Blind No More: Constant Time Non-Random Improving Moves and Exponentially Powerful Recombination

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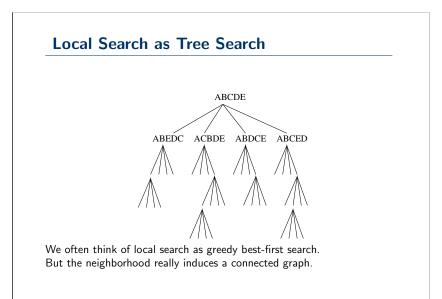
What is a Landscape?

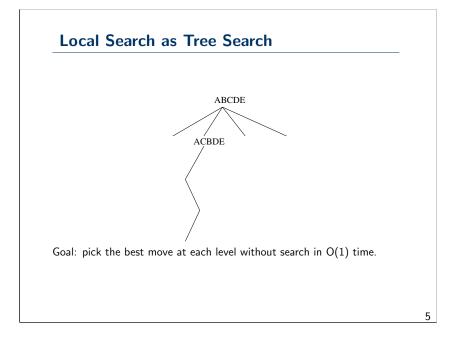


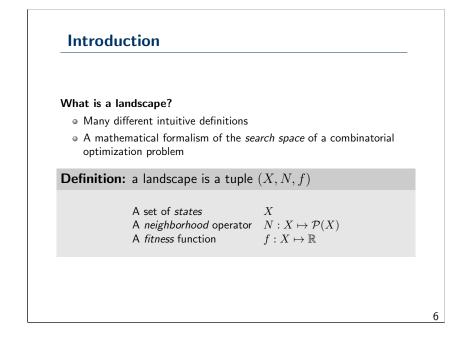
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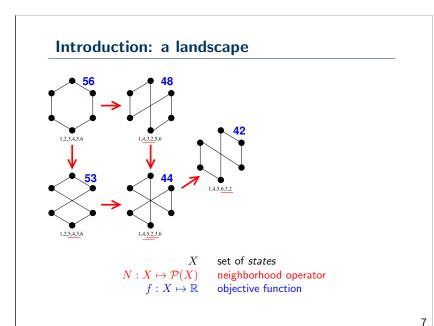
What is a Landscape?

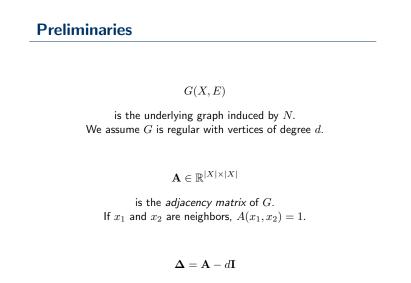












is the Laplacian of G.

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The Wave Equation: definition 1

Average change

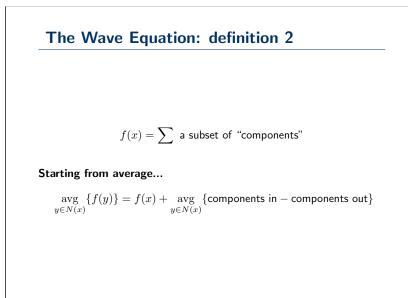
$$\Delta f = (\mathbf{A} - d\mathbf{I})f = k(\bar{f} - f)$$

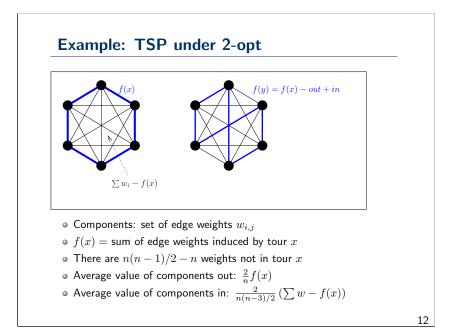
$$\Delta f(x) = \sum_{y \in N(x)} (f(y) - f(x)) = k(\bar{f} - f(x))$$

Average value

$$\sup_{y \in N(x)} \{f(y)\} = \frac{1}{d} \sum_{y \in N(x)} f(y)$$

= $f(x) + \frac{1}{d} \left(\sum_{y \in N(x)} f(y) - f(x) \right)$
= $f(x) + \frac{1}{d} \Delta f(x)$
= $f(x) + \frac{k}{d} (\bar{f} - f(x))$
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The Components and \bar{f}

Let C denote the set of components

 $0 < p_3 < 1$ is the proportion of the components in C that contribute to the cost function for any randomly chosen solution

$$\bar{f} = p_3 \sum_{c \in C} c$$

For the TSP:

$$\bar{f} = \frac{n}{n(n-1)/2} \sum_{w_{i,j} \in C} w_{i,j}$$
$$\bar{f} = \frac{2}{n-1} \sum_{w_{i,j} \in C} w_{i,j}$$

The Wave Equation: definition 2

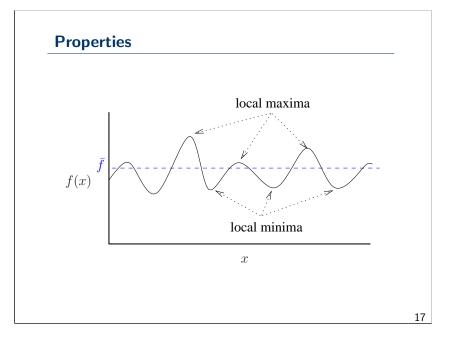
$$\begin{split} \sup_{y \in N(x)} \{f(y)\} &= f(x) + \frac{2}{n(n-3)/2} \left(\sum w - f(x) \right) - \frac{2}{n} f(x) \\ &= f(x) + \frac{2}{n(n-3)/2} \left((n-1)/2\bar{f} - f(x) \right) - \frac{2}{n} f(x) \\ &= f(x) + \frac{(n-1)}{n(n-3)/2} (\bar{f} - f(x)) \\ &= f(x) + \frac{k}{d} (\bar{f} - f(x)) \end{split}$$

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	ab	bc	cd	de	ae	ас	ad	bd	be	ce
ABCDE	1	1	1	1	1	 0	0	0	0	0
ABEDC	1	0	1	1	0	1	0	0	1	0
ABCED	1	1	0	1	0	0	1	0	0	1
ABDCE	1	0	1	0	1	0	0	1	0	1
ACBDE	0	1	0	1	1	1	0	1	0	0
ADCBE	0	1	1	0	1	0	1	0	1	0

Looking	at th	ie nei	-	rs in a	agg	regat				
ab	bc		de	ae		ас	ad	bd	be	ce
1	1	1	1	1		0	0	0	0	0
1	1	1	1	1		0	0	0	0	0
1	1	1	1	1		0	0	0	0	0
0	0	0	0	0		1	1	1	1	1
0	0	0	0	0		1	1	1	1	1

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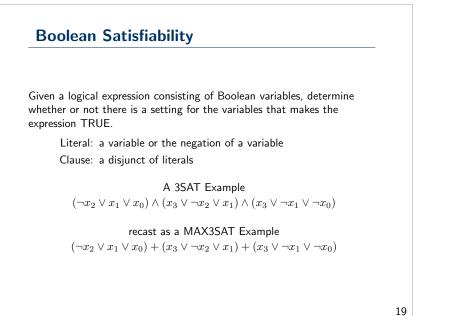
Walsh Functions

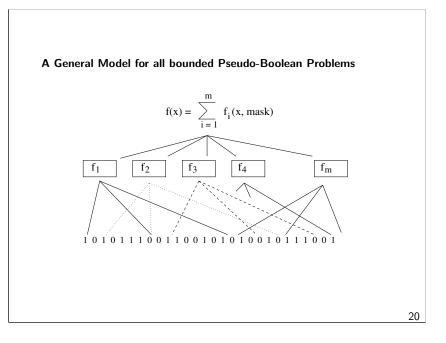
The Walsh Decomposition

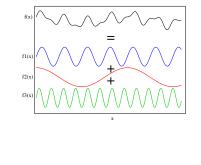
$$f(x) = \sum_{j=0}^{2^n - 1} w_j \psi_j(x)$$

Let bc(j) count the number of 1 bits in string j:

$$\begin{split} \psi_j(x) &= (-1)^{bc(j\wedge x)} \\ \text{If } bc(j\wedge x) \text{ is odd, then } \psi_j(x) &= -1 \\ \text{If } bc(j\wedge x) \text{ is even, then } \psi_j(x) &= 1. \\ w_j &= \frac{1}{2^n} \sum_{i=0}^{2^n-1} f(i) \psi_j(i) \end{split}$$







Walsh Analysis

Every n-bit MAXSAT or NK-landscape or P-spin problem is a sum of m subfunctions, $f_i\colon$

$$f(x) = \sum_{i=1}^{m} f_i(x)$$

The Walsh transform of f is is a sum of the Walsh transforms of the individual subfunctions.

$$W(f(x)) = \sum_{i=1}^{m} W(f_i(x))$$

Each subfunction f_i contributes only 2^K Walsh coefficients. Assuming m is O(n) then the number of Walsh coefficients is O(n).

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MAX-3SAT decomposition

MAX-3SAT is a superposition of 3 elementary landscapes

Walsh span of order p

$$\varphi^{(p)} = \sum_{\{i : bc(i)=p\}} w_i \psi_i$$

The p^{th} Walsh span is an elementary landscape

$$\Delta \varphi^{(p)} = -2p\varphi^{(p)}$$

MAX-3SAT decomposition

Recall that we can express f as:

$$f(x) = \sum_{i=1}^{m} \sum_{j=1}^{2^{k}} w_{m(i,j)} \psi_{m(i,j)}(x)$$

Grouping the Walsh decomposition results in

$$f(x) = \sum_{p=0}^{3} \varphi^{(p)}(x)$$

Thus MAX-3SAT is a superposition of 3-elementary landscapes

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Superpositions of Elementary Landscapes

$$\begin{split} f(x) &= f1(x) + f2(x) + f3(x) + f4(x) \\ f1(x) &= f1_a(x) + f1_b(x) + f1_c(x) \\ f2(x) &= f2_a(x) + f2_b(x) + f2_c(x) \\ f3(x) &= f3_a(x) + f3_b(x) + f3_c(x) \\ f4(x) &= f4_a(x) + f4_b(x) + f4_c(x) \end{split}$$
$$\begin{split} \varphi^{(1)}(x) &= f1_a(x) + f2_a(x) + f3_a(x) + f4_a(x) \\ \varphi^{(2)}(x) &= f1_b(x) + f2_b(x) + f3_b(x) + f4_a(x) \\ \varphi^{(3)}(x) &= f1_c(x) + f2_c(x) + f3_c(x) + f4_a(x) \\ f(x) &= \varphi^{(1)}(x) + \varphi^{(2)}(x) + \varphi^{(3)}(x) \end{split}$$

Constant Time Steepest Descent Let vector w' store the Walsh coefficients including the sign relative to solution x. $w'_i(x) = w_i \psi_i(x)$ Flip bit p such that $y_p \in N(x)$. Then if $p \subset i$ then $w'_i(y_p) = -w'_i(x)$ otherwise $w'_i(y_p) = w'_i(x)$ For MAX-kSAT and NK-Landscapes flipping one bit changes the sign of only a constant number of Walsh coefficients.

Constant Time Steepest Descent Construct a vector S such that $S_p(x) = \sum_{\forall b, \ p \subset b} w_b'(x)$ In this way, all of the Walsh coefficients whose signs will be changed by flipping bit p are collected into a single number $S_p(x)$.

Constant Time Steepest Descent

Lemma 1. Let $y_p \in N(x)$ be the neighbor of string x generated by flipping bit p.

$$f(y_p) = f(x) - 2(S_p(x))$$

If $p \subset b$ then $\psi_b(y_p) = -1(\psi_b(x))$ and otherwise $\psi_b(y_p) = \psi_b(x)$.

Corollary:

Because f(x) is constant wrt p: Maximizing $S_p(x)$ minimizes the neighborhood of f(x).

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Constant Time Steepest Descent

To make this easy, assume such that every variable occcurs exactly the same number of times. Then each variable appears in km/N = kc subfunctions.

This easy case analysis also exactly corresponds to the average complexity case (with mild restrictions on the frequency of bit flips).

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Constant Time Steepest Descent

When one bit flips, it impacts $k c \ {\rm subfunctions.}$

At most ck(k-1) terms in vector S change.

When one bit flips, at most $ck(2^{k-2})$ nonlinear Walsh coefficients change, and only 1 linear term changes.

Thus, the update take O(1) time.

The locations of the updates are obvious

$$S_{1}(y_{p}) = S_{1}(x)$$

$$S_{2}(y_{p}) = S_{2}(x)$$

$$S_{3}(y_{p}) = S_{3}(x) + \sum_{\forall b, (p \land 3) \subset b} w'_{b}(x)$$

$$S_{4}(y_{p}) = S_{4}(x)$$

$$S_{5}(y_{p}) = S_{5}(x)$$

$$S_{6}(y_{p}) = S_{6}(x)$$

$$S_{7}(y_{p}) = S_{7}(x)$$

$$S_{8}(y_{p}) = S_{8}(x) + \sum_{\forall b, (p \land 8) \subset b} w'_{b}(x)$$

$$S_{9}(y_{p}) = S_{9}(x)$$

"Old" and "New" improving moves

A "new" improving move must be a new updated location in S. Checking these takes ${\cal O}(1)$ time on average.

There can be previously discovered "old" moves stored in a buffer.

For MAX-kSAT we use a fixed number of buffers to track "old" moves. This can be done (virtually always) in O(1) time.

Next Ascent

If we want to do Next Ascent instead of Steepest Ascent, we just all of the improving moves into a buffer and pick one. Again, this takes ${\cal O}(1)$ time.

Identifying Local Optima

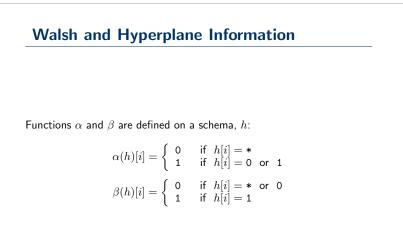
If there are no improving moves, the point is a local optimum. The point is automatically identified: there are no "old" improving moves and no update is an improving move.

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Speed Results for MAXSAT Solvers

	AdaptG2WSAT	GSAT	Walsh
UR-1000000	698.86	32.13	1.80
UR-2000000	3458.06	140.37	3.88
UR-3000000	8157.01	319.95	6.05
mem-ctrl2	4120.52	54.11	4.17
wb_4m8s-48	7339.77	83.16	6.06

Table: Time in seconds require to reach a Local Optima for several stochastic local search algorithms for MAX-kSAT problems.



Walsh and Hyperplane Information

$$f(h) = \frac{1}{|h|} \sum_{x \in h} f(x) = \sum_{j \subseteq \alpha(h)} w_j \psi_j(\beta(h))$$

 $\begin{array}{l} \alpha(h) \text{ is a mask used to select } 2^{o(h)} \text{ relevant coefficients.} \\ \beta(h) \text{ extracts the 1 bits from the respective coefficients.} \\ \text{An odd number of 1 bits yields a negative sign.} \\ \text{Example: Let } h = **01** \text{ and compute } f(h) \end{array}$

 $\alpha(**01**) = 001100 \text{ and } \beta(**01**) = 000100$

 $j \in \{$ 000000, 000100, 001000, 001100 $\}$

$$f(**01**) = w_0 - w_4 + w_8 - w_{12}.$$

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Hyperplane Initialization

The Hyperplane Advantages:

Start from 1) a good solutions and 2) in a good subspace For each clause, select the order-3 hyperplane which yields the best average evaluation.

Use this hyperplane information to select a starting point for search (which is guaranteed to be below average).

$$f(****010) = w_0 + w_1 - w_2 + w_4 - w_3 + w_5 - w_6 - w_7.$$

Calculations take 23 additions (FFT/WFT Butterfly) per clause.

$$f(****010) = ((w_1) - (w_2 + w_4)) - ((w_3 - w_5) + (w_6 + w_7)).$$

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Results for MAXSAT Solvers

	HyperWalsh	Walsh	GSAT	AdaptG2WSat
div-8	5467 ± 197	13761	13066 ± 187	10795 ± 93
c2-1	12819 ± 80	19524	19595 ± 116	16056 ± 251
b15	24517 ± 149	30803	31509 ± 149	27920 ± 176
mrisc	6435 ± 258	40851	39628 ± 588	34301 ± 768
rsd-37	22976 ± 167	92361	87911 ± 533	64162 ± 355
mem-c2	29649 ± 368	75729	73071 ± 584	38277 ± 535
3sat-1m	29249 ± 125	41511	40418 ± 165	30856 ± 134
3sat-2m	58415 ± 186	82898	80696 ± 220	61466 ± 182

Table: Mean and standard deviation of evaluations of solutions found after \boldsymbol{n} bit flips by several algorithms.

Steepest Descent over Neighborhood Means

We have the vector \boldsymbol{S} such that

$$S_p(x) = \sum_{\forall b, \ p \subset b} w'_b(x)$$

Also construct the vector Z such that

$$Z_p(x) = \sum_{\forall b, \ p \subset b} \quad order(b) \ w'_b(x)$$

Note that S and Z and U all update at exactly the same locations.

Lemma 2.

$$Avg(N(y_p)) = Avg(N(x)) - 2(S_p(x)) + \frac{4}{N}Z_p(x)$$

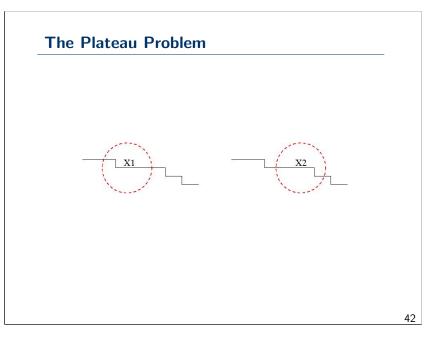
Steepest Descent over Neighborhood Means

Let
$$U_p(x) = -2(S_p(x)) + \frac{4}{N}Z_p(x)$$

 $Avg(N(y_p)) = Avg(N(x)) + U_p(x)$

The vector U(x) can now be used as a proxy for Avg(N(x))Maximizing $U_p(x)$ minimizes the neighborhood of $Avg(N(y_p))$.

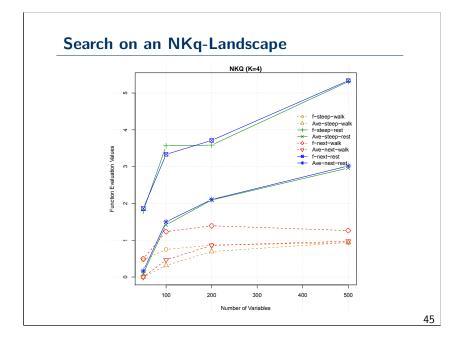


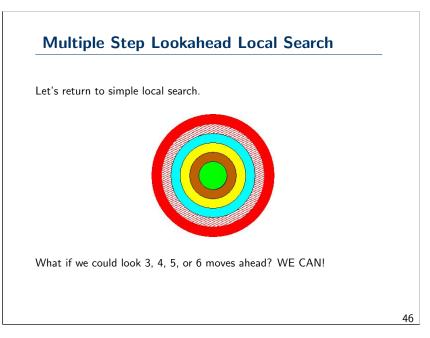


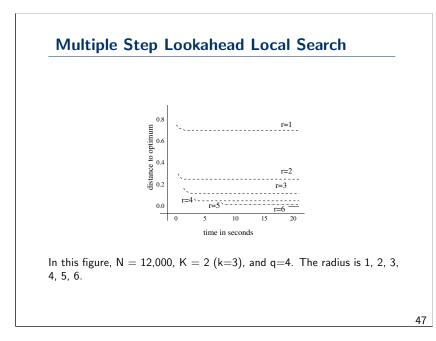
The locations of the updates are obvious $U_1(y_p) = U_1(x)$ $U_2(y_p) = U_2(x)$

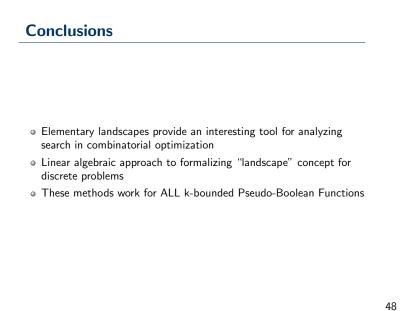
$$egin{array}{rcl} U_2(y_p) &=& U_2(x) \ U_3(y_p) &=& U_3(x) + Update \ U_4(y_p) &=& U_4(x) \ U_5(y_p) &=& U_5(x) \ U_6(y_p) &=& U_6(x) \ U_7(y_p) &=& U_7(x) \ U_8(y_p) &=& U_8(x) + Update \ U_9(y_p) &=& U_9(x) \end{array}$$

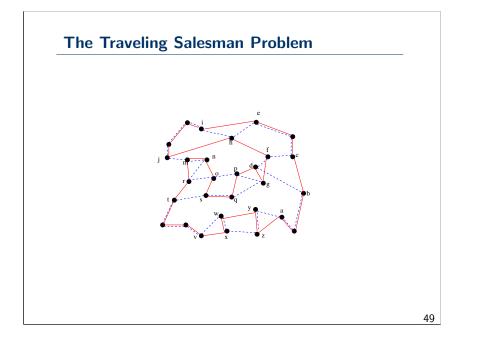
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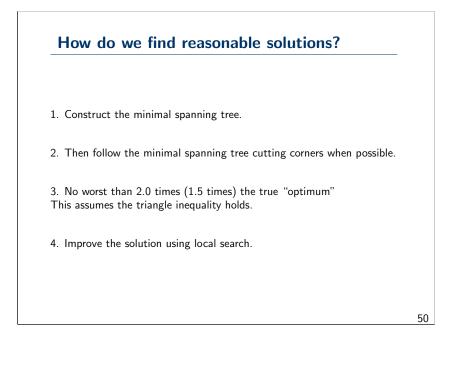


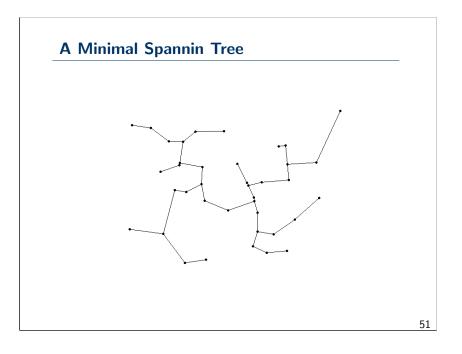




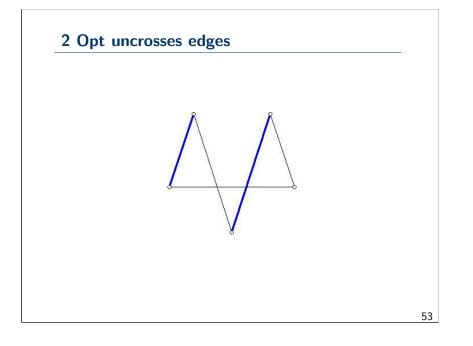








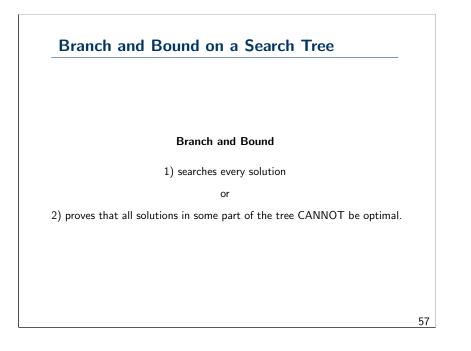
2 Opt	
A	
A B C D E F G H I J K L M N O P Q S T U V W X Y Z	
A B C D E F G P O N M L K J I H Q S T U V W X Y Z	
Do this forall pairs of break points. $O(N^2)$	
$O(N^2)$	

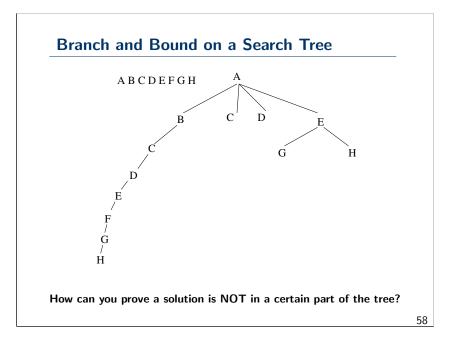


3 Opt	
A B C D E F G H I J K L M N O P Q S T U V W X Y Z	
A B C D E F G V U T S Q H I J K L M N O P W X Y Z	
Do this forall triples of break points.	
$O(N^3)$	

Lin-Kernighan K-Opt

Partial Eva	luation
our X: A B C D	E F GH I J K L M N O PQ S T U V W X Y Z
our Y: A B C D I	E F GP O N M L K J I HQ S T U V W X Y Z
(Y) = F(X) - edg	ge(G,H) - $edge(P,Q)$ + $edge(G,P)$ + $edge(H,Q)$
(1) time evalutio	n of ${\cal O}(n^2)$ neighbors.





B C	$egin{array}{c} w_{a,b} \ w_{a,c} \end{array}$	$w_{b,c}$				
D E	$w_{a,d}$ $w_{a,e}$	$w_{b,d}$ $w_{b,e}$	$w_{c,d}$ $w_{c,e}$	$w_{d,e}$	$\frac{w_{e,f}}{E}$	
F	$w_{a,f}$	$\frac{w_{b,f}}{B}$	$\frac{w_{c,f}}{C}$	$\frac{w_{d,f}}{D}$	$\frac{w_{e,f}}{F}$	
		D	C	D	L	

How can we speed up local search?

Only use the shortest edges. Usually only need 10 percent of the edges.

В	XXX				
С	XXX	$w_{b,c}$			
D	$w_{a,d}$	$w_{b,d}$	XXX		
Е	$\begin{array}{c} XXX\\ XXX\\ w_{a,d}\\ w_{a,e} \end{array}$	$w_{b,e}$	$w_{c,e}$	XXX	
F	$w_{a,f}$	XXX	XXX	$w_{d,f}$	$w_{e,f}$
	A	В	С	D	E

On the famous ATT532 city problem, there are 532*531/2 edges. Use the 25 shortest edges for each city (532*25). This set includes the global optimum.

Evolutionary Algorithms

- 1. We generate a population of solutions
- 2. We take 2 parents out of the population and create 2 offspring
- 3. We evaluate the new offspring

4. Using "Truncation Selection" we keep the best solutions found so far (or apply some other form of selection).

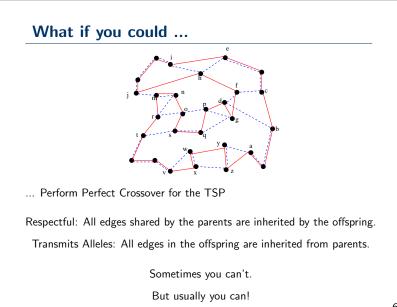
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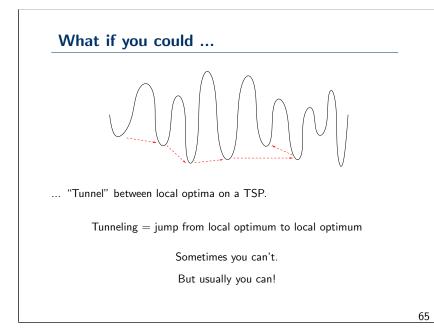
Evolutionary Algorithms

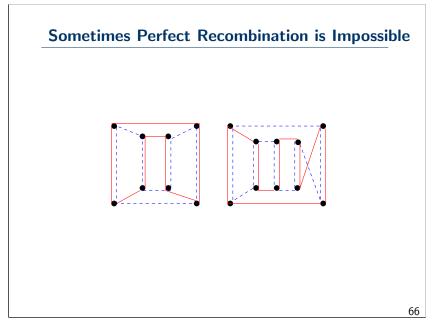
For bit strings, recombination is easy.

Parent One:	00000000000000000 - 00000000000
Parent Two:	111111111111111111111111111111111111111
Child:	00000000000000000 - 111111111111

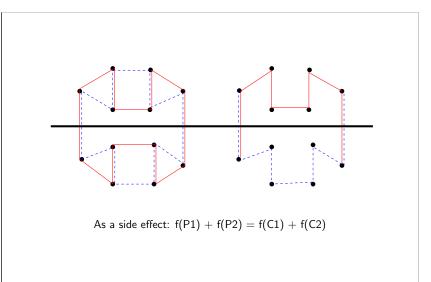
Evolutionary Algorithms But you can't just cut and paste permutations. Parent One: A B C D E F G - H I J K L Parent Two: D H A F I J B - A L C E G Child??: A B C D E F G - A L C E G

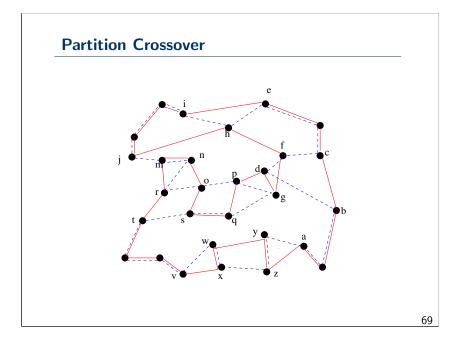


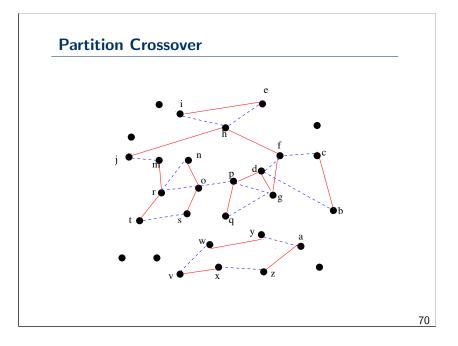


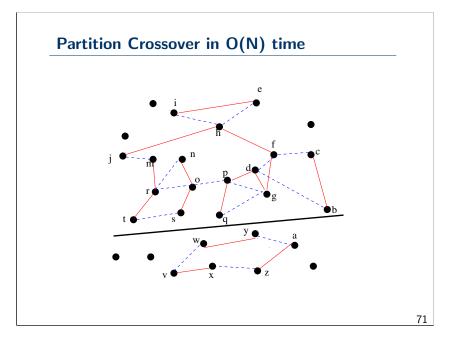


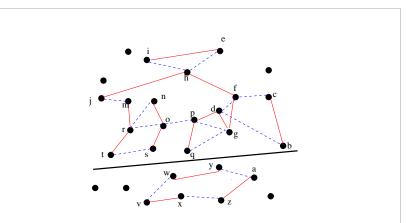
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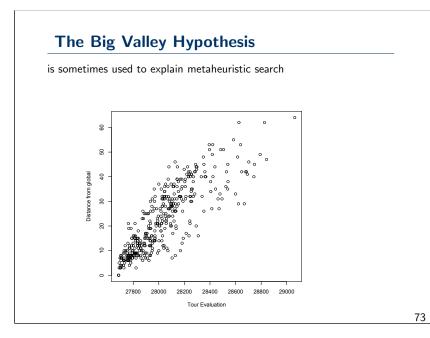






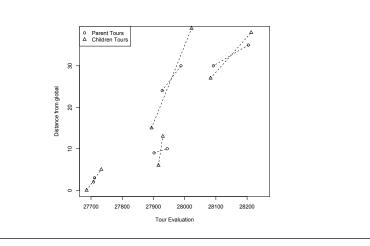
Why are the offspring usually local optima? Because the "pieces" that are recombined are already locally optimal, and they are inherited intact.

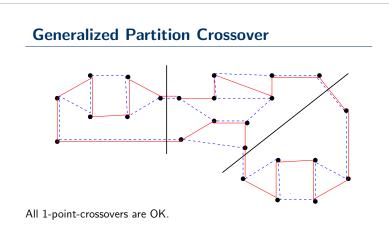
Only if 2-opt moves vertices across the partition is improvement possible.



Tunneling Between Local Optima

Local Optima are "Linked" by Partition Crossover





Generalize Partition Crossover is always feasible if the partitions have 2 exits (same color in and out). If a partition has more than 2 exits, the "colors" must match.

This will automatically happen if all of the partitions have cut two.

Instance	att532	nrw1379	rand1500	u1817
2-opt	3.3 ± 0.2	3.2 ± 0.2	3.7 ± 0.3	5.0 ± 0.3
3-opt	10.5 ± 0.5	11.3 ± 0.5	24.9 ± 0.2	26.2 ± 0.7
LK-search	5.3 ± 0.2	5.2 ± 0.3	10.6 ± 0.3	13.3 ± 0.4

Table: Average number of *partition components* used by GPX in 50 recombinations of random local optima found by 2-opt, 3-opt and LK-search.

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	1 be a randomly generated population;
	2 be a temporary child population;
	P1: apply LK-search and evaluate;
1	. Recombine best tour of $P1$ with the remaining $t-1$ tours;
	this generates a set of up to $2t$ offspring.
2	. If recombination was not feasible
	mutate tour i and place in population $P2$;
3	Place the best solution found so far in population $P2$;
4	Select offspring to fill population $P2$;
5	For each member of $P2$: apply LK-search and evaluate;
6	P1 = P2; If stopping condition not met, goto 1.
	Figure: The Hybrid GA; the GA is generational, but elitist.
6	

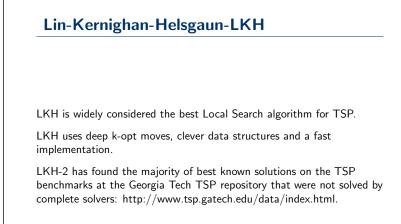
	rand500	att532	nrw1379	rand1500	u1817
Hybrid GA	50/50	26/50	1/50	12/50	1/50
Chained-LK	38/50	16/50	1/50	2/50	0/50

Table: The number of times the global optimum is found by each algorithm after 1010 calls to LK-search over 50 experiments.

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	Global Edges	Clobal Edges	Unique Edges
	U U	Global Edges	Unique Edges
	in Population	in Minimum Tour	in Population
rand500	500 ± 0	449.68 ± 1.98	941.56 ± 1.56
att532	532 ± 0	464.1 ± 2.11	979.54 ± 1.47
nrw1379	1378.9 ± 0.04	1162.3 ± 3.44	2709.34 ± 2.25
rand1500	1500 ± 0	1301.02 ± 4.15	2871.9 ± 3.14
u1817	1815.12 ± 0.18	1562.44 ± 3.22	3616.92 ± 4.71

Table: Results obtained by running the hybrid GA for only 5 generations and *without* mutation.



LKH-2 and Clustered Instances

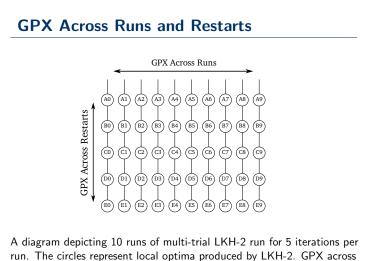
Empirical experiments show that LKH-2 performs significantly worse on random clustered instances than uniform random instances. We conjecture that its performance on clustered instances could be improved by exploiting crossover.

Iterative Partial Transcription and GPX

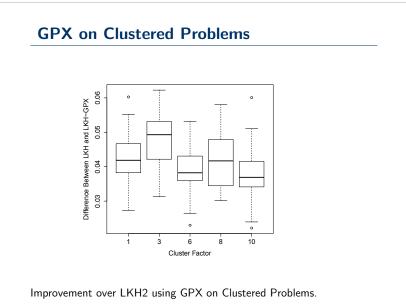
Instance	C3k.0	C3k.1	C10k.0	C10k.1	C31k.0	C31k.1
LKH-2 no x-over	0.660	0.863	1.143	1.009	1.489	1.538
LKH-2 w IPT	0.622	0.656	1.040	0.873	1.280	1.274
LKH-2 w GPX	0.622	0.651	1.031	0.872	1.270	1.267

The minimum percentage above the Held-Karp Bound for several clustered instances of the TSP of solutions found by ten random restarts of LKH-2 without crossover, with IPT and with GPX. Best values for each instance are in boldface. Sizes range from 3000 to 31,000 cities.

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A diagram depicting 10 runs of multi-trial LKH-2 run for 5 iterations per run. The circles represent local optima produced by LKH-2. GPX across runs crosses over solutions with the same letters. GPX across restarts crosses over solutions with the same numbers.



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