# Fitness Landscapes and Problem Difficulty

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# Talk Outline

- What is a fitness landscape?
- Why should algorithm designers care about the fitness landscape?

- How do you tell if a fitness landscape feature matters?
  - Instance versus ensemble-level problem difficulty
  - How important are “well-known” landscape features?

- Linking fitness landscape structure and algorithm run-time dynamics
  - An illustrative example from Job-Shop Scheduling

- Future research areas in fitness landscape analysis

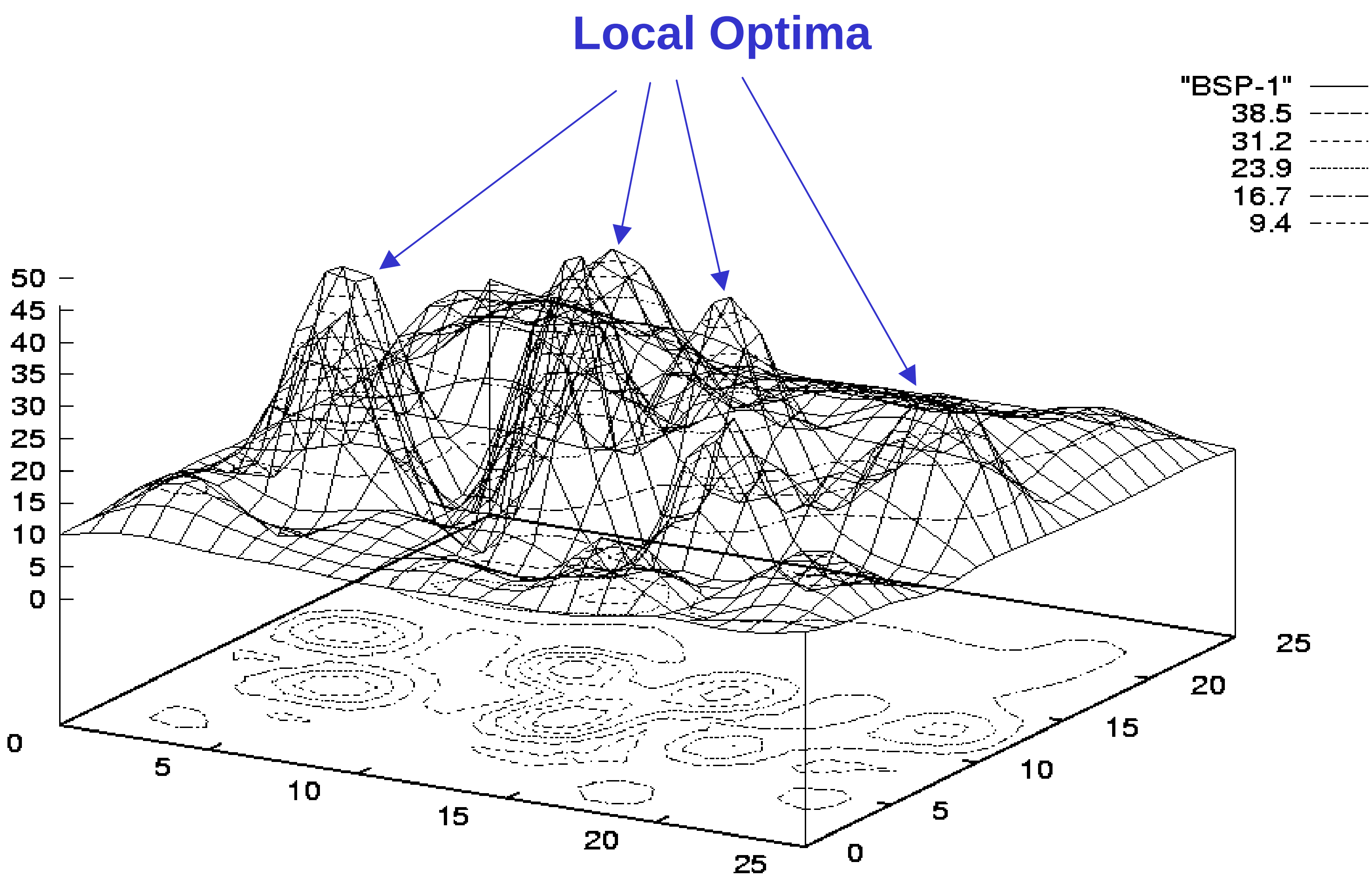
- Conclusions

# What is a Fitness Landscape?

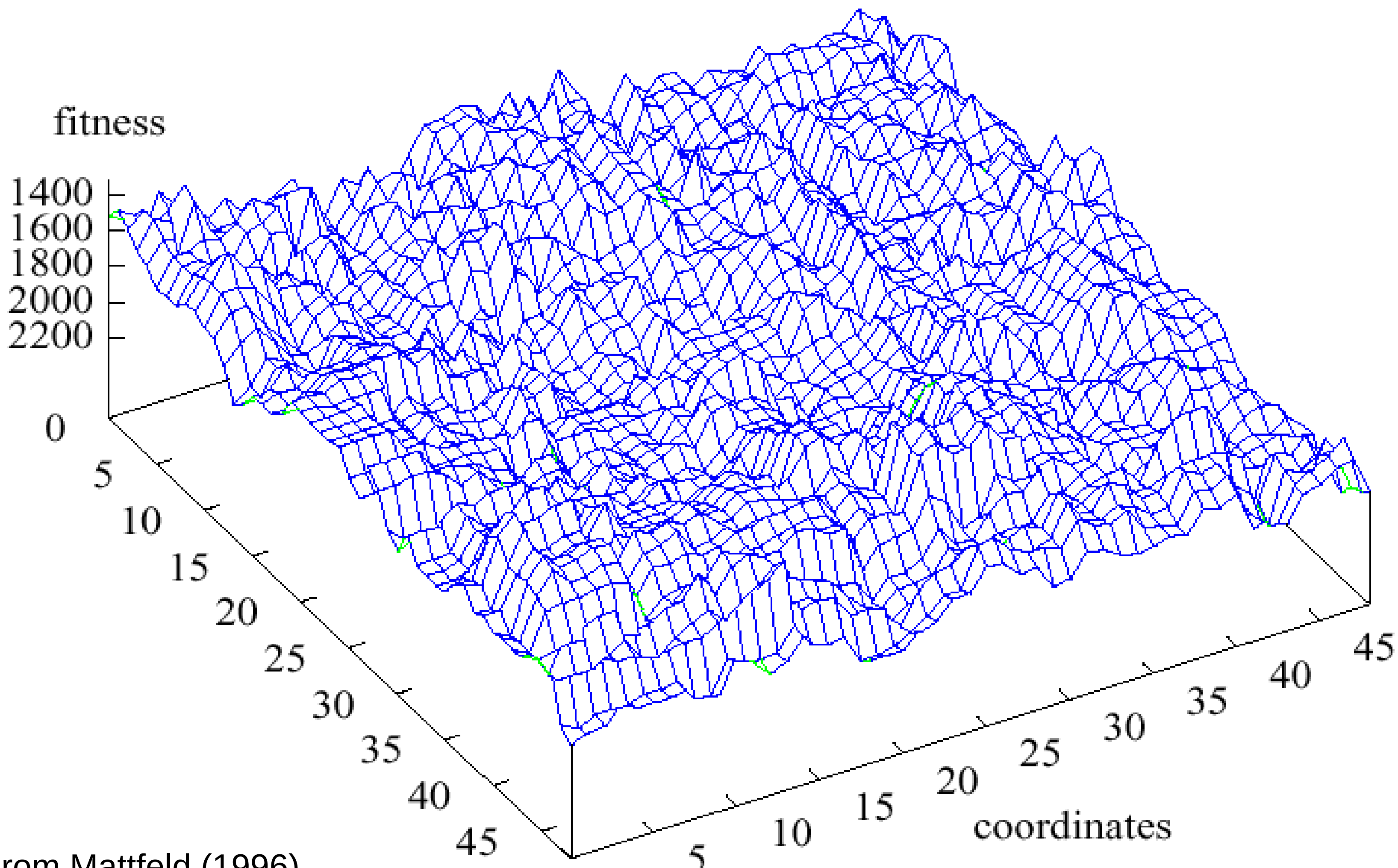
- For typical local search methods (tabu search, simulated annealing)
  - A vertex-weighted graph!
  - Three core components
    - A search space *S*
    - A fitness or objective function f:*S->R*
    - A move operator *N*:*S->P(S)*
  - *To a first-order approximation* – see Reeves (1998) for critique

- For evolutionary algorithms
  - The picture is significantly less clear
  - Multiple move operators
  - Move operators that take multiple solutions (e.g., crossover)
  - See Jones (1995) for a great discussion of these and other related issues

# Local Search and the Fitness Landscape



# A (Slightly) More Realistic Example




Taken From Mattfeld (1996)

# More Complexities and Subtleties

- Two qualitatively different types of fitness landscape
- "Type 1" Fitness Landscapes
  - Dominated by large plateaus of equally fit solutions
  - Different terminology (e.g., benches and exits)
  - Not hard to find in combinatorial optimization
    - E.g., MAX-SAT and flow-Shop Scheduling
- "Type 2" Fitness Landscapes
  - Dominated by local optima, distinct neighbor fitness values
  - Different terminology (e.g., barriers and depth)
  - Pervasive in function/global optimization
  - The "other half" of combinatorial optimization problems
    - E.g., the TSP
- See Hoos and Stutzle (2005) for further information

# Why Should You Care About Fitness Landscapes?

- *The* motivating observation
  - Algorithm performance depends on the ability of a search strategy to exploit the structure of the underlying fitness

- Implications
  1. Knowledge of fitness landscape structure is the *only* way to design algorithms in a *targeted* fashion, i.e., not hacking
  2. Algorithms are necessarily "tuned" to a particular class of fitness landscapes => you have to know your problem!

- Caveat
  - Fitness landscape structure is important, but cannot in truth be studied independently of the algorithm under consideration
  - *Algorithm behavior and fitness landscape structure are linked*

# Fitness Landscape Features: An Overview (1)

- Correlation length
  - Weinberger, Stadler
  - Generate a fitness time-series via a random walk
  - Autocorrelation measures ruggedness
  - Rugged landscapes => more difficulty for adaptive algorithms

- Fitness-distance correlation
  - Kirkpatrick and Toulouse, Boese et al, Jones and Forrest
  - Generate a large sample of random local optima
  - Compute the correlation between
    - Distance-to-best or average distance to other optima
    - Fitness
  - Strong correlation => good solutions are clustered
    - The “big-valley” structure
  - Weak correlation => adaptive search will lead you astray

# Fitness Landscape Features: An Overview (2)

- Barrier structure
  - The entire simulated annealing research community!
  - How much of a fitness decrease is required to escape the attractor basin of a local optimum?
  - Barrier trees (Stadler)
    - Is search likely to be trapped in certain regions of the search space?
    - Leonard-Jones clusters

- The average distance between local optima
  - Mattfeld
  - What is the average distance between local optima?
  - Quantifies search space “diameter” or “width”
  - Large search spaces => higher degree of difficulty

# Fitness Landscape Features: An Overview (3)

- The number of optimal solutions
  - Clark et al.
  - How many *globally* optimal solutions are there?
  - More optimal solutions => they should be easier to find
  - Popularized in the context of MAX-SAT

- Backbone size
  - Slaney and Walsh, Singer et al.
  - How many solution attributes are found in *all* optimal solutions?
  - Large backbone => once you “solve” the backbone, the rest of the problem should be easy

- The average distance between local optima and optimal solutions
  - Singer et al.
  - What is the average distance between local optima and the *nearest* optimal solution?
  - Simultaneously accounts for both search space size and the number of “targets” embedded within the sub-space

# How To Tell If a Fitness Landscape Feature “Matters”?

- Intuition
  - A fitness landscape feature is important if its presence is highly correlated with the difficulty of locating an optimal solution
  - In other words, if the presence of the feature impedes an search algorithm from operating effectively

- Some things to consider before undertaking analysis
- Do you care about ensemble-level differences in problem difficulty?
  - E.g., 30-city TSPs versus 100-city TSPs
- Do you care about instance-level differences in problem difficulty?
  - E.g., 1000 instances of 100-city TSPs

- An observation
  - Cost to solve 100-city TSPs varies over 8 *orders of magnitude*
- An opinion
  - If you can’t account for such huge differences at the instance level, you can’t hope to explain differences at the ensemble level

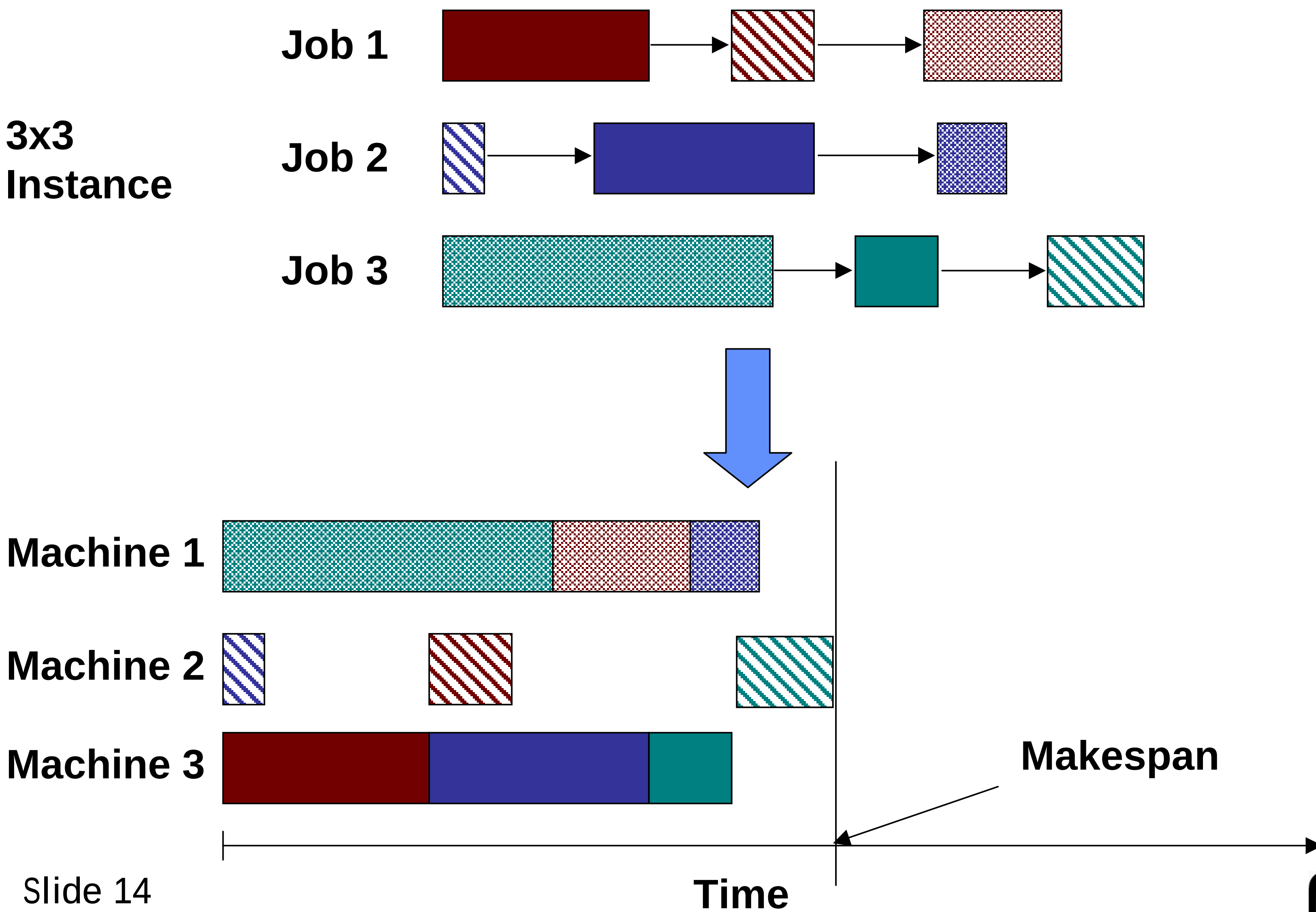
# Static Cost Models of Problem Difficulty

- A static cost model
  - Accounts for the variability in problem difficulty observed in a set of fixed-dimension problem instances
- The “static” modifier derives from the fact that algorithm dynamics are not explicitly taken into account
- Problem difficulty
  - How much does it cost on average to locate an optimal solution to a given problem instance?
- Fixed-dimension problem instances
  - E.g., a set of 100 random Euclidean TSP instances
- Linear regression of landscape feature versus problem difficulty
- The $r^2$ value of the resulting model quantifies the proportion of variability in problem difficulty accounted for by the model

# Static Cost Models: The Current Situation

- *Most well-known search space features are only weakly correlated with problem difficulty*
  - Correlation length
  - The number of optimal solutions
  - The average distance between local optima
  - The backbone size
  - Fitness-distance correlation
- These features *at best* account for 25%-50% of the total variability in problem difficulty on *small* problems
  - And often much less
- Accuracy rapidly drops as problem size increases

# Experimental Domain: Job-Shop Scheduling (JSP)

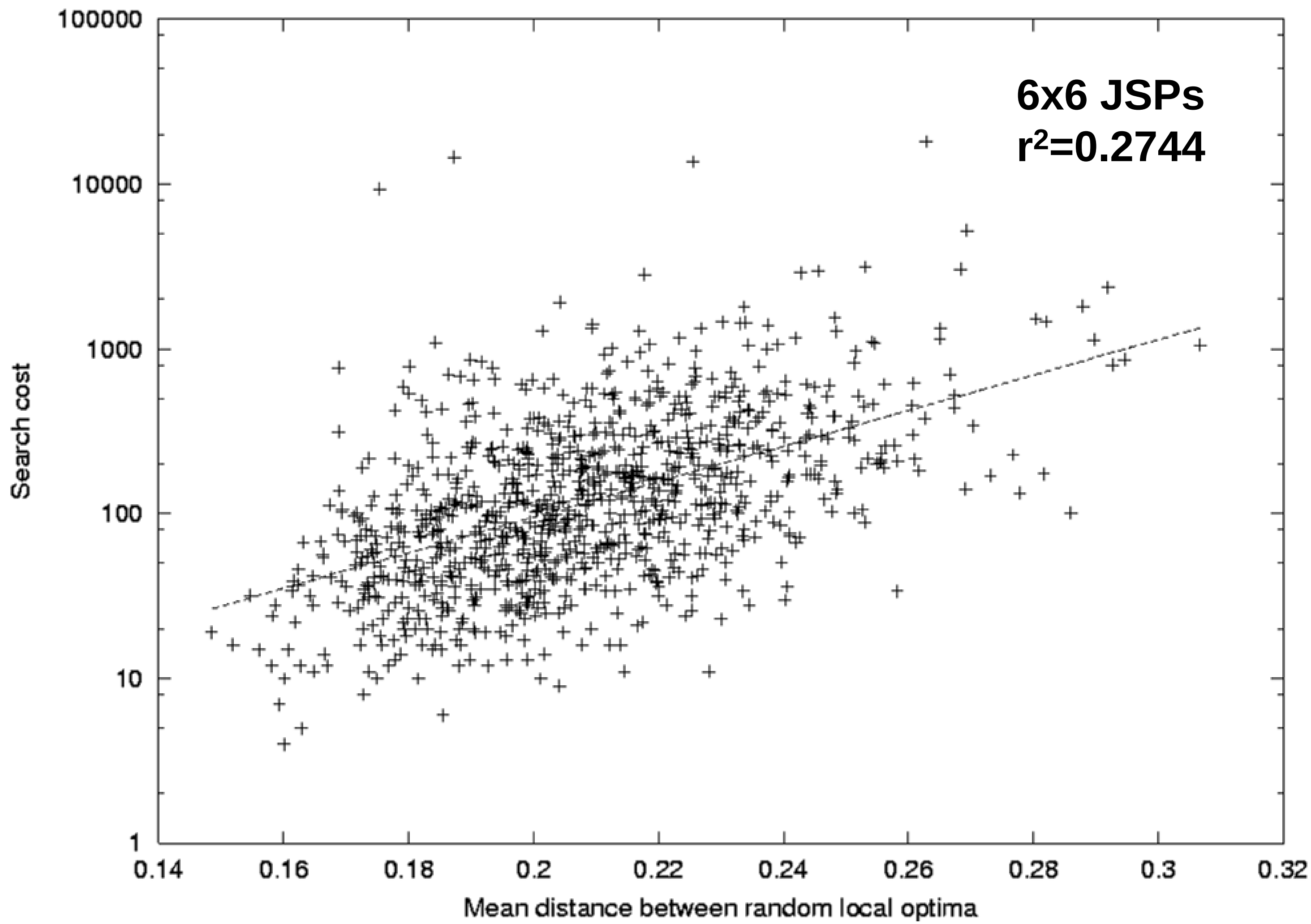


# Performance of Static Cost Models on the JSP

- Consider a set of 1000 6-job, 6-machine instances
  - Small in comparison to any “real” benchmark problems
- Static cost model accuracy for widely studied measures
  - Correlation length $r^2=0.0$
  - The number of globally optimal solutions $r^2=0.2223$
  - The backbone size $r^2=0.2231$
  - Average distance between local optima $r^2=0.2744$
  - Fitness-distance correlation $r^2=0.1211$
- Only account for about 25% of the total variability
  - Why are these popular and widely studied?

- *Things get worse for larger problems*, e.g., 10-jobs, 10-machines

# The Best of the Lot…



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# A More Effective Static Cost Model (1)

- Hypothesis:
  - Problem difficulty is proportional to the *effective* size of the search space

- Must simultaneously account for both
  1. The absolute size of the search space
  2. The number and distribution of solutions within the search space

- New /unexplored measure: $\overline{d}_{lopt-opt}$
  - The mean distance between random local optima and the nearest optimal solution



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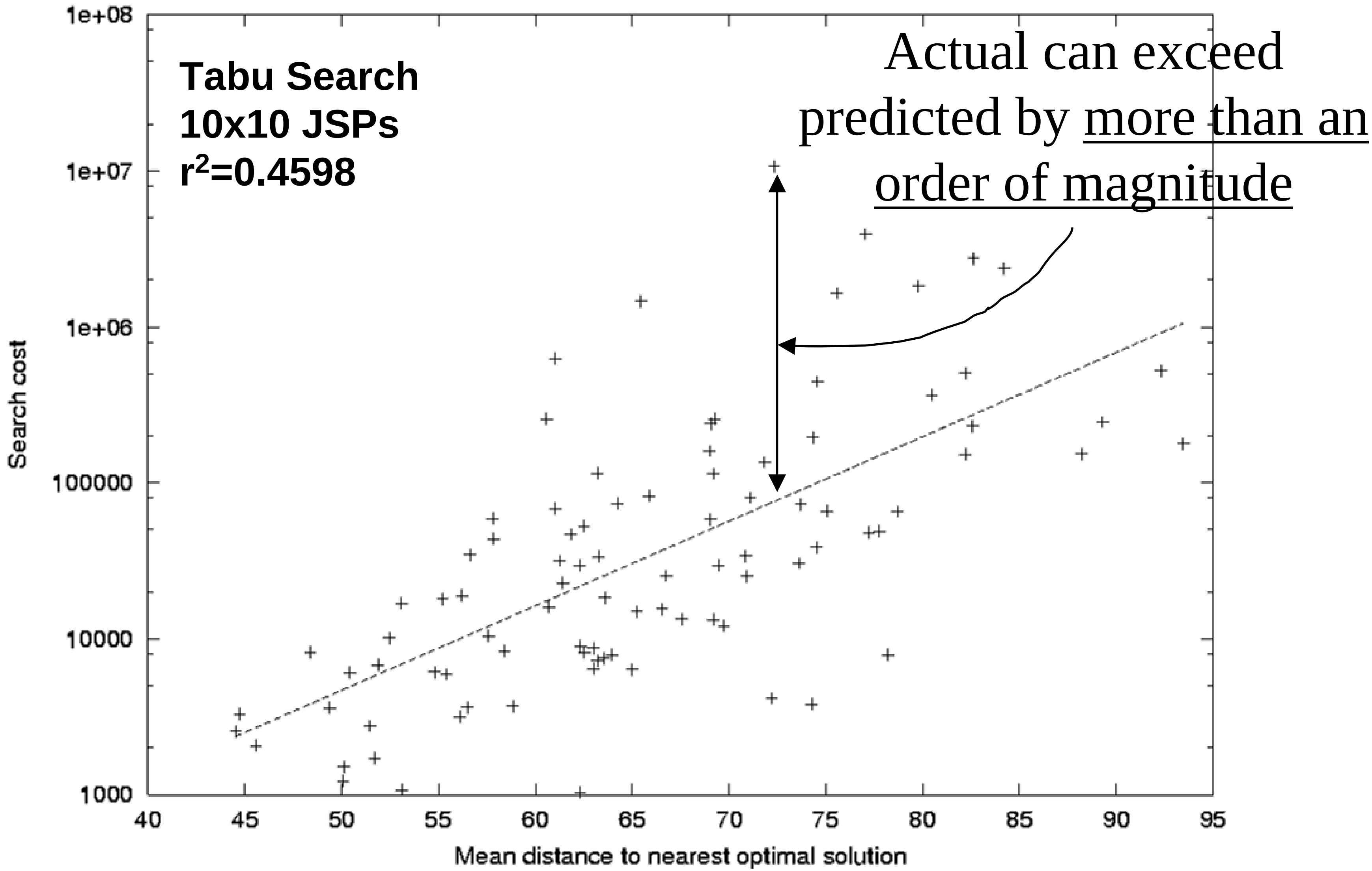
# A More Effective Static Cost Model (2)




$\overline{d}_{lopt-opt}$



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# Static Cost Models and Landscape Features: Discussion

- It is not enough to simply posit that a specific fitness landscape feature plays an important role in problem difficulty
  - Intuition suggests that a particular feature “should” be important
  - Intuition is often wrong than right in science

- It is easy enough to subject these hypotheses to rigorous testing
  - Static cost models via linear regression

- A common theme
  - Features that are “thought” to be important for many widely-used algorithms aren’t all that important at all

- Implication
  - Landscape analysis is not a “solved” research area

# Beyond Static Cost Models: The Test Subjects

- Tabu search
  - Steepest-descent local search, but…
  - … prevents search from “undoing” recent moves
- Metropolis sampling (aka MCMC)
  - Always accept improving/equal moves
  - Probabilistically accept worse moves
- Iterated local search
  - Generate large “kick-moves” to escape local optima
  - Apply greedy descent and iterate…

# Modeling Objectives

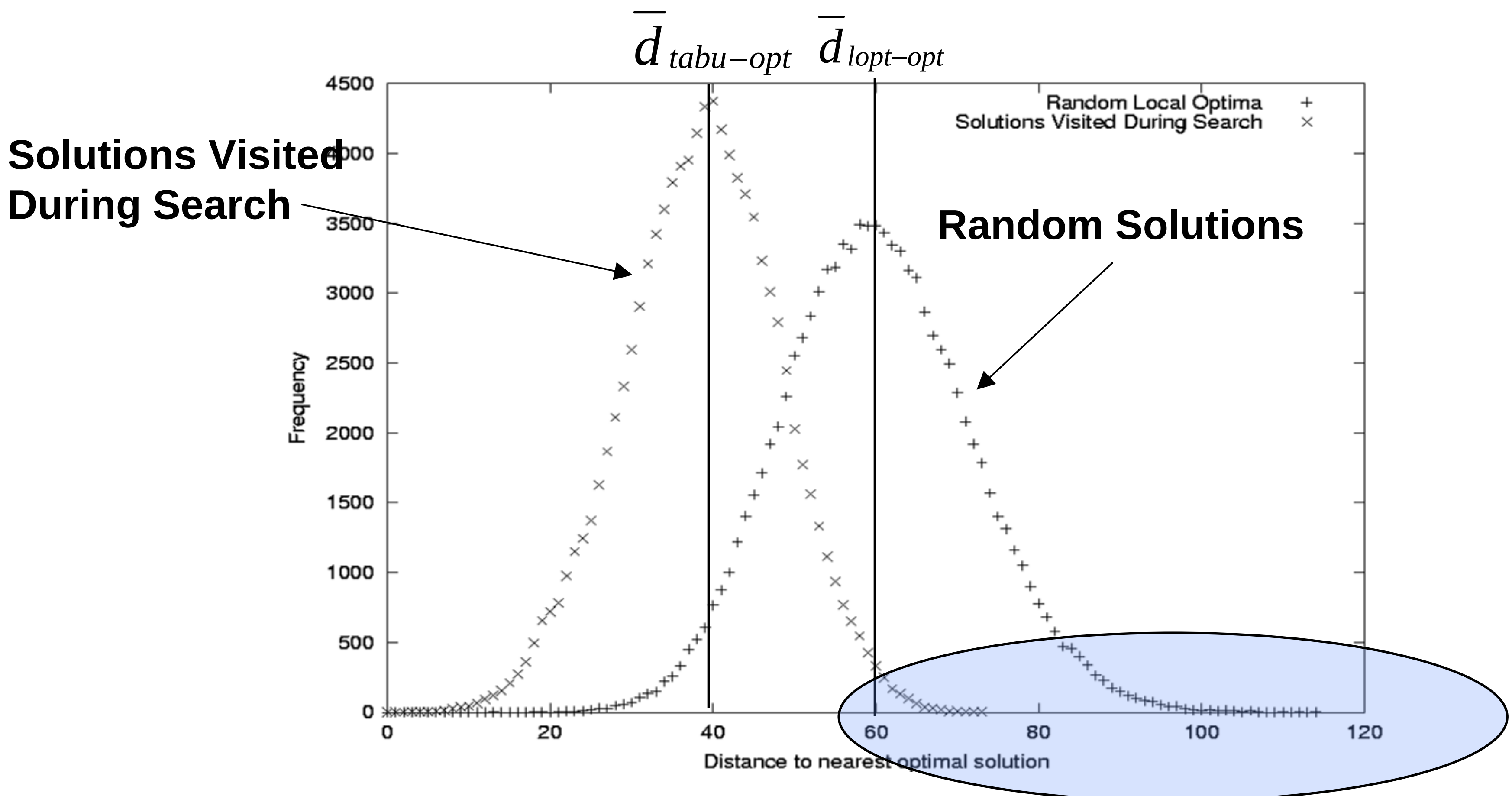
1. To account for variability in problem difficulty
   – Difficulty = cost to locate an optimal solution
   – *Cost models* of local search algorithms
2. To characterize the relationship between search space structure and problem difficulty
   – What features cause problems for local search?
3. To model the run-time behavior of local search algorithms
   – What is the high-level search strategy?

# Static Cost Models for the JSP: Summary

- New measure accounts for 65%-90% of the variability in problem difficulty for small JSPs…
- … but only 40-45% of the variability in large JSPs
- Conclusion
  - Problem difficulty is proportional to the effective size of the search space
  - But <u>only</u> to a first-order approximation
- Universal drawbacks to static cost models
  - Accuracy fails to scale to larger JSPs
  - No insight into run-time dynamics

# Bias and Tabu Search in the JSP

<u>Observation:</u> Random local optima are *not* necessarily representative of the set of solutions visited *during* search




Large differences in maximal distance!



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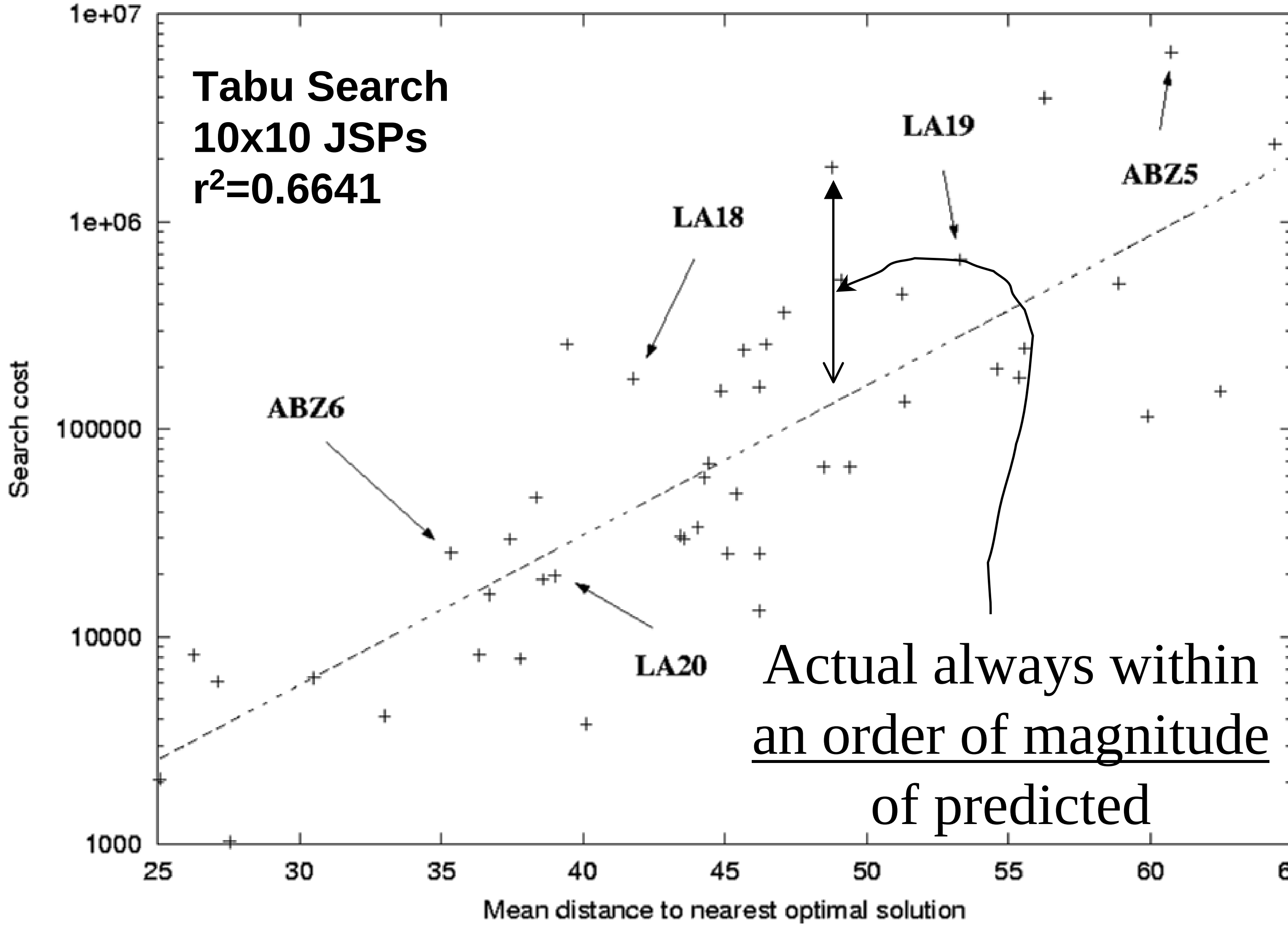
# Accuracy of the Quasi-Dynamic Model



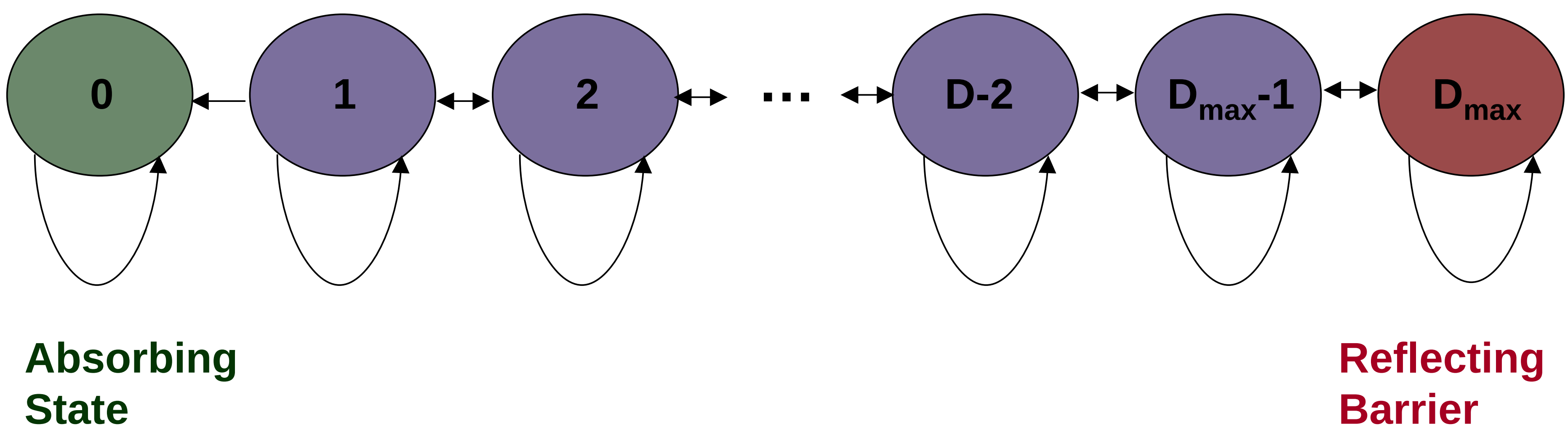

$\overline{d}_{tabu-opt}$

# Dynamic Cost Models

- Any local search algorithm can *in principle* be modeled as a Markov chain
  - Finite number of states
  - Exact transition probabilities
- Is this approach tractable?
  - No!
- Key issues in developing tractable Markov models
  - How to aggregate solutions?
  - How to model short-term memory? (if applicable)

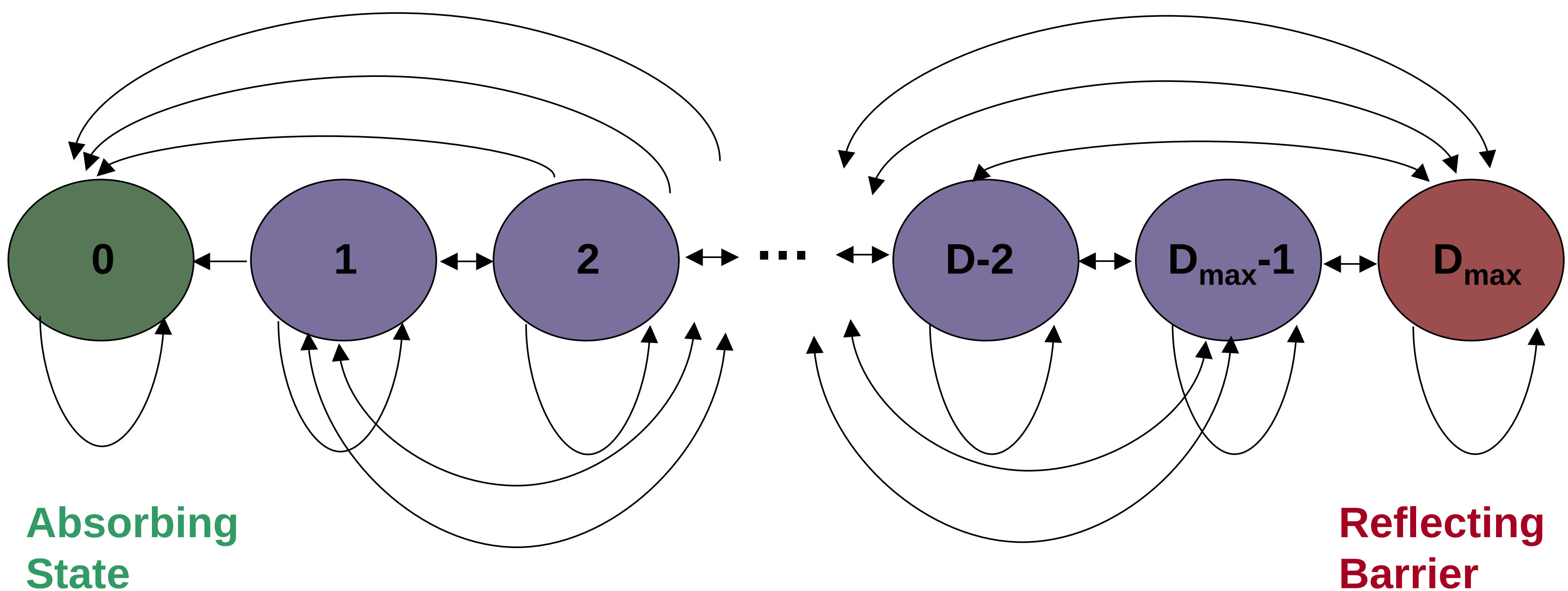
# A Markov Model of Metropolis Sampling

- Aggregate solutions based on their distance to the nearest optimal solution
- A simple one-dimensional random walk
- Equivalent to the Gambler's Ruin problem



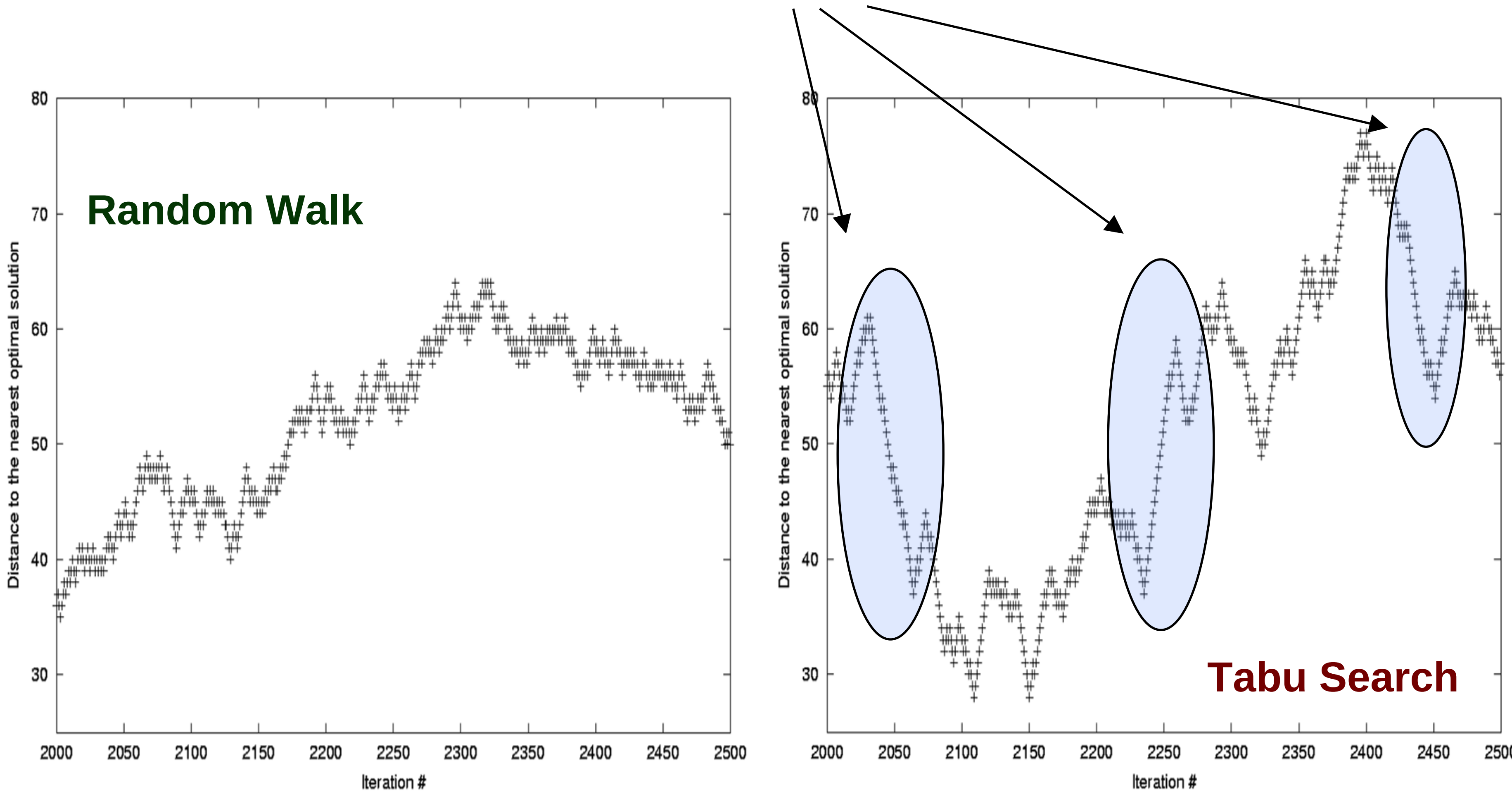
# A Markov Model of Iterated Local Search

- A generalized one-dimensional random walk…
- … but with restricted transition probabilities
- Large-distance jumps are highly unlikely



## Short-Term Memory and the Dynamics of Tabu Search

- Short-term memory consistently biases search either away from or toward the nearest optimal solution



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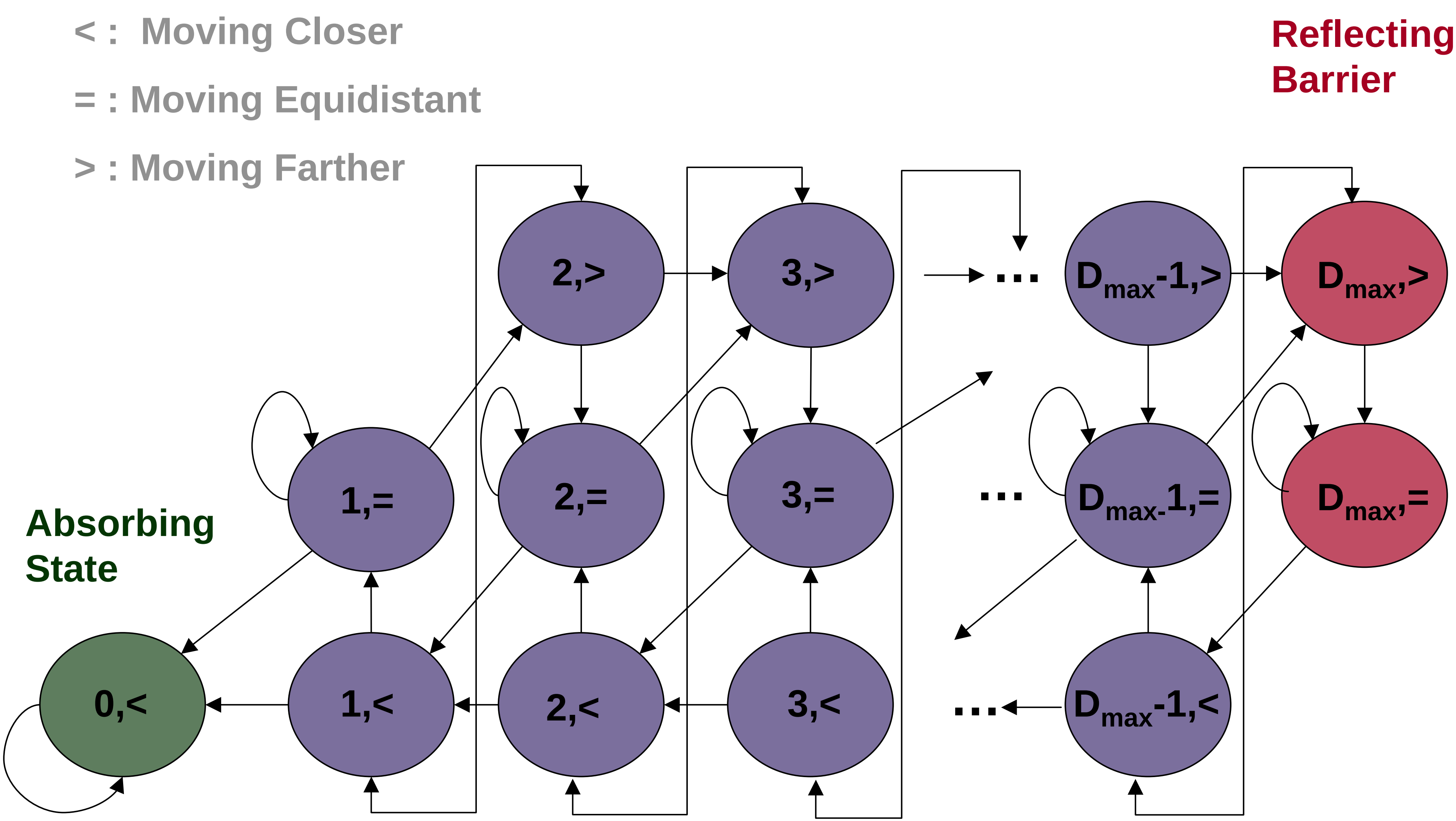
# A Markov Model of Tabu Search



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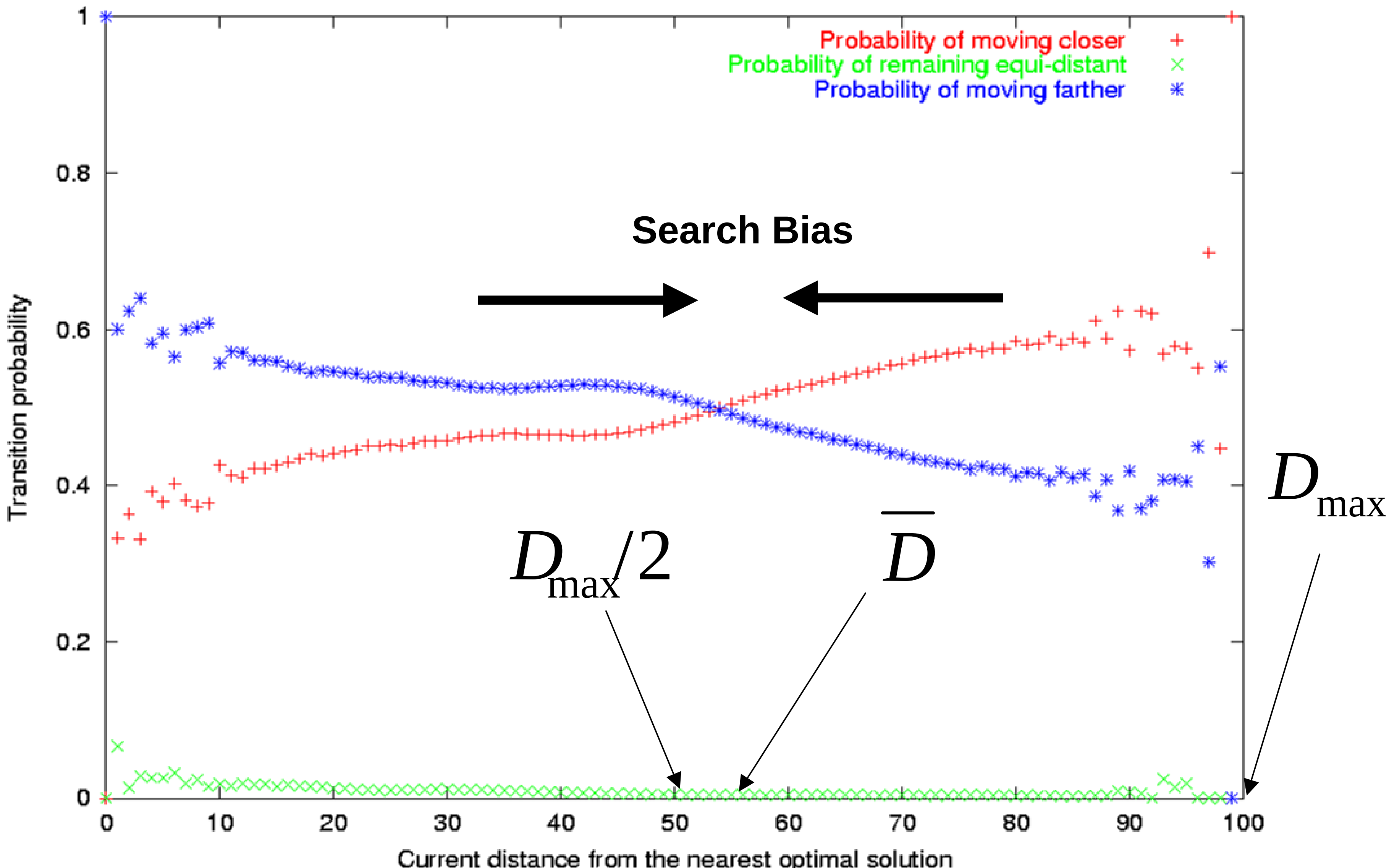
# Transition Probabilities Under Metropolis Sampling



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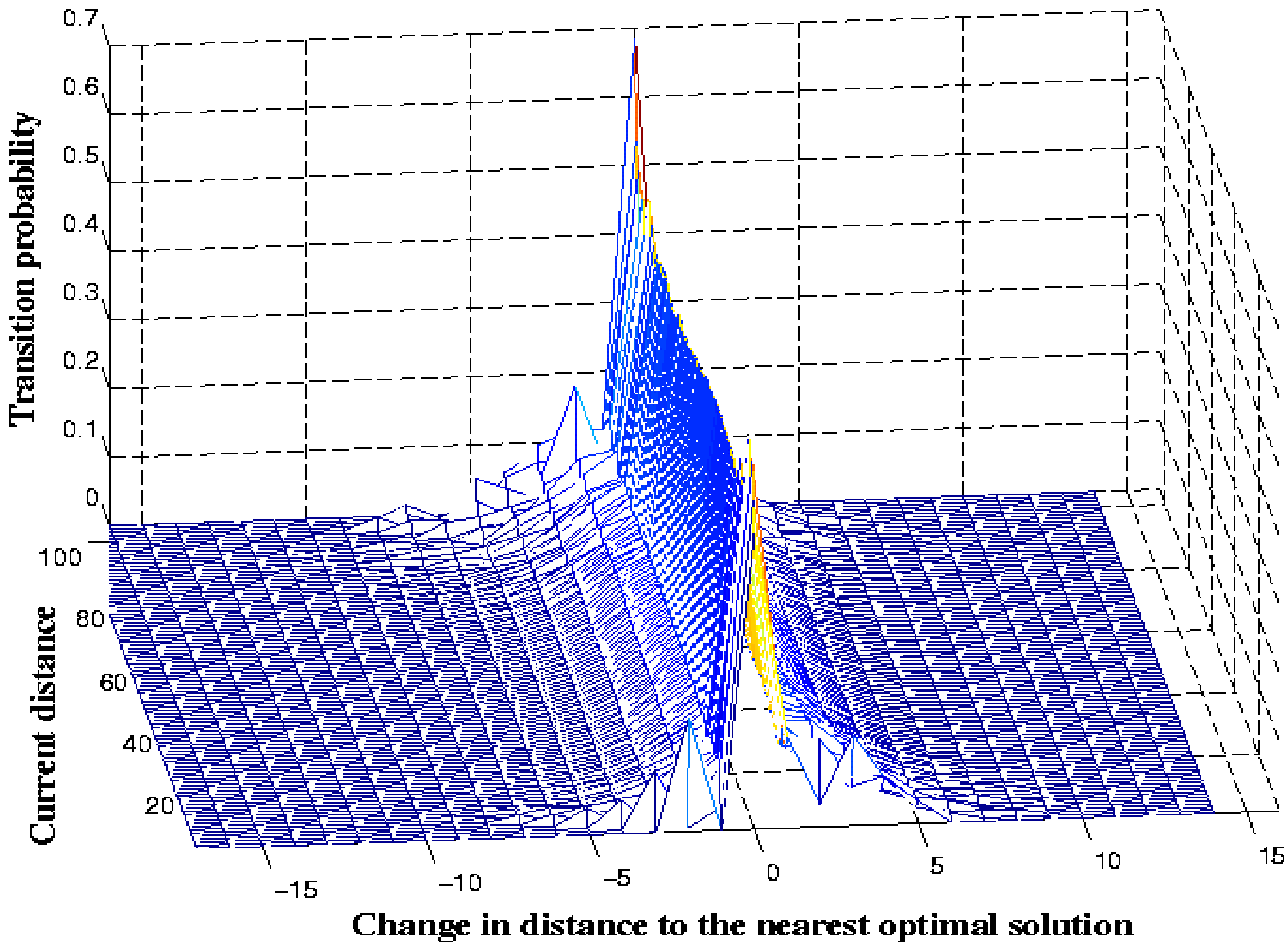
# Transition Probabilities Under Iterated Local Search



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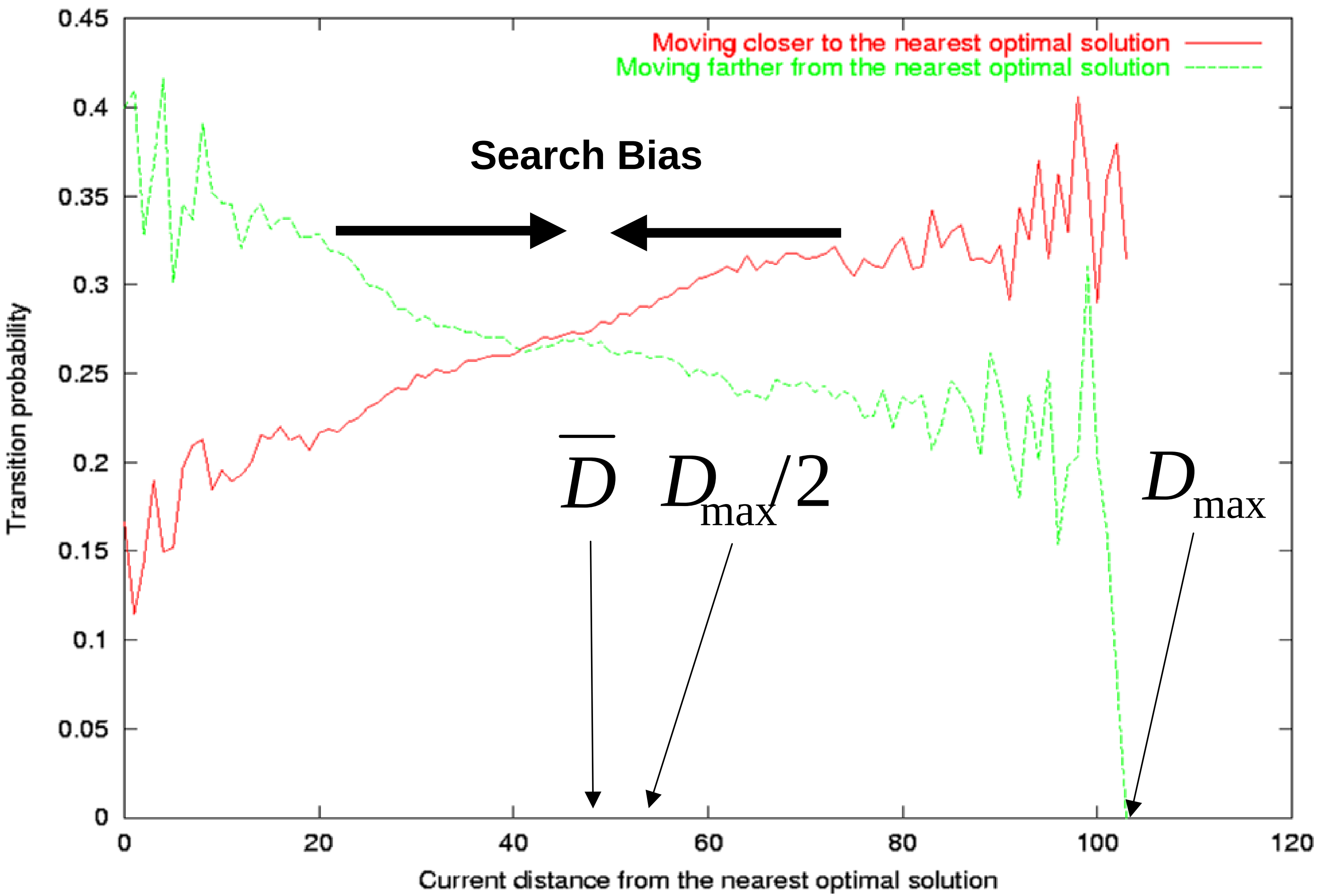
# Transition Probabilities Under Iterated Local Search



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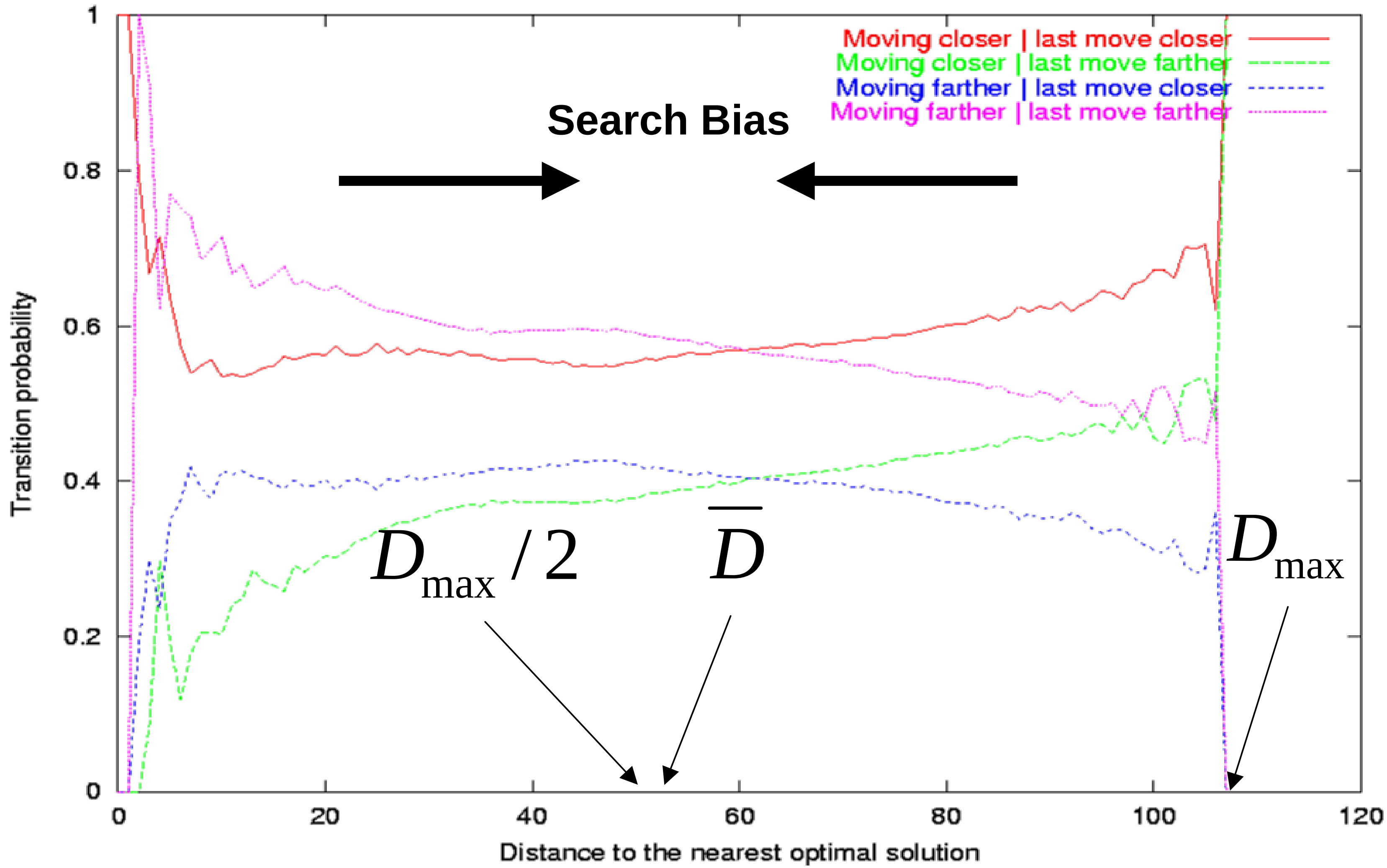
# Transition Probabilities Under Tabu Search



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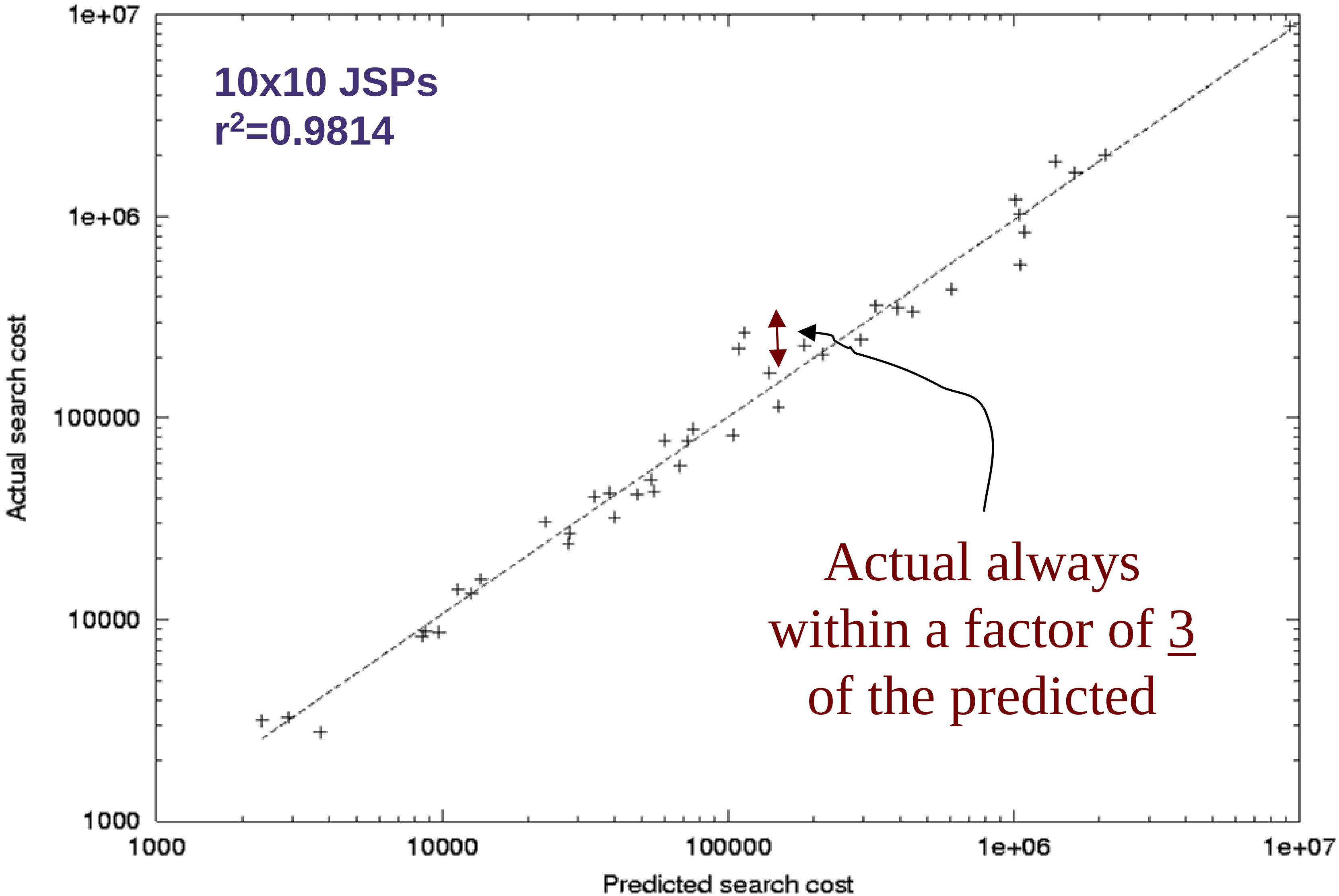
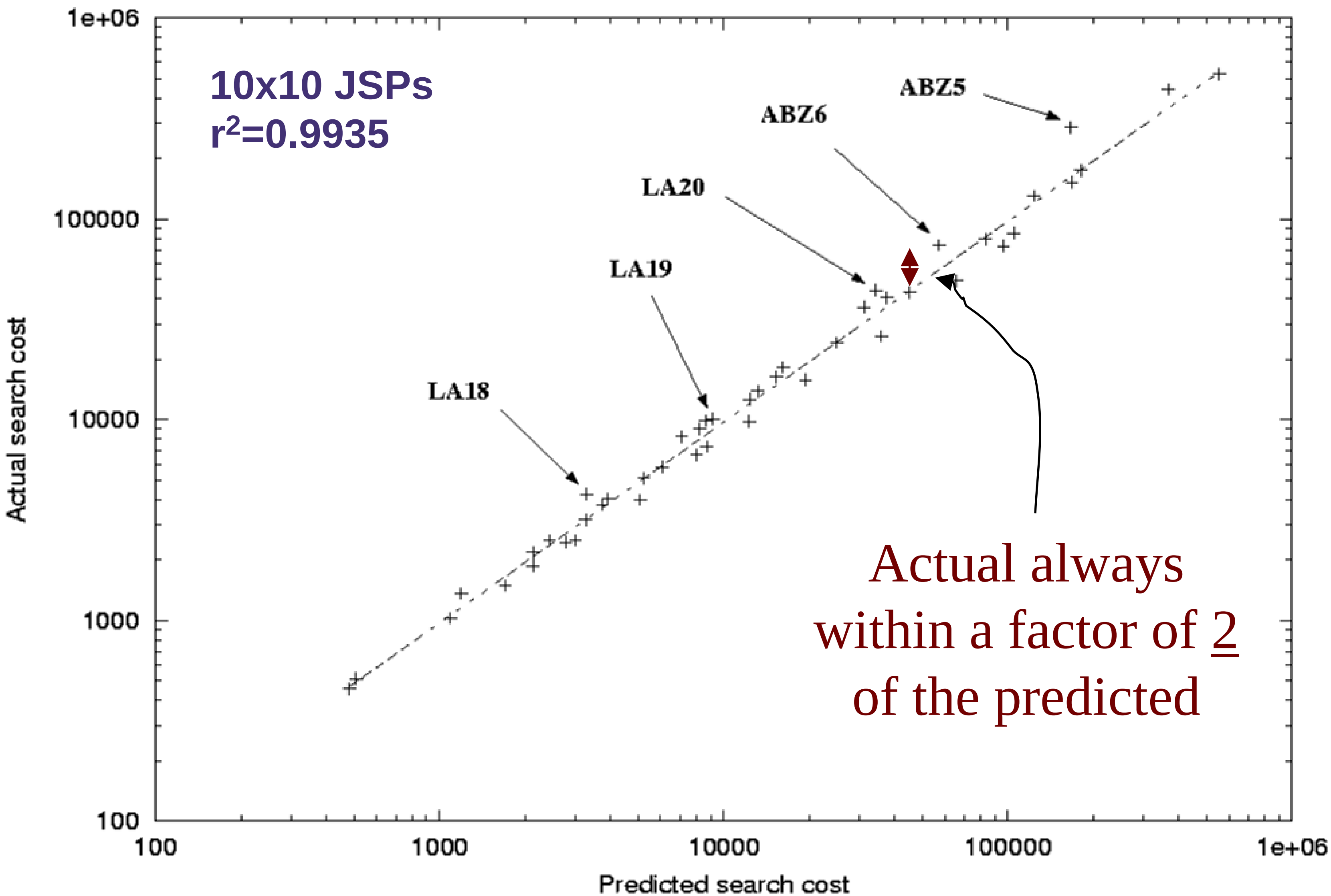
# Dynamic Cost Model Accuracy: Metropolis Sampling



# Dynamic Cost Model Accuracy: Iterated Local Search



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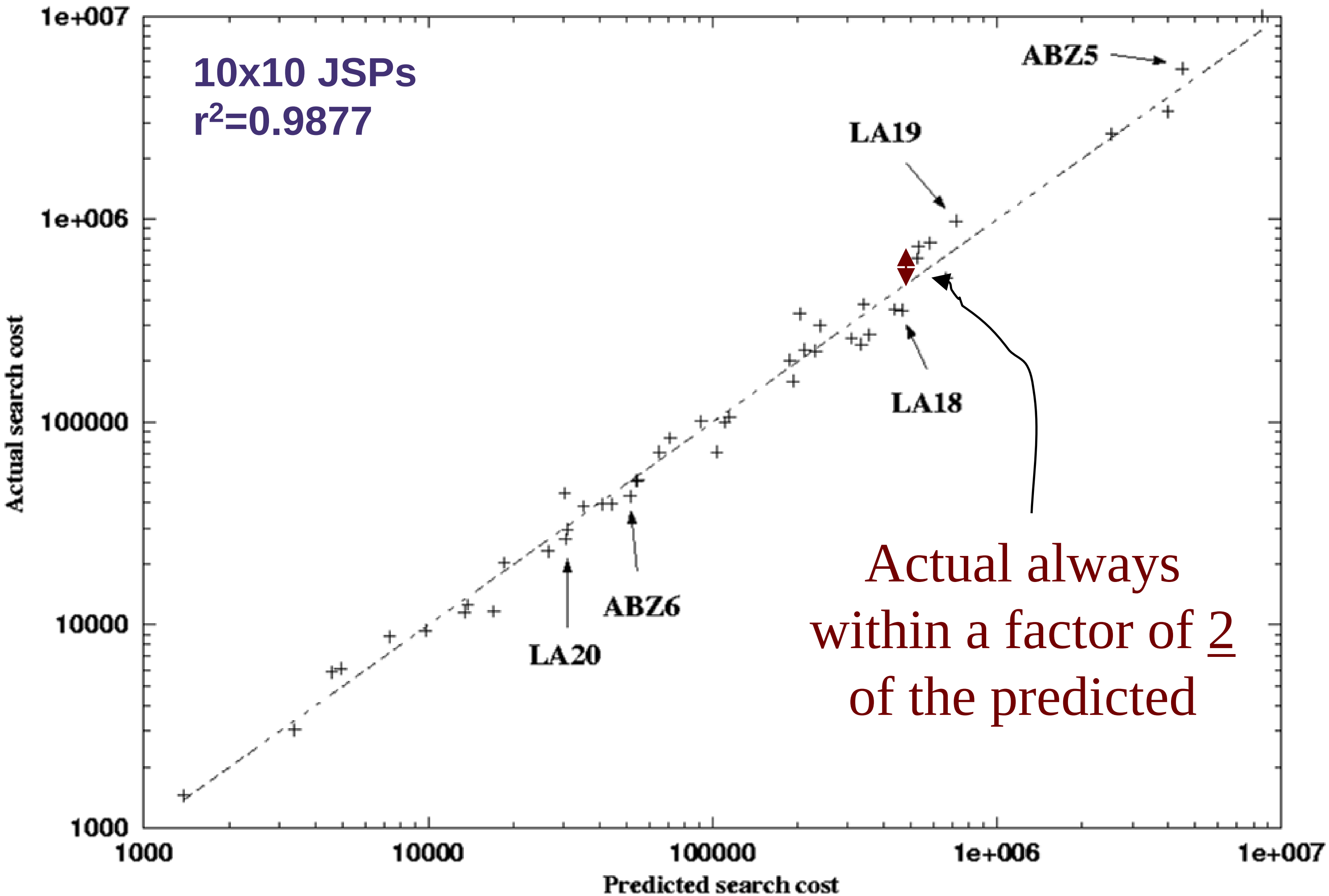
# Dynamic Cost Model Accuracy: Tabu Search



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# The Relationship Between the Cost Models

1. Search is biased toward solutions that are distance $\overline{D}$ from the nearest globally optimal solution
2. Search is biased toward solutions that are *approximately* distance $D_{\max}/2$ from the nearest globally optimal solution

=> $D_{\max} \approx 2\overline{D}$ !

- $\overline{D}$ *estimates* a key parameter of the dynamic model

- The static and quasi-dynamic models provide increasingly accurate estimates of $\overline{D}$

- Implication: Landscape structure and run-time dynamics are tightly linked

# Future Research Opportunities

- Generalization to other algorithms?
- Generalization to other problems?
- How does problem structure impact cost models?
- Applications
  - Can we estimate bias strength and $D_{max}$?
  - Can we *predict* search cost?
  - With what level of accuracy?
- Algorithm design
  - How can we minimize the impact of search space bias?
  - Do different representations induce different biases?

- *The analysis of fitness landscape structure and problem difficulty is effectively an open area*

# Closing Thoughts

- Fitness landscape structure is a key determinant in problem difficulty for a wide range of algorithmic search paradigms
  - *Ignoring structure in algorithm design leads to "iterated hacking"*
- Many landscape features thought to be highly correlated with problem difficulty aren't
  - *Always test your hypotheses*
- There can be very clear relationships between fitness landscape structure and algorithm run-time behavior
  - But these can only be identified via careful experimentation and analysis
- This research area is largely open
  - A lot of papers sound conclusive, but if you look more closely…