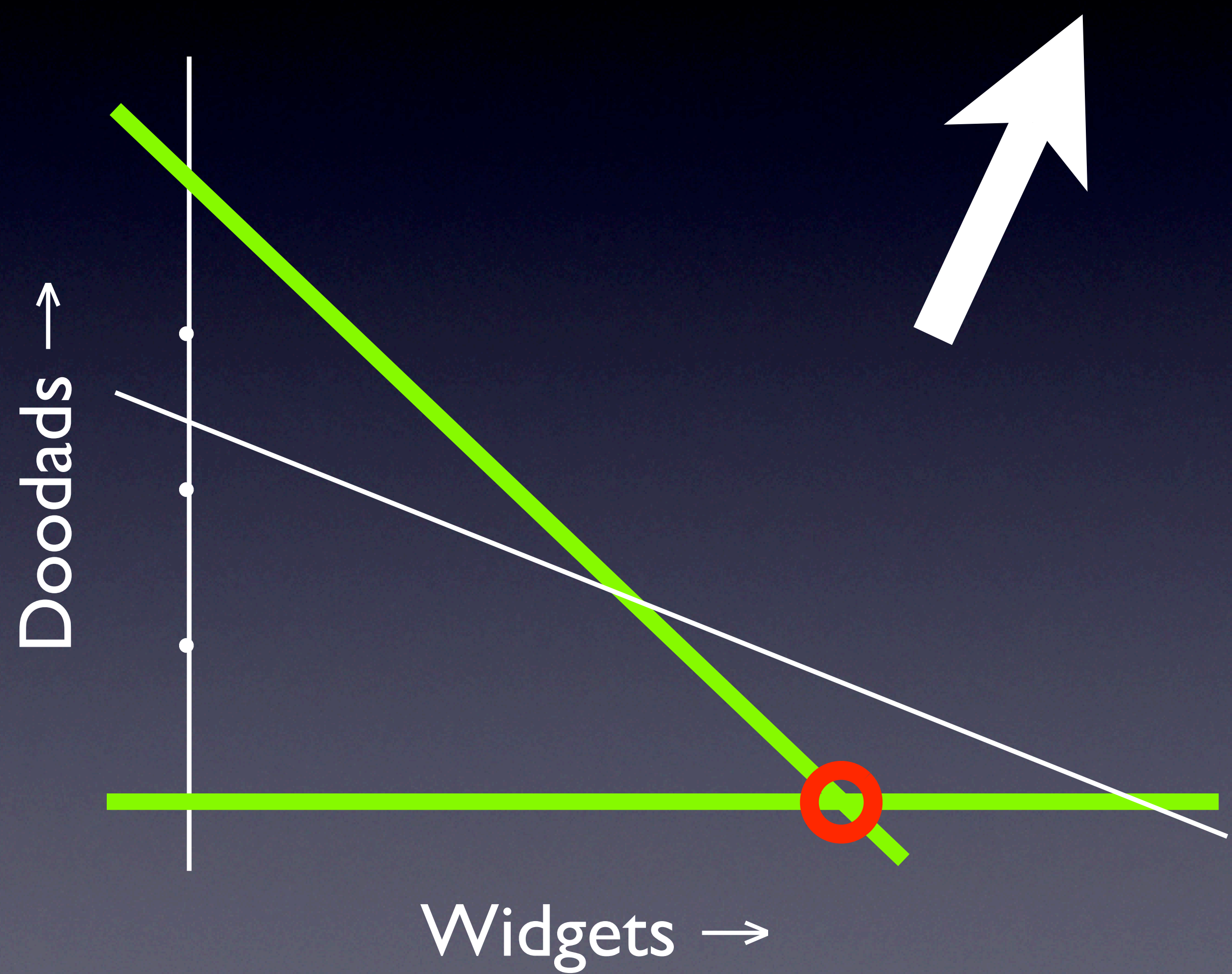
Neighboring bases

- Two bases are neighbors if they share (n-1) of n constraints
- Expanding a node in our search picks one constraint to add and another to delete

Neighbors



Neighbors



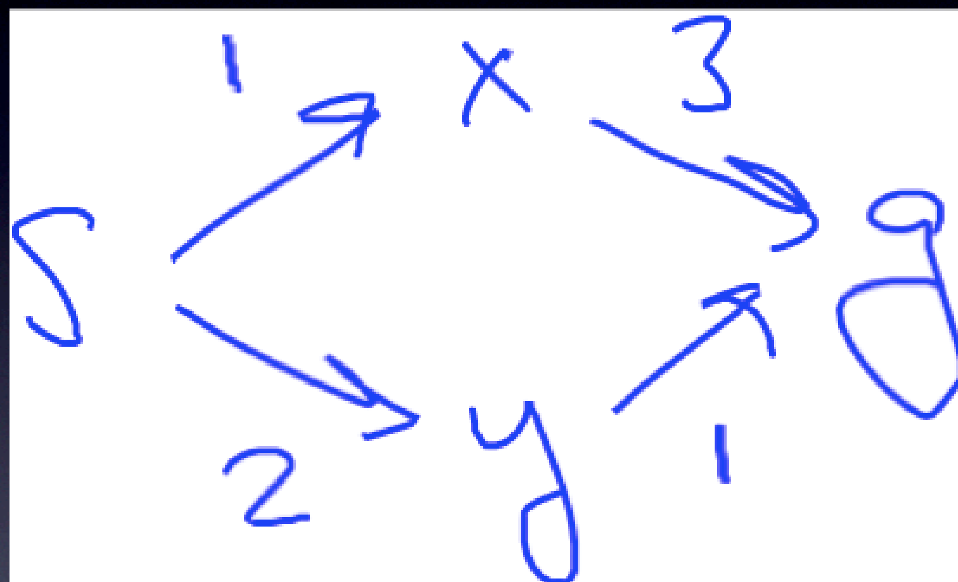
Neighbors

Simplex

- Notice that the objective increased monotonically throughout search
- Turns out, this is always possible—leads to a lot of pruning!
- We have just defined the simplex algorithm
  - if we pretend that arbitrary vertices are feasible, with an objective that penalizes infeasibility heavily

Duality example

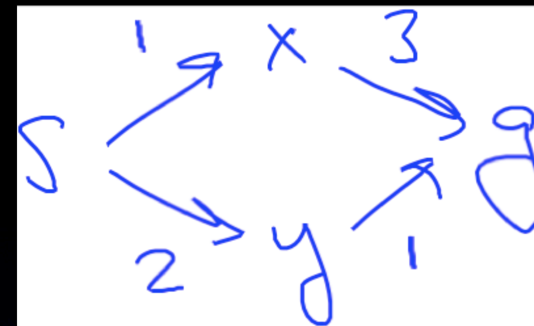
Path planning LP



- Find the min-cost path: variables

$$P_{sx}, P_{sy}, P_{xg}, P_{yg} \geq 0$$

Path planning LP



min

$$p_{sx} + 3p_{xg} + 2p_{sy} + p_{yg}$$

st

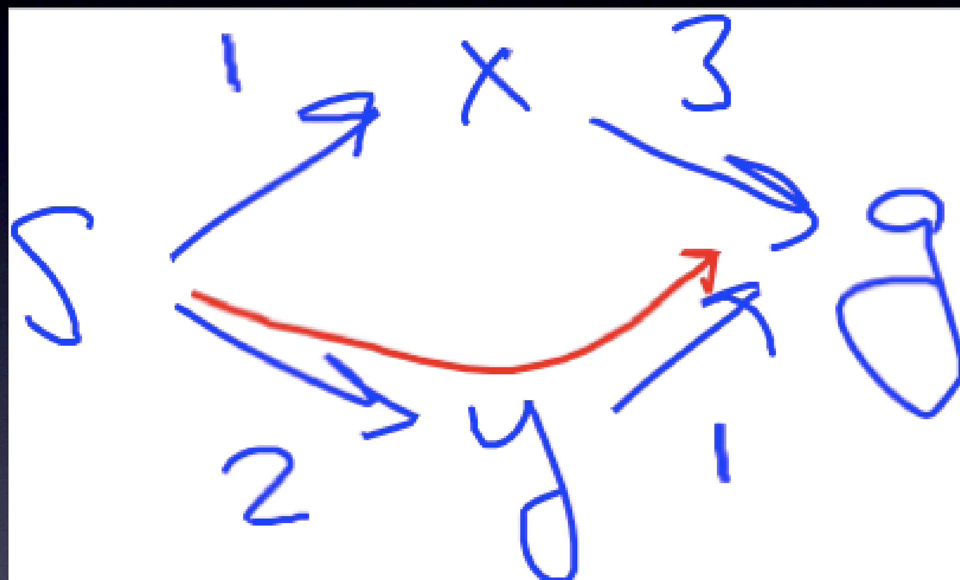
$$p_{sx} + p_{sy} = 1$$

$$-p_{sx} + p_{xg} = 0$$

$$-p_{sy} + p_{yg} = 0$$

$$-p_{xg} - p_{yg} = -1$$

Optimal solution



$p_{sy} = p_{yg} = 1, \quad p_{sx} = p_{xg} = 0, \quad \text{cost } 3$

Matrix form

$$\min \begin{pmatrix} 1 & 3 & 2 & 1 \end{pmatrix} p$$

st

$$\begin{pmatrix} 1 & 0 & 1 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 \\ 0 & -1 & 0 & -1 \end{pmatrix} p = \begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix}$$

$$p \geq 0$$

Dual

$$(\lambda_s\ \lambda_x\ \lambda_y\ \lambda_g)\begin{pmatrix} 1 & 0 & 1 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 \\ 0 & -1 & 0 & -1 \end{pmatrix}$$

$$\leq (1\ 3\ 2\ 1)$$

Dual objective

- To get tightest bound, maximize:

$$\begin{pmatrix}\lambda_s & \lambda_x & \lambda_y & \lambda_g\end{pmatrix}\begin{pmatrix}1\\0\\0\\-1\end{pmatrix}$$

Whole thing

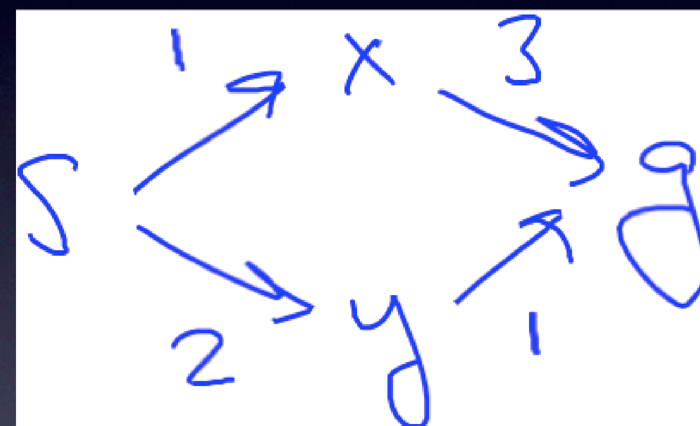
$$\max \quad \lambda_s - \lambda_g$$

$$\text{st} \quad \lambda_s - \lambda_x \le 1$$

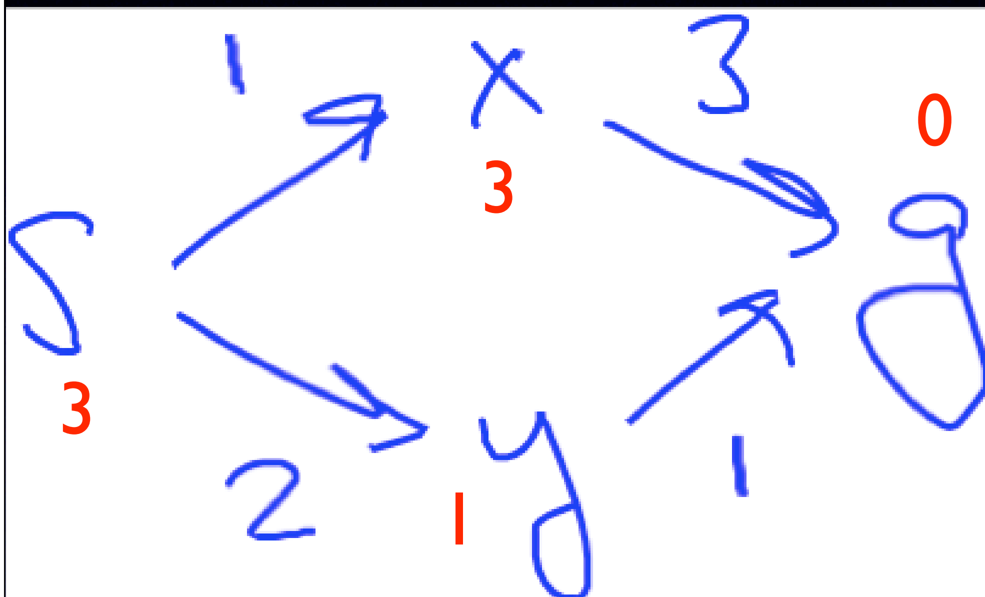
$$\lambda_x - \lambda_g \le 3$$

$$\lambda_s - \lambda_y \le 2$$

$$\lambda_y - \lambda_g \le 1$$



Optimal dual solution



$$\max \ \lambda_s - \lambda_g$$

st

$$\lambda_s - \lambda_x \le 1$$
$$\lambda_x - \lambda_g \le 3$$
$$\lambda_s - \lambda_y \le 2$$
$$\lambda_y - \lambda_g \le 1$$

Any solution which adds a constant to all λs also works

Similarly, could reduce λ_x as far as 2

Interpretation

- Dual variables are prices on nodes: how much does it cost to start there?
- Dual constraints are local price constraints: edge xg (cost 3) means that node x can't cost more than 3 + price of node g

Search in ILPs

Simple search algorithm (from last class)

- Run DFS
  - node = partial assignment
  - neighbor = set one variable
- Prune if a constraint becomes unsatisfiable
  - E.g., in 0/1 prob, setting $y = 0$ in $x + 3y \geq 4$
- If we reach a feasible full assignment, calculate its value, keep best

Pruning

- Suggested increasing pruning by adding constraints
- Constraint from best solution so far: objective ≥ M (for maximization problem)
- Constraint from optimal dual solution: objective ≤ M
- Can we find more pruning to do?

First idea

- Analogue of constraint propagation or unit resolution
- When we set a variable x, check constraints containing x to see if they imply a restriction on the domain of some other variable y
- E.g., setting x to 1 in implication constraint $(1\text{-}x) + y \geq 1$

Example

- 0/1 variables x, y, z
- maximize x subject to

  $2x + 2y - z \leq 2$

  $2x - y + z \leq 2$

  $-x + 2y - z \leq 0$

Example search

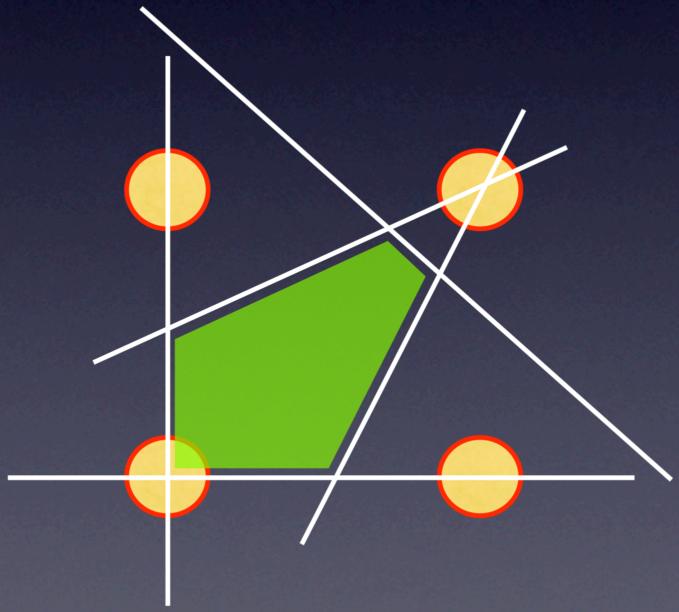
Problem w/ constraint propagation

- Constraint propagation doesn't prune as early as it could:

  $$2x + 2y - z \leq 2$$

  $$2x - y + z \leq 2$$

  $$-x + 2y - z \leq 0$$



- Consider $z = 1$

Branch and bound

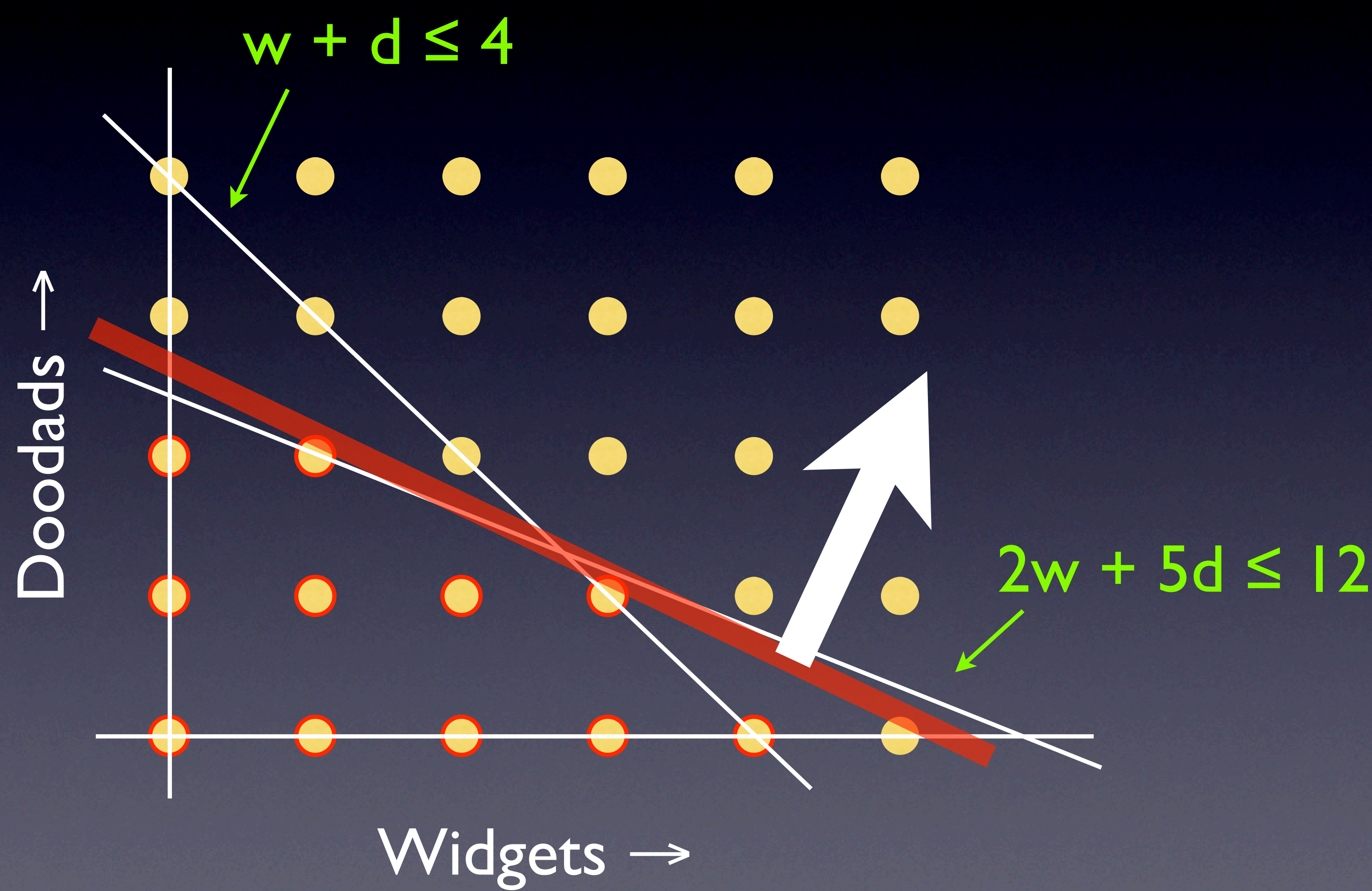
- Each time we fix a variable, solve the resulting LP
- Gives a tighter upper bound on value of objective in this branch
- If this upper bound < value of a previous solution, we can prune
- Called **fathoming** the branch

Can we do more?

- Yes: we can make bounds tighter by looking at the…

Duality gap

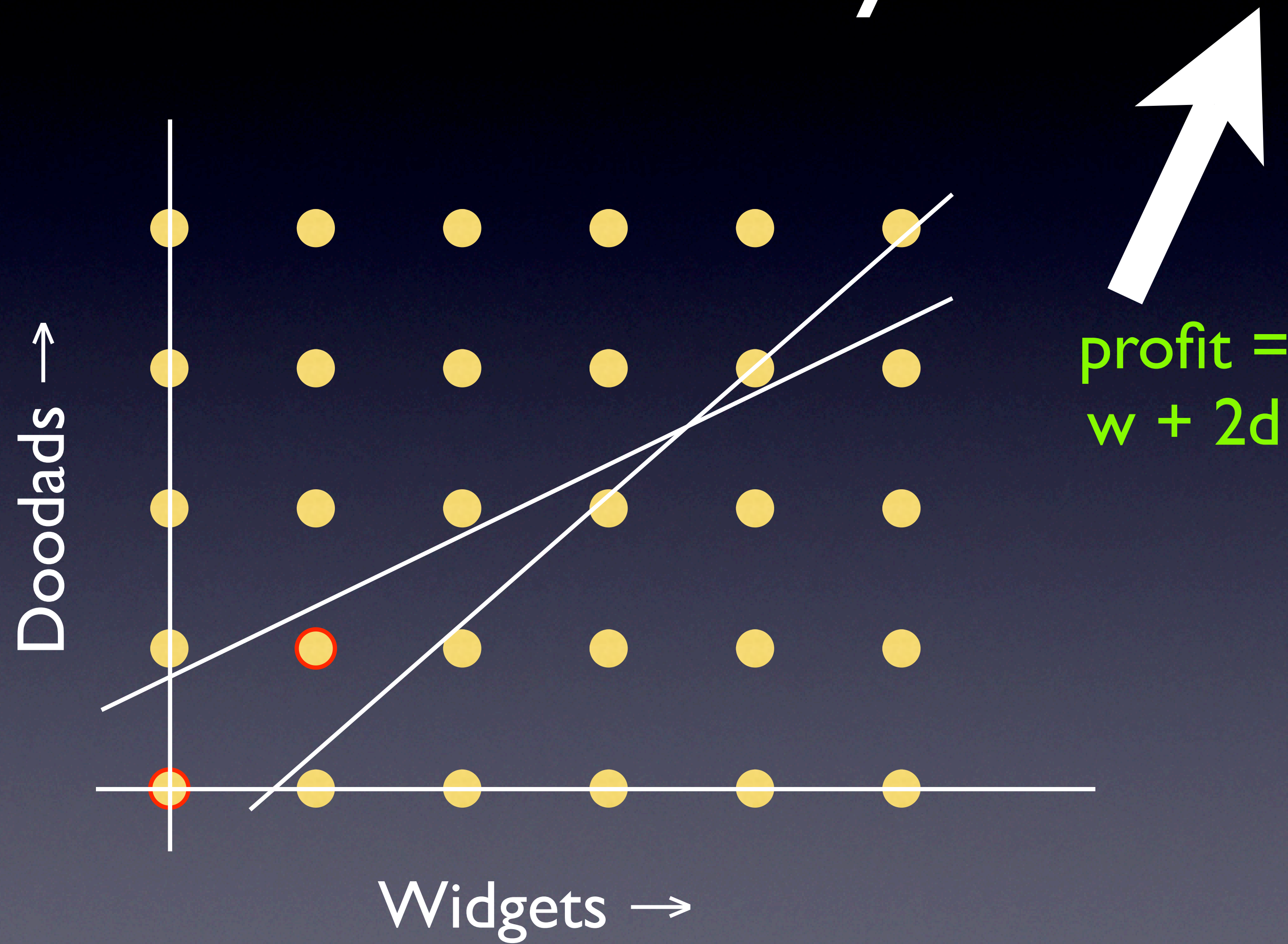
Factory LP



Duality gap

- We got bound of 5 1/3 either from primal LP relaxation or from dual LP
- Compare to actual best profit of 5 (respecting integrality constraints)
- Difference of 1/3 is **duality gap**
  - Term is also used for ratio 5 / (5 1/3)
- Pretty close to optimal, right?

Unfortunately…



Bad gap

- In this example, duality gap is 3 vs 8.5, or about a ratio of 0.35
- Ratio can be arbitrarily bad
- Aside: can often bound it for classes of ILPs
  - e.g., straightforward ILP from **MAX SAT** has gap no worse than $1-1/e = 0.632\ldots$

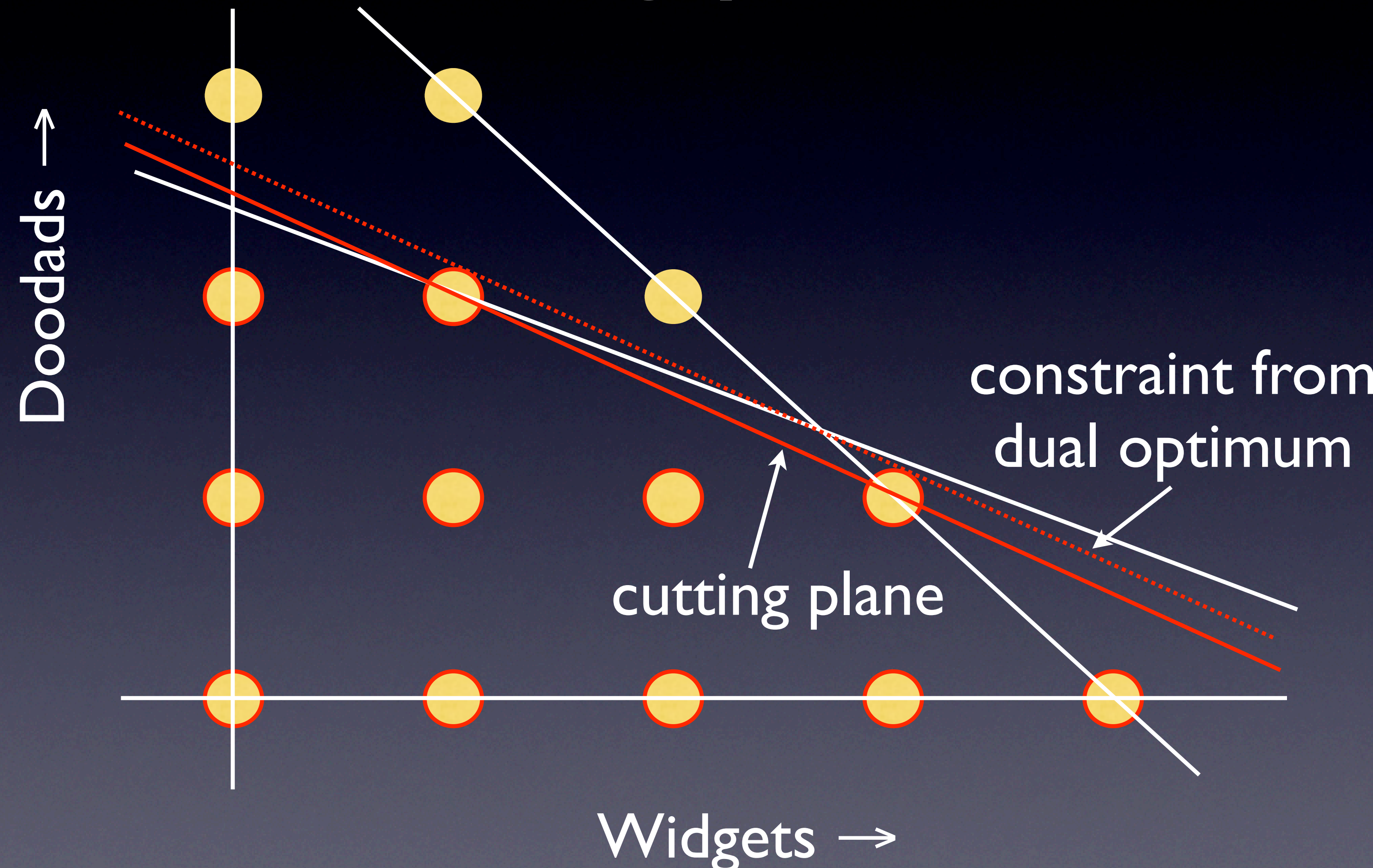
Early stopping

- A duality gap this large won’t let us prune or stop our search early
- To fix this problem: **cutting planes**

Cutting plane

- A cutting plane is a new linear constraint that
  - cuts off some of the non-integral points in the LP relaxation
  - while leaving all integral points feasible

Cutting plane



How did we find it?

- Recall our optimal dual multipliers (1/3, 1/3):

  $1/3\ (w + d - 4) + 1/3\ (2w + 5d - 12) \leq 0$

  $w + 2d \leq 16/3 = 5\ 1/3$

- Since w, d are integers, so is $w + 2d$
- So if $w + 2d \leq 5\ 1/3$, we also have

  $w + 2d \leq 5$

Gomory cuts

- This cutting plane is the **Gomory cut**
- First general recipe to find a cut in poly time that's guaranteed to cut off at least a minimal amount of the LP relaxation's feasible region
- Might have fractions on both LHS and RHS:
  - $2\ 1/2\ w + 3\ d \leq 5\ 1/3$

Gomory cuts

- Find cut for: $2\ 1/2\ w + 3\ d \leq 5\ 1/3$
- Rounding down fractions on LHS can only weaken inequality:
  - $2w + 3d \leq 5\ 1/3$
- And as before, LHS is now integral so RHS fraction is irrelevant:
  - $2w + 3d \leq 5$

Other cuts

- In our example, the Gomory cut was perfect: the vertices of the LP are now the solutions of the ILP
- How good is the Gomory cut in general?
- Sadly, not so great.
- Other cuts (not discussed here): intersection cut, problem specific cuts

Cutting planes recipe

- Solve LP relaxation
- Use optimal primal and dual variables to generate a cut
- Add cut to LP (giving a less-relaxed LP) and re-solve
- Repeat until LP's primal solution is integral

When does gap = 0?

- gap = 0 is often called **strong duality**
- Many people have defined sufficient conditions
- Most common: Slater's condition
  - problem is convex
  - there exists a **strictly feasible** point

Strictly feasible

- minimize $f(x)$ st

  $g_i(x) \leq 0, \; i = 1, 2, \ldots, m$

  $Ax = b$

- Strictly feasible point has $g_i(x) < 0$ for all i
- Generalization: strict feasibility need not hold if $g_i(x)$ is linear
  - so all feasible LPs have gap = 0

Branch and Cut

Branch and cut

- Cutting planes recipe doesn't use branching
- What if we try to interleave search with cut generation?
- Resulting **branch and cut** methods are some of the most popular algorithms for solving ILPs and MILPs

Recipe

- DFS as for branch and bound
- At each node, solve the LP relaxation
  - detect "fathomed" branches
  - while not bored
    - use dual vars to generate cut, re-solve
- Branch on next variable
  - after a branch it may become easier to generate more cuts

Cut generation

- Cuts at a node N are valid at N's children
  - so it's worth spending more effort higher in the search tree
- General techniques for cut generation are often expensive and/or generate weak cuts
  - so people often use problem-specific cuts

Cut lifting

- Sometimes a cut for one branch can be **lifted** to apply to other branches
- Or we can learn a cut in lifted form to start with
- These cuts are like constraint learning
- Try to compile some of the results of our search to save branching later

Lifted example

- Two constraints from a SAT instance:
  - $x + y + (1-z) \geq 1, \quad y + z + w \geq 1$
- Adding them yields
  - $x + 2y + w \geq 1$
- **Trimming** yields a cut:
  - $x + y + w \geq 1$

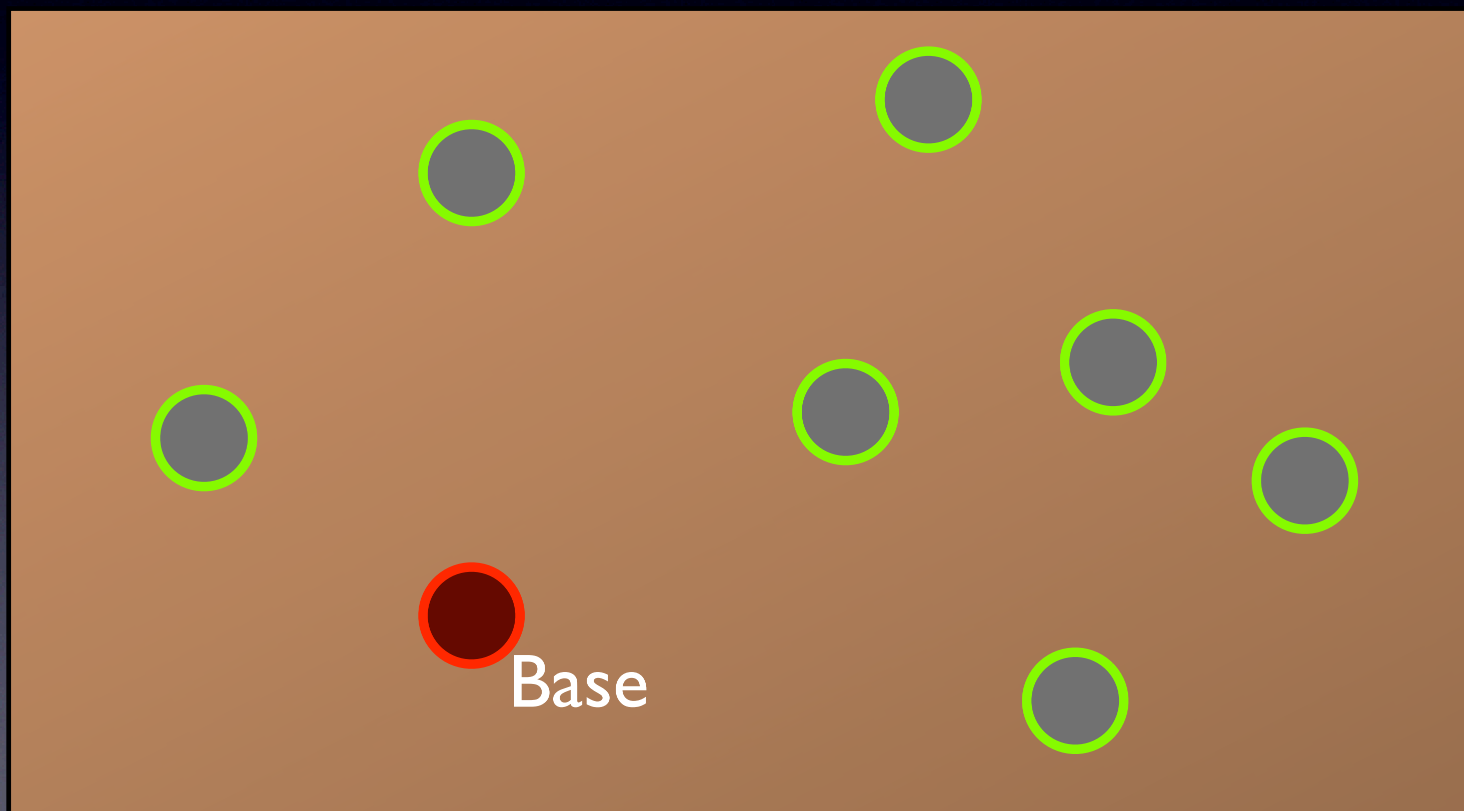
More generally

- If a variable appears with opposite sign in two constraints, sum them
  - $x + 2y + z \geq 1, \quad 2x + y \geq 1$
  - $3x + 3y + z \geq 2$
- Then trim the result:
  - $2x + 2y + z \geq 2$

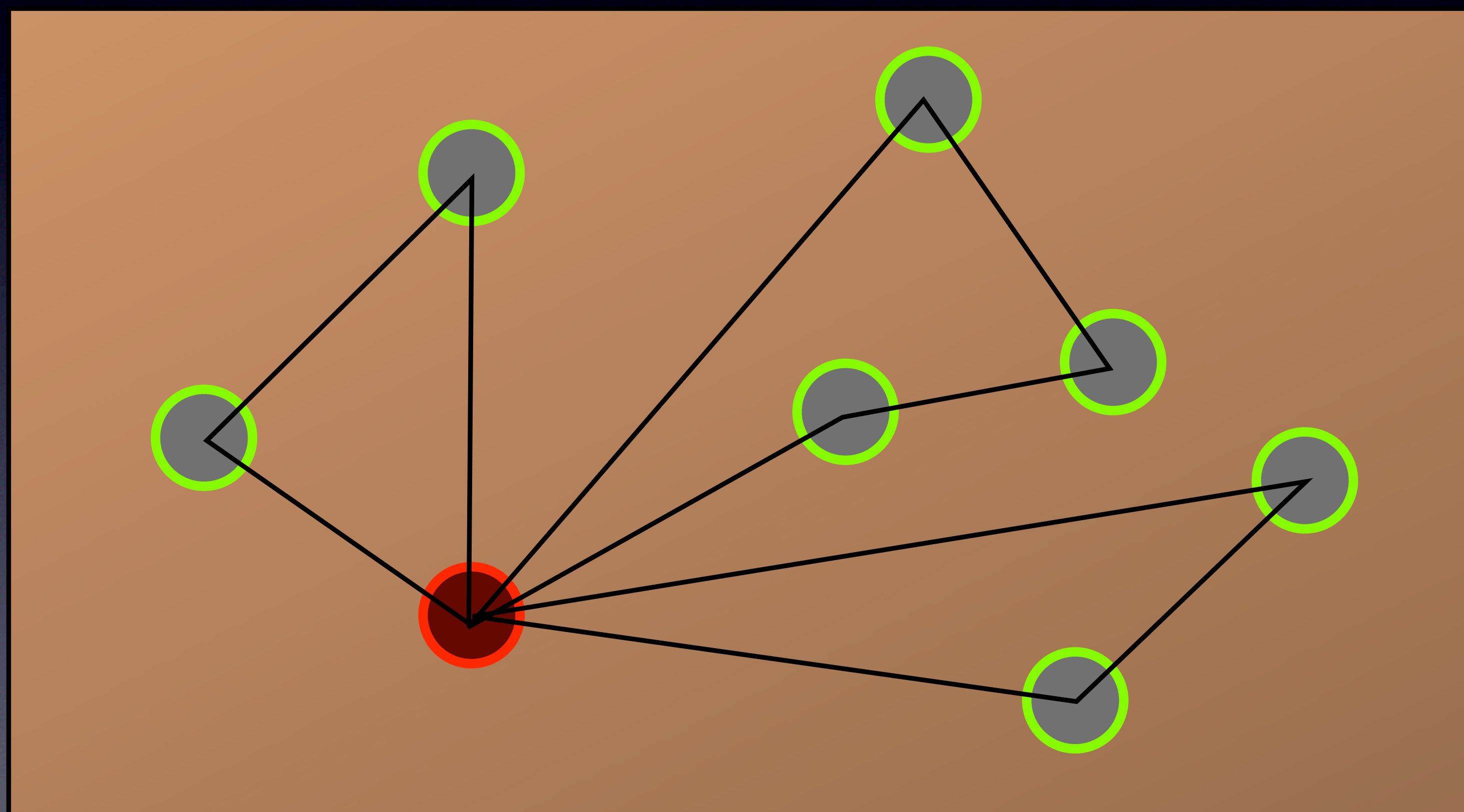
Example: robot task assignment

- Team of robots must explore unknown area

Points of interest



Exploration plan



ILP

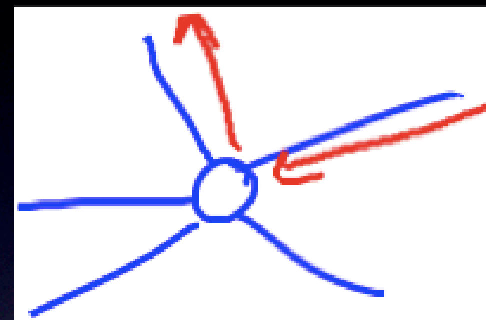
- Variables (all 0/1):
  - z_{ij} = task j assigned to robot i
  - x_{ijk} = robot i uses edge jk
- Cost = path cost - task bonus
  - $\sum x_{ijk} c_{ijk} - \sum z_{ij} t_{ij}$

Constraints

- For all i, j: $\sum_k x_{ijk} \geq z_{ij}$
- For each i, x_{ijk} forms a tour from base:
  - subtour elimination constraints

Subtour elimination

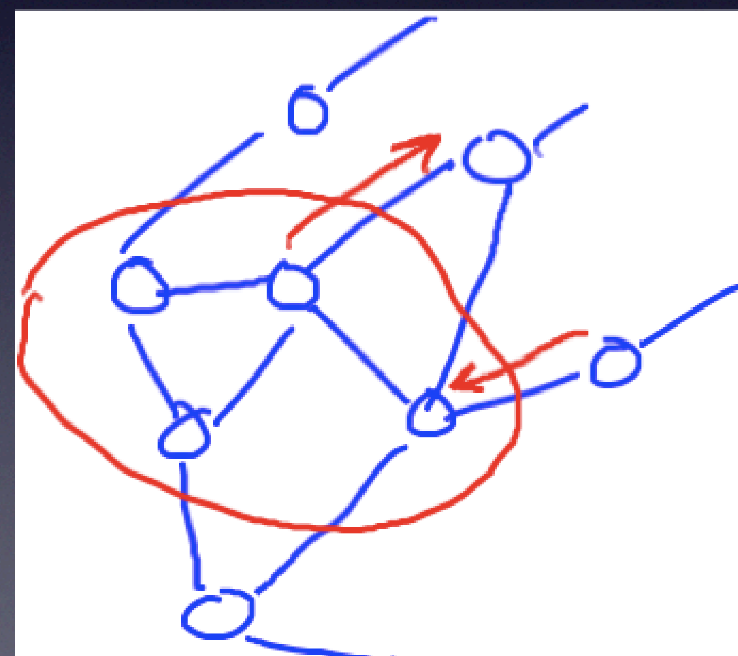
$$\sum_i x_{si} \geq 2$$



$$\forall S \quad \sum_{i \in S} \sum_{j \notin S} x_{ij} \geq 2$$
$$s \notin S$$

or

$$\sum_{i,j \in S} x_{ij} = 0$$



Game search

Games

- We will consider games like checkers and chess:
  - sequential
  - zero-sum
  - deterministic, alternating moves
  - complete information
- Generalizations later

Chess

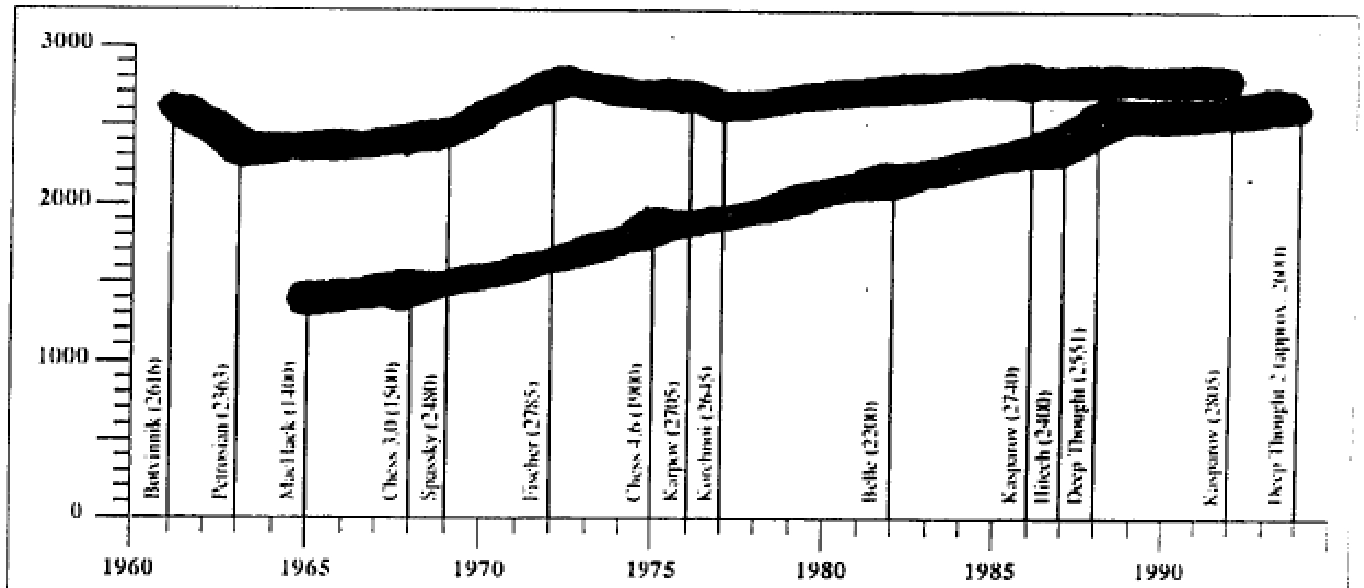


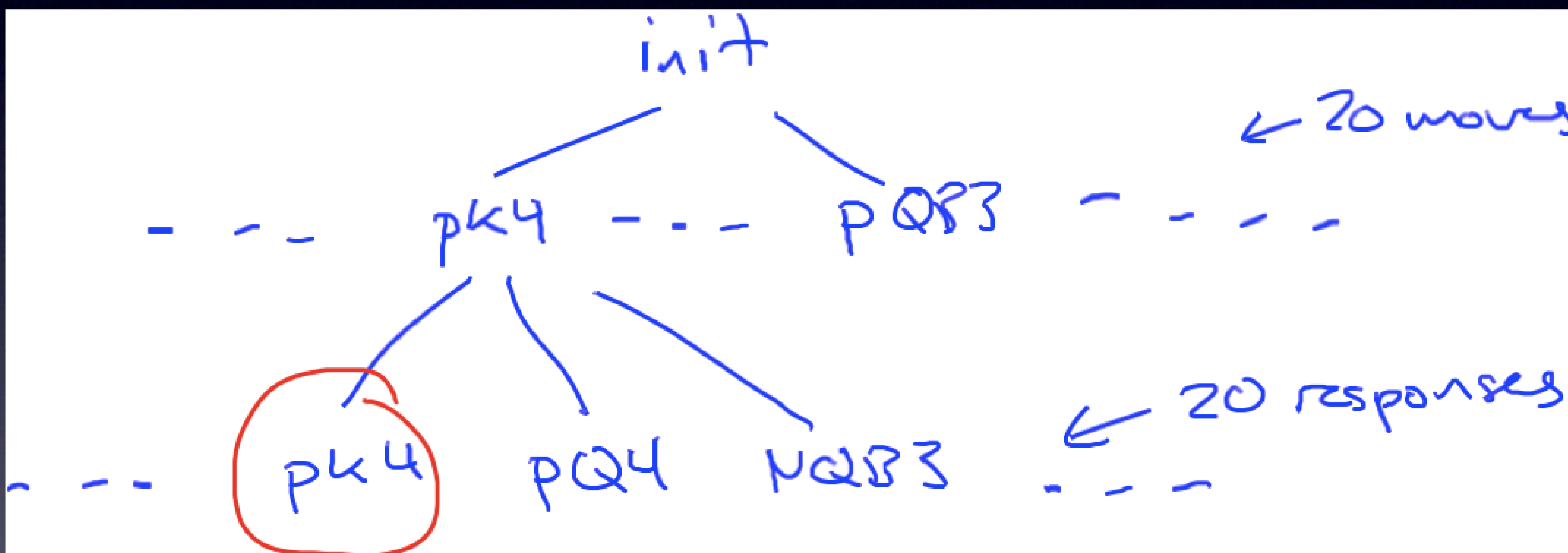
Figure 5.12 Ratings of human and machine chess champions.

- Classic AI challenge problem
- In late '90s, Deep Blue became first computer to beat reigning human champion

History:

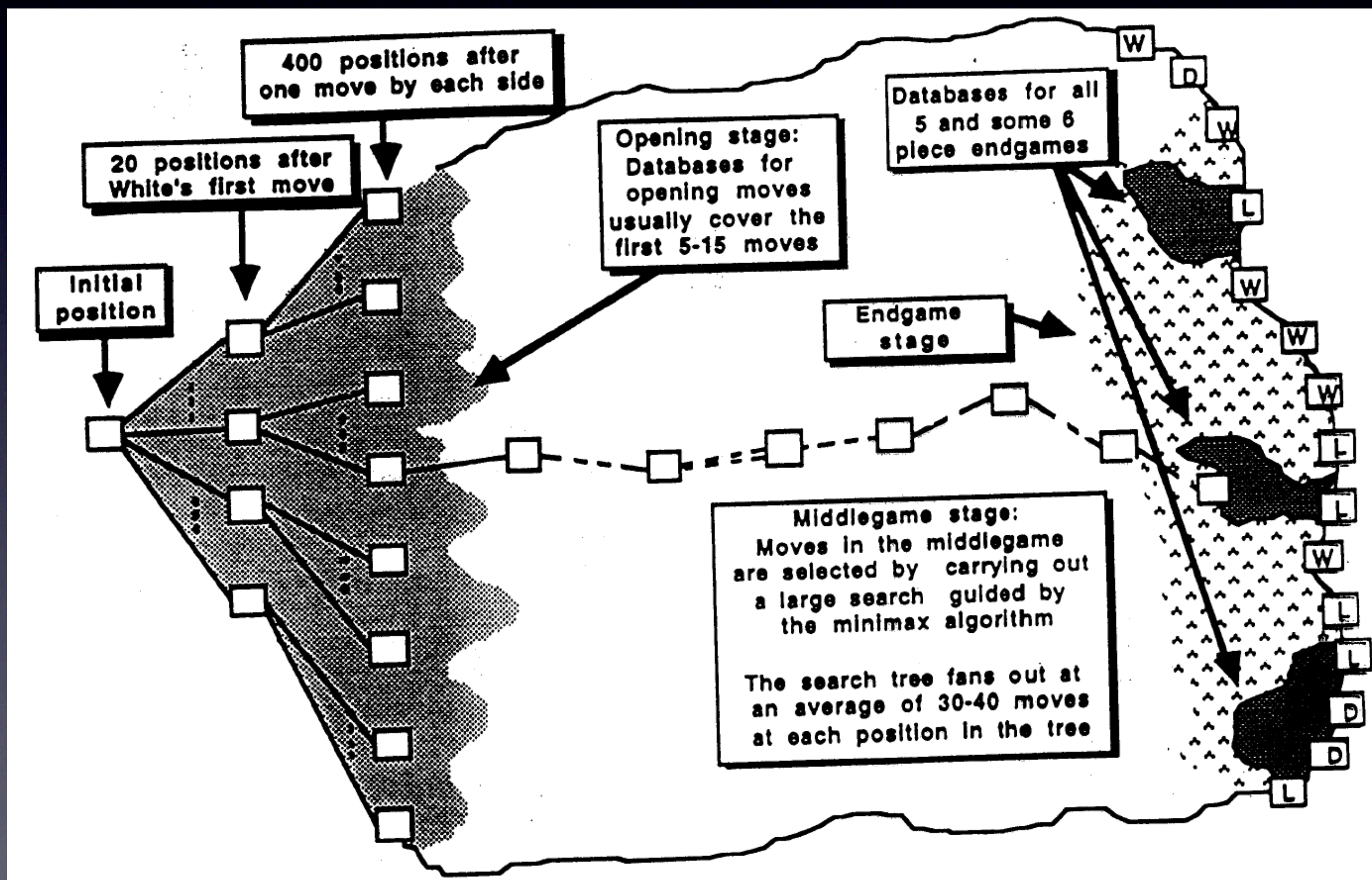
- Minimax with heuristic: 1950
- Learning the heuristic: 1950s (Samuels' checkers)
- Alpha-beta pruning: 1966
- Transposition tables: 1967 (hash table to find dups)
- Quiescence: 1960s
- DFID: 1975
- End-game databases: 1977 (all 5-piece and some 6)
- Opening books: ?

Game tree




8
7
6
5
4
3
2
1
a b c d e f g h

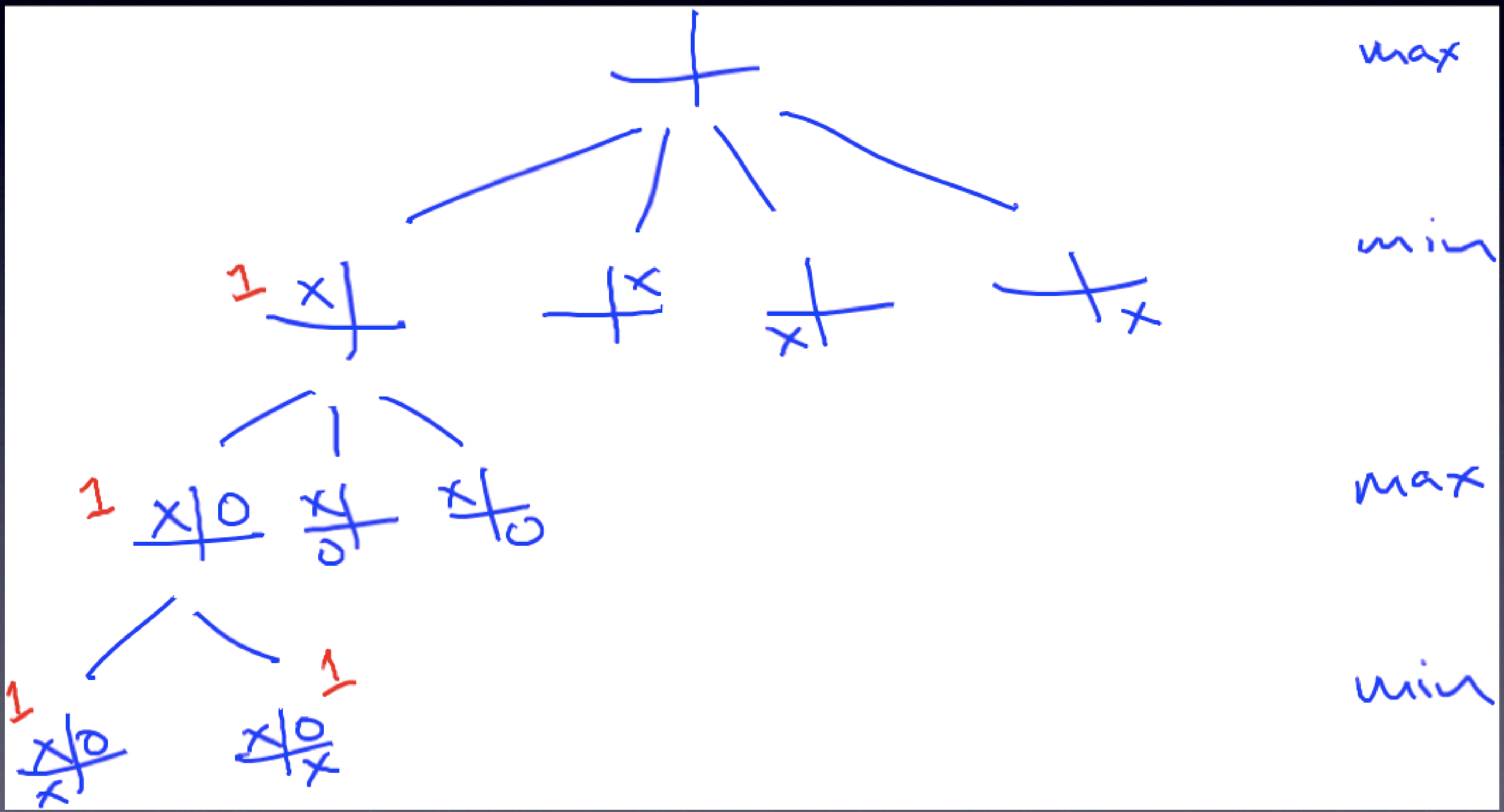
Game tree for chess



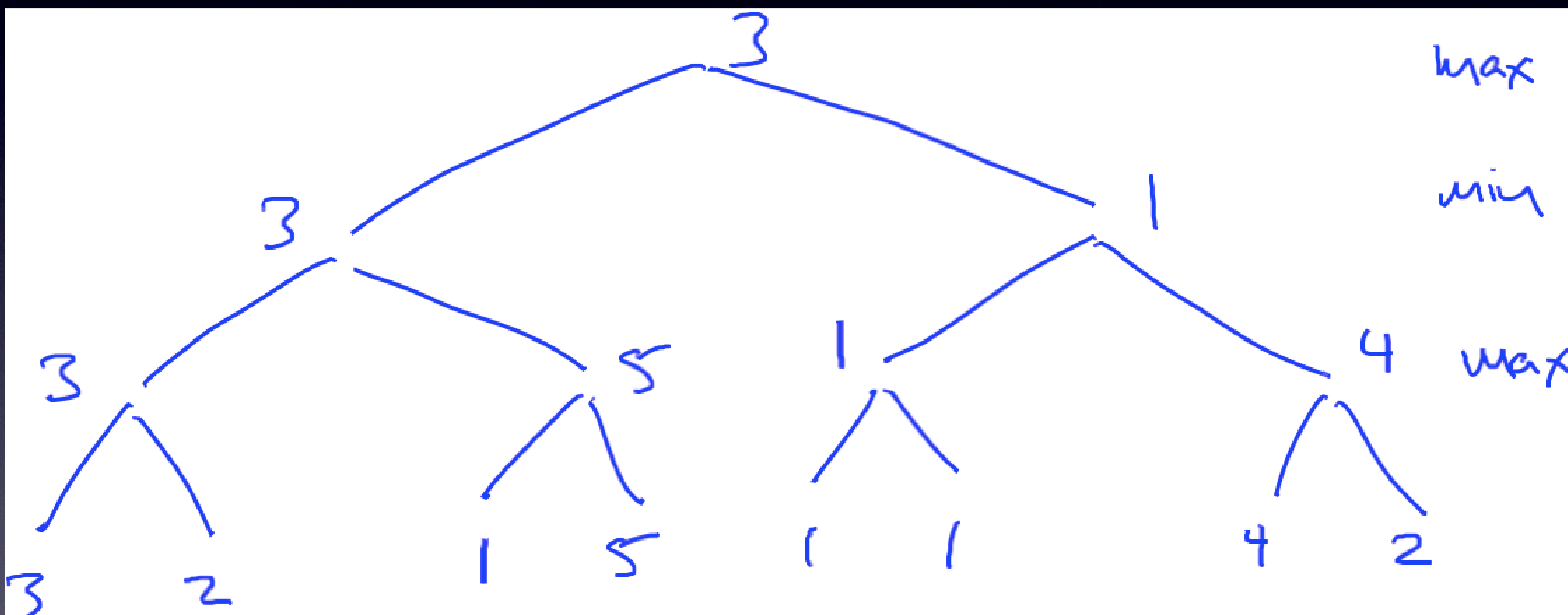
Minimax search

- For small games, we can determine the value of each node in the game tree by working backwards from the leaves
- My move: node's value is maximum over children
- Opponent move: value is minimum over children

Minimax example: 2x2 tic tac toe



Synthetic example



Principal variation