THE UBIQUITOUS SEARCH (METHODS TO ESCAPE FROM LOCAL MINIMA)

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Outline

- Characteristics of
  - Search Problems
  - Search Algorithms
- Existing methods to
  - Help escape from local minima
  - Handle constraints
- NOVEL: Nonlinear Optimization With External Lead
- Applications of NOVEL
  - Nonlinear continuous constrained optimization problems
  - Filter bank design problems
  - Nonlinear discrete satisfiability problems
  - Feedforward neural network learning problems

Motivations

- Many real-world applications
  - Artificial intelligence
  - Logic
  - Computer aided design
  - Database query processing
  - Planning
  - Scheduling
- Complete methods cannot handle large problems
- Global search versus local search

Characteristics of Search Problems

- Levels of search problem
  - Problem instance level
  - Meta level: generalization of solution
- Search space
  - Finite/infinite
- Variables
  - Fixed and well defined/undefined (and possibly unbounded)
  - Discrete/continuous/mixed/symbolic

Characteristics of Search Problems (cont'd)

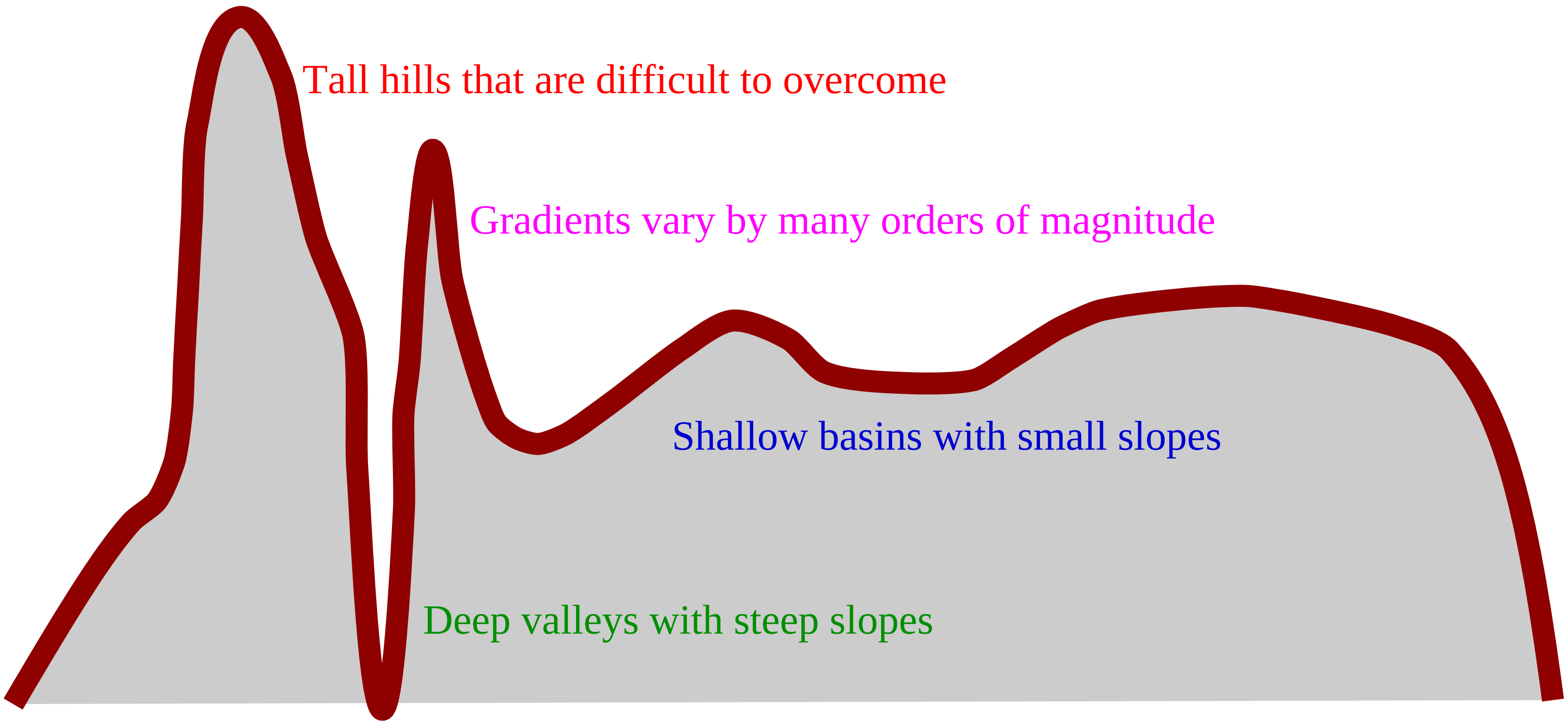
- Objective
  - Well defined/undefined
  - Linear/nonlinear/symbolic
- Objective measures
  - Deterministic/probabilistic
  - Resource measures
- Constraints
  - Hard/soft constraints
  - Linear/nonlinear/symbolic
  - Resource constraints

Characteristics of Search Algorithms

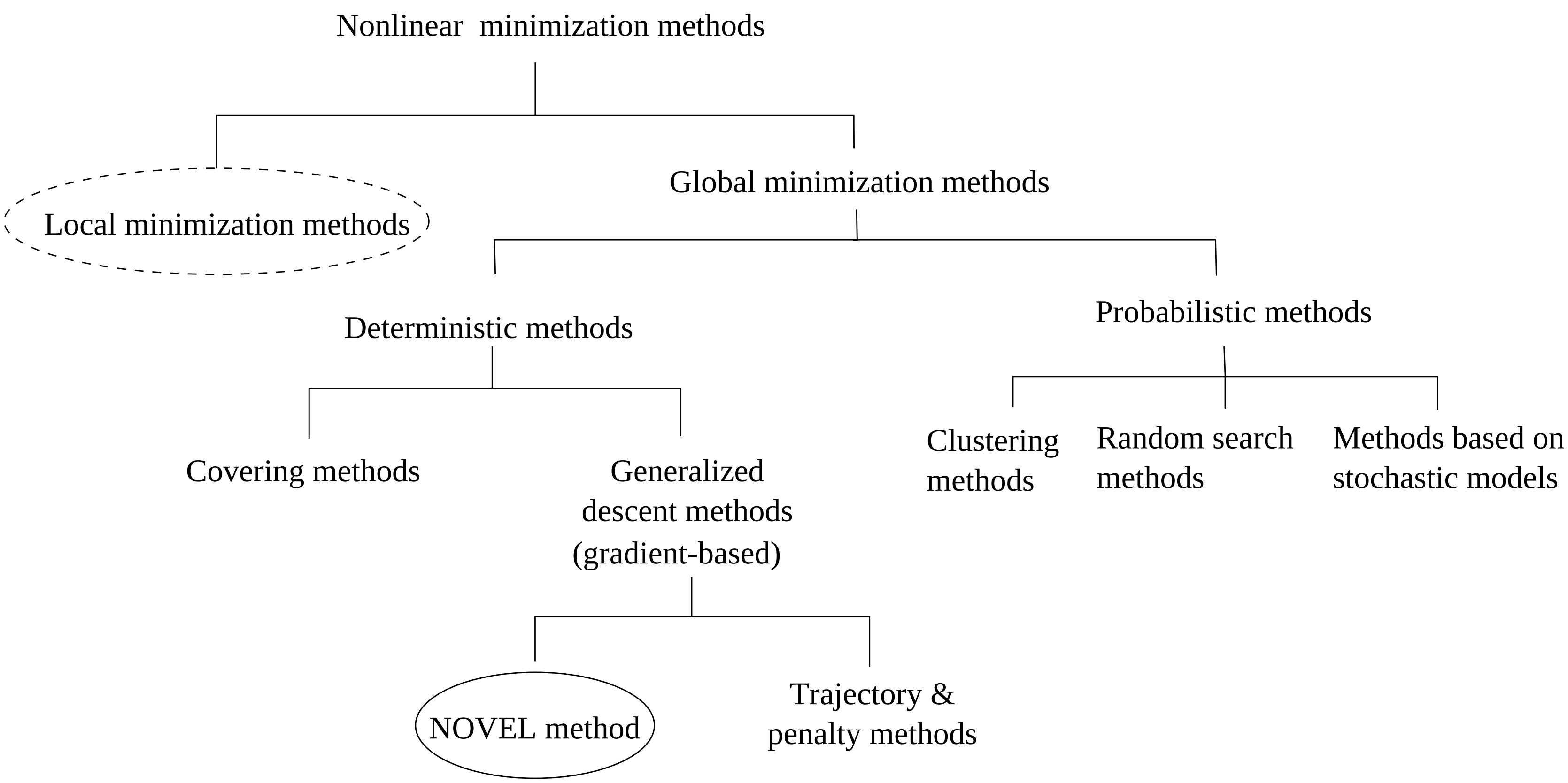
- Representation of search space
  - Search complexity
- Decomposition strategies
- Heuristic predictor or direction finder
  - Relaxation algorithms
- Mechanisms to help escape from local minima
- Mechanisms to handle constraints
- Stopping conditions
- Resource scheduling strategies

METHODS TO HELP ESCAPE FROM LOCAL MINIMA

Local Minima



Existing Methods to Help Escape from Local Minima



Existing Methods (cont'd)

Deterministic methods

- Covering – Detect regions not containing global minima and exclude them
- Trajectory – Modify differential equations modeling local descents
- Penalty – Modify objective function to avoid redetermination of the same local minima

Probabilistic methods

- Clustering – Group points around local minima (difficult when terrain is rugged)
- Random – Single start, multi-start, random line search, adaptive random search, evolutionary algorithms, simulated annealing
- Stochastic – Use random variables to model unknown values of objective (Bayesian)

Existing Methods: Summary

- Covering methods and methods based on stochastic models are inefficient in dealing with problems with more than 20 variables
- Generalized descent methods and clustering methods are inefficient in dealing with problems with many local minima
  - Descent methods get trapped in local minima
- Random search methods are inefficient due to randomness and redetermination of local minima

HANDLING CONSTRAINTS

Existing Methods for Handling Constraints

- Non-transformational approaches
  - Discarding methods
  - Back-to-feasible-region methods
- Transformational approaches
  - Penalty methods
    - Optimize sum of objective and constraints weighted by penalties
    - Penalize suboptimal solutions weighted by penalties in objective
  - Barrier methods: add new barriers during search
  - Lagrange-multiplier methods

Lagrangian Methods

- Optimization problem

$$\begin{aligned} \text{minimize} \quad & f(x) \\ \text{subject to} \quad & h(x) = 0 \end{aligned}$$

- Lagrangian/Augmented Lagrangian functions

$$\begin{aligned} L(x, \lambda) &= f(x) + \lambda^T h(x) \\ \mathcal{L}(x, \lambda) &= f(x) + ||h(x)||_2^2 + \lambda^T h(x) \end{aligned}$$

- Sufficient conditions for optimality: System of differential equations

$$\begin{aligned} \nabla_x L(x, \lambda) = 0 \\ \nabla_\lambda L(x, \lambda) = 0 \end{aligned}$$

Lagrangian Methods (cont'd)

- Two counteracting forces to converge to saddle points
  - Gradient descent in x space ($\frac{dx}{dt} = -\nabla_x \mathcal{L}(x, \lambda)$)
    - When constraints are violated: minimize violation
    - When constraints are not violated: minimize objective (λ carries no weight)
  - Gradient ascent in λ space ($\frac{d\lambda}{dt} = \nabla_\lambda \mathcal{L}(x, \lambda)$)
    - When constraints are violated, increase λ to increase weight of violation
- More effective than penalty methods in adjusting λ
- Handling inequality constraints
  - Slack variable method
  - MaxQ method

Discrete Lagrangian Methods

- Discrete optimization problem

$$\begin{aligned} \text{minimize} \quad & f(x) \\ \text{subject to} \quad & h(x) = 0, \quad x \in Z \end{aligned}$$

- Discrete Lagrangian function: $L(x, \lambda) = f(x) + \lambda^T h(x)$
- Dynamic system

$$\begin{aligned} x_{k+1} &= x_k - \Delta_x L(x_k, \lambda_k) \\ \lambda_{k+1} &= \lambda_k + h(x_k) \end{aligned}$$

- Discrete Saddle-Point Theorem: $F(x^*, \lambda) \leq F(x^*, \lambda^*) \leq F(x, \lambda^*)$
- Fixed Point Theorem: Feasible solution is reached if dynamic system terminates

NOVEL: NONLINEAR OPTIMIZATION VIA EXTERNAL LEAD

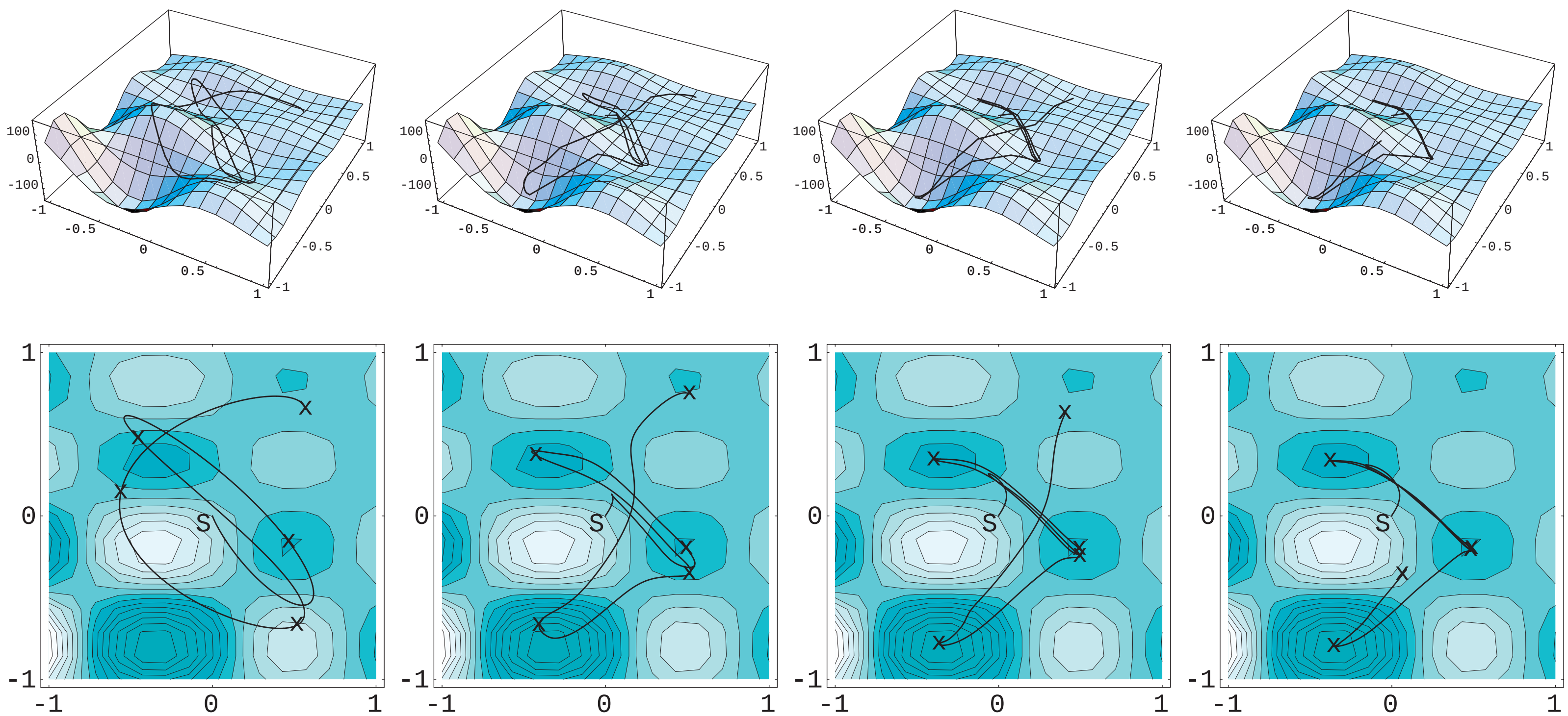
Features of NOVEL

- Global search: locating promising regions
  - A user-defined trace function leading the search
  - Local minima attracting the search trajectory
- Local search
  - Gradient descent
  - Lagrangian search

A Simple Example

- Minimizing Levy's No. 3 function of two variables

$$f_{l_3}(x) = \sum_{i=1}^{5} i\, cos[(i-1)x_1 + i] \sum_{j=1}^{5} j\, cos[(j+1)x_2 + j]$$



Framework of *NOVEL*

- Global search phase
  - Three stages in tandem to explore search space
  - Locate promising regions with good local minima
- Local search phase
  - Descent methods, e.g. gradient descent
  - Conjugate gradient
  - Quasi-Newton's method

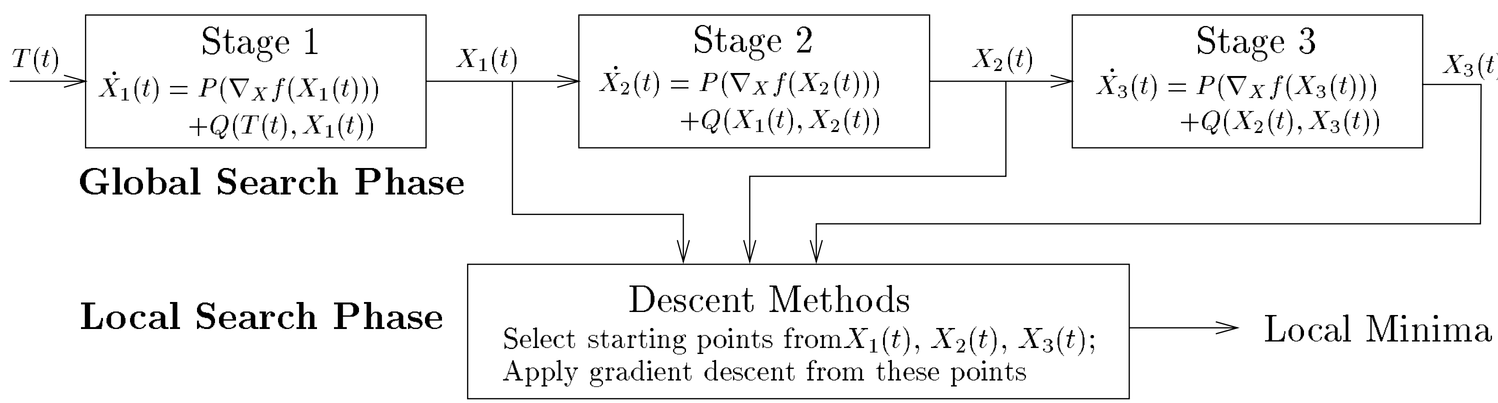
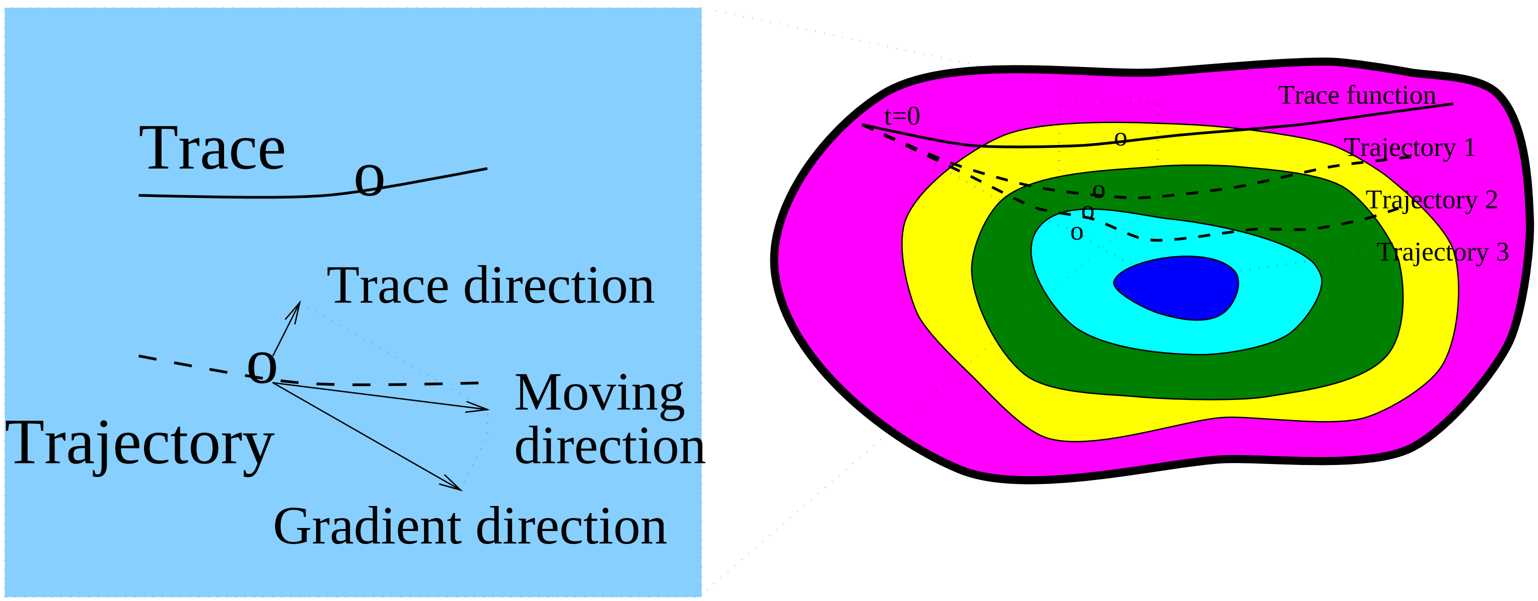


Illustration of Global Search Phase



Uniform Traversal of Search Space by $T(t)$

- For each dimension, search the whole space from coarse to fine
- $T(t)$ — Aperiodic **trace** function searching from coarse to fine

  $$= \rho\, sin \left[2\pi \left(\frac{t}{2}\right)^{0.95 - \frac{0.45(i-1)}{n})} + \frac{2\pi(i-1)}{n} \right]$$

  - t: autonomous variable
  - n: number of dimensions
  - i: i'th dimension
  - ρ: search range

Mathematical Formulation of Global Search Phase

- Generic formulation to specify a trajectory through variable space X.

$$\frac{d\,X(t)}{dt} = P(\nabla_X f(X(t))) + Q(T(t), X(t))$$

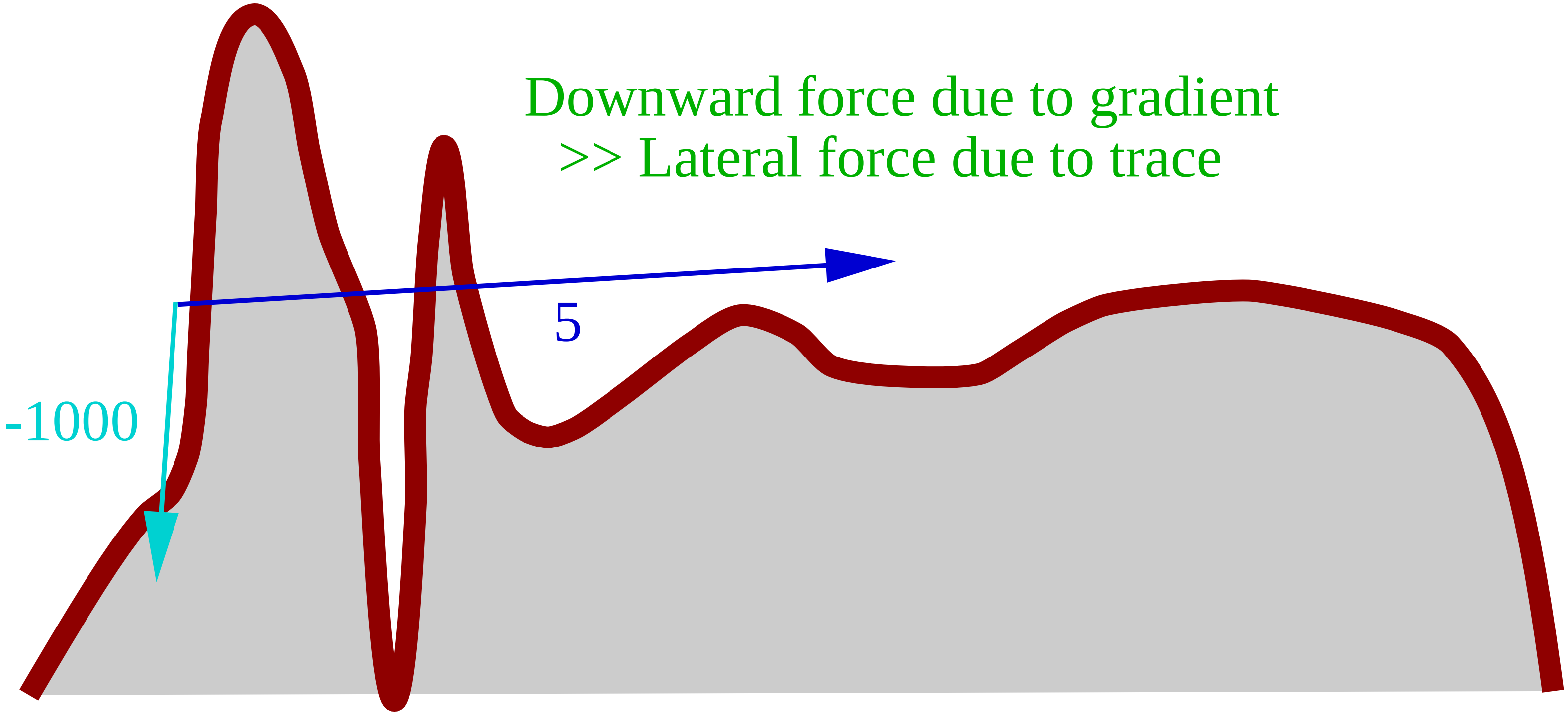
  - $f(X)$: Error function to be minimized
  - $\nabla_X f(X)$: Gradient of $f(X)$
  - $P(\nabla_X f(X(t)))$ enables gradient to attract the trajectory
  - $Q(T(t), X(t))$ allows trace function $T(t)$ to lead the trajectory

- One simple trajectory through variable space X

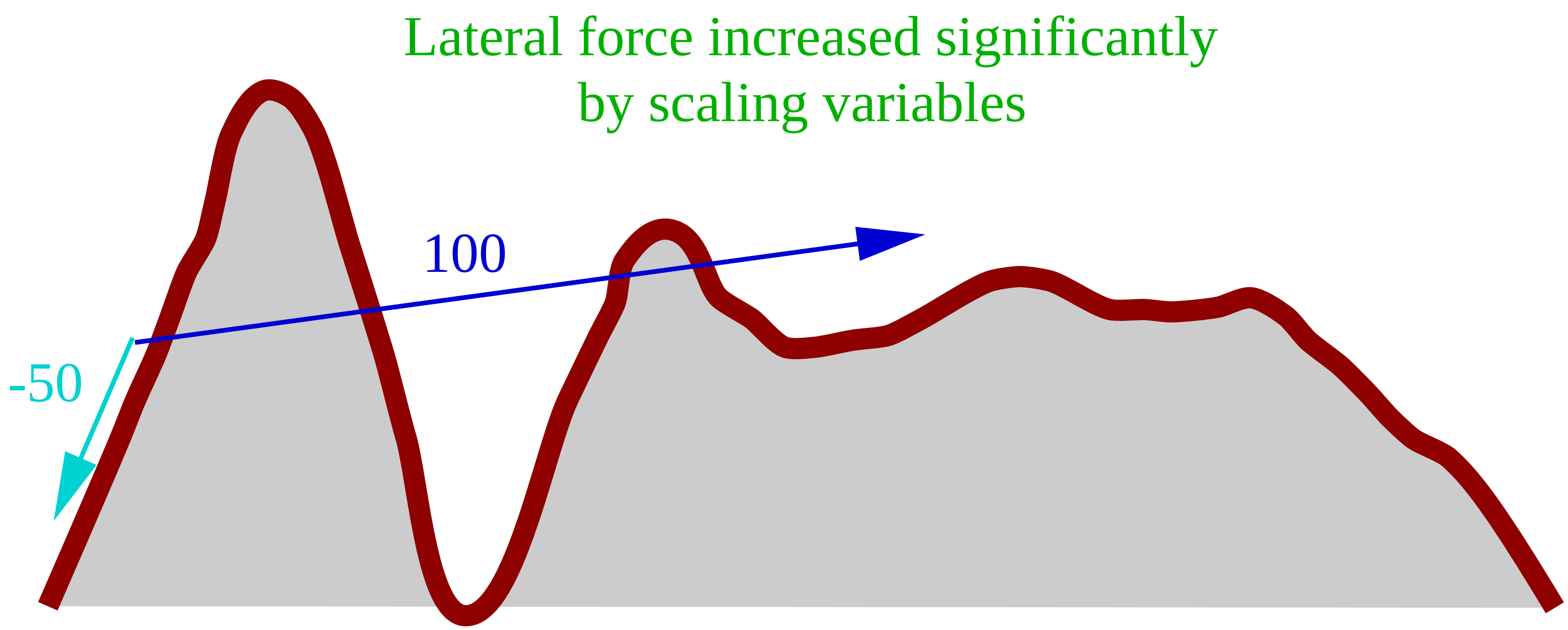
$$\frac{d\,X(t)}{dt} = -\mu_g \nabla_X f(X(t)) - \mu_t (X(t) - T(t))$$

  - μ_g and μ_t are positive real numbers

Insufficient Lateral Force



After Scaling Variables



Solution Methods

- Differential equation solver, e.g. LSODE package for solving ordinary differential equations from netlib
  - Slow
  - Accurate
- Finite difference equation solver

$$X(t + \delta t) = X(t) + \delta t\{-\mu_g \nabla f(X) - \mu_t[X(t) - T(t)]\}$$

  - Fast
  - Approximate

APPLICATION 1: NONLINEAR CONTINUOUS CONSTRAINED OPTIMIZATION

Lagrangian Search and Trace

- Dynamic system

$$\begin{aligned}\frac{dx}{dt} &= -\nabla_x \mathcal{L}(x(t), \lambda(t)) + w * [\mathcal{L}_x(x(t), \lambda(t)) - T(x(t))] \\ \frac{d\lambda}{dt} &= \nabla_\lambda \mathcal{L}(x(t), \lambda(t))\end{aligned}$$

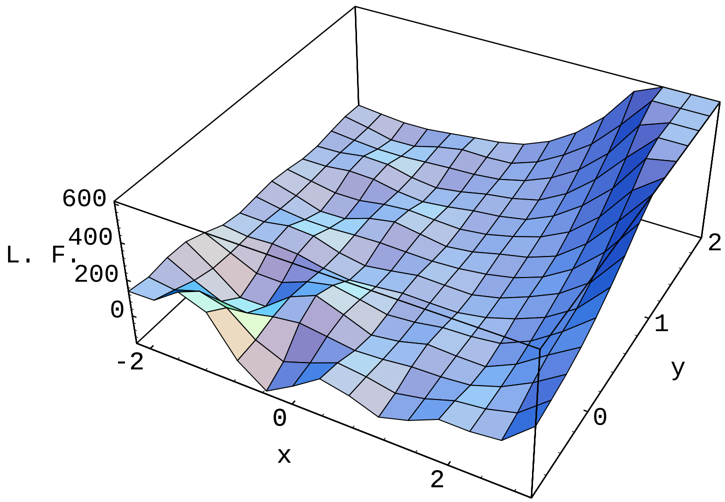
- Lyupunov function as stopping condition

$$F(x, \lambda) = || - \nabla_x \mathcal{L}(x, \lambda)||^2 + ||\nabla_\lambda \mathcal{L}(x, \lambda)||^2.$$

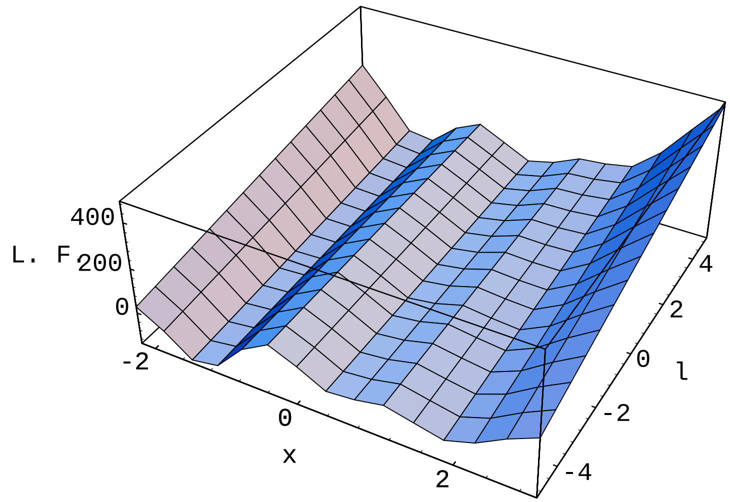
- Handling inequality constraint $g(x) \leq 0$

$$\left[max^2(0, \mu_i + g_i(X)) - \mu_i^2\right] = 0$$
$$[\mu_i max^{q_i}(0, g_i(X))] = 0$$

Example: Levy's No. 3 Function & Elliptic Constraint

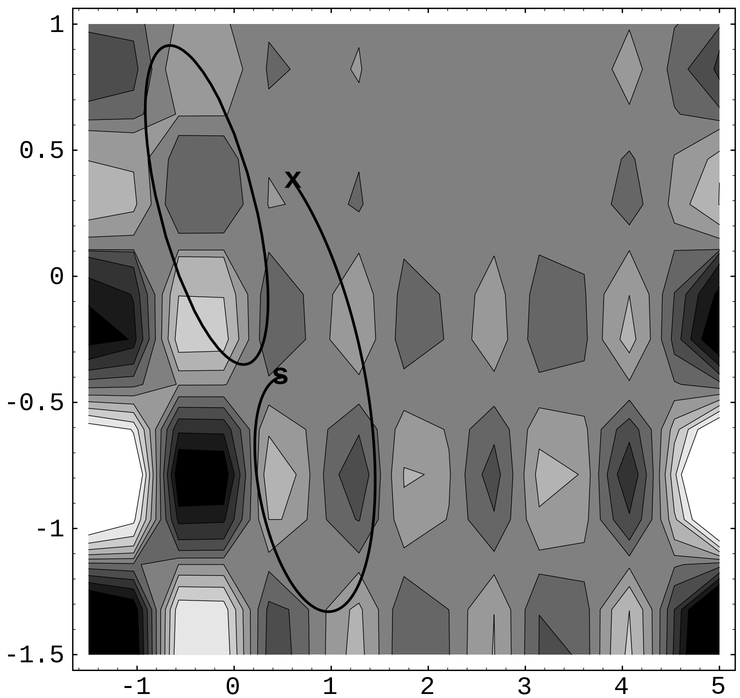


x-y plot

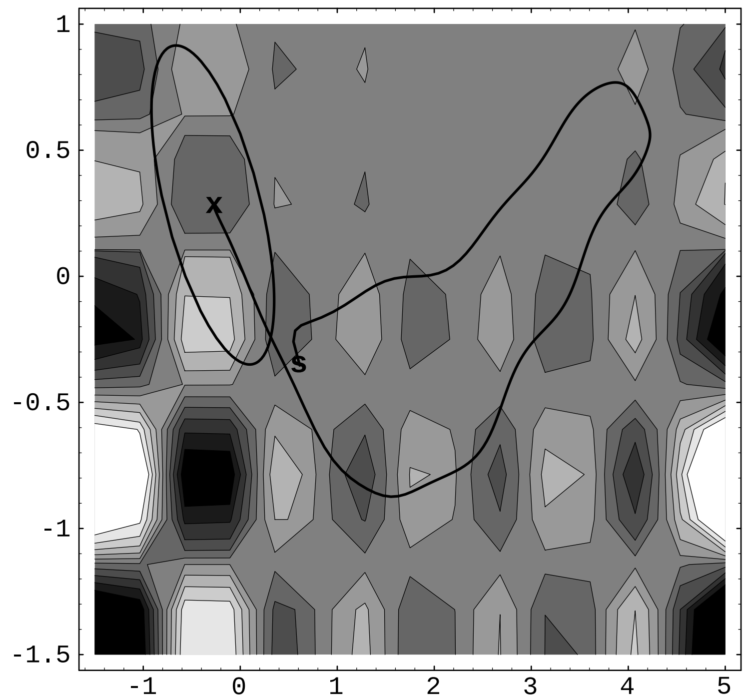


x-λ plot

Example (cont'd)



Objective, constraint, & trace



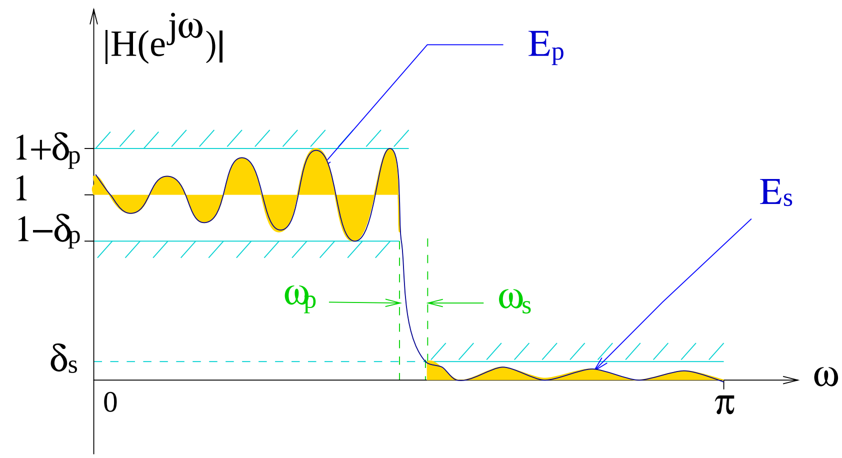
Objective, constraint, & trajectory

Problem ID	Search Range	*NOVEL* Search Time Limit	Best Known Solutions	Epperly's Solutions	Slack w/o Scaling Solutions	Slack w/ Scaling Solutions	MaxQ Solutions
2.1.1	1.0	3279	-17.00	-17.00	-	-17.00	-17.00
2.2.1	10.0	5856	-213.00	-213.00	-	-213.00	-213.00
2.3.1	10.0	57404	-15.00	-15.00	-	-15.00	-15.00
2.4.1	10.0	29829	-11.00	-11.00	-11.00	-11.00	-11.00
2.5.1	1.0	2937	-268.00	-268.00	-	-268.00	-268.00
2.6.1	1.0	3608	-39.00	-39.00	-	-39.00	-39.00
2.7.1(1)	40.0	68563	-394.75	-394.75	-	-394.75	-394.75
2.7.1(2)	40.0	51175	-884.75	-884.75	-	-884.75	-884.75
2.7.1(3)	40.0	170751	-8695.00	-8695.00	-	-8695.00	-8695.00
2.7.1(4)	40.0	203	-754.75	-754.75	-	-754.75	-754.75
2.7.1(5)	40.0	97470	-4150.40	-4150.40	-	-4150.40	-4150.40
2.8.1	25.0	158310	15990.00	15990.00	-	$\boxed{15639.00}$	$\boxed{15639.00}$
3.1.1	5000.0	352305	7049.25	-	-	7049.25	7049.25
3.2.1	50.0	47346	-30665.50	-30665.50	-	-30665.50	-30665.50
3.3.1	10.0	803	-310.00	-310.00	-	-310.00	-310.00
3.4.1	5.0	199	-4.00	-4.00	-	-4.00	-4.00
4.3.1	5.0	20890	-4.51	-4.51	-4.51	-4.51	-4.51
4.4.1	5.0	73	-2.217	-2.217	-2.217	-2.217	-2.217
4.5.1	5.0	16372	-11.96	$\boxed{-13.40}$	-	$\boxed{-13.40}$	$\boxed{-13.40}$
4.6.1	5.0	4435	-5.51	-5.51	-5.51	-5.51	-5.51
4.7.1	5.0	423	-16.74	-16.74	-16.75	-16.75	-16.75
5.2.1	50.0	240829	1.567	-	1.567	1.567	1.567
5.4.1	50.0	374850	1.86	-	1.86	1.86	1.86
6.2.1	100.0	3017	400.00	400.00	400.00	400.00	400.00
6.3.1	100.0	2756	600.00	600.00	600.00	600.00	600.00
6.4.1	100.0	3340	750.00	750.00	750.00	750.00	750.00
7.2.1	100.0	162643	56825.00	-	56825.00	56825.00	56825.00
7.3.1	150.0	228320	46266.00	-	-	46266.00	$\boxed{44903.00}$
7.4.1	150.0	631029	35920.00	-	-	35920.00	35920.00

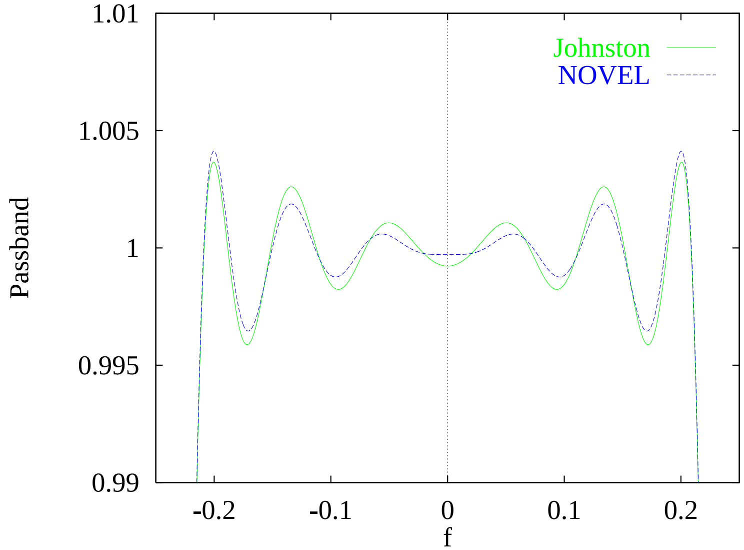
APPLICATION 2: QMF FILTER-BANK DESIGN

QMF Filter Bank Design

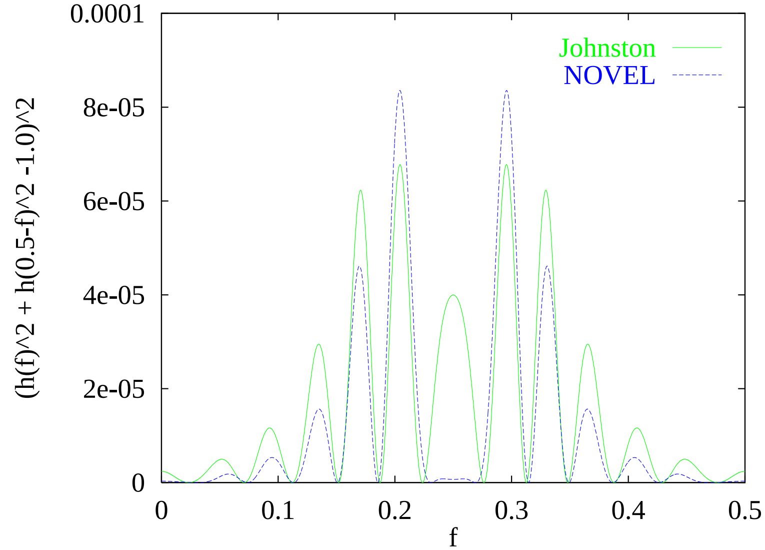
Filter	Design Objectives
Overall Filter Bank	Min amplitude distortion
	Min aliasing distortion
	Min phase distortion
Single Filter	Min stopband ripple (δ_s)
	Min passpand ripple (δ_p)
	Min transition band error (E_t)
	Min stopband energy (E_s)
	Max passband flatness (E_p)



Example: 24D QMF Design



Passband frequency response

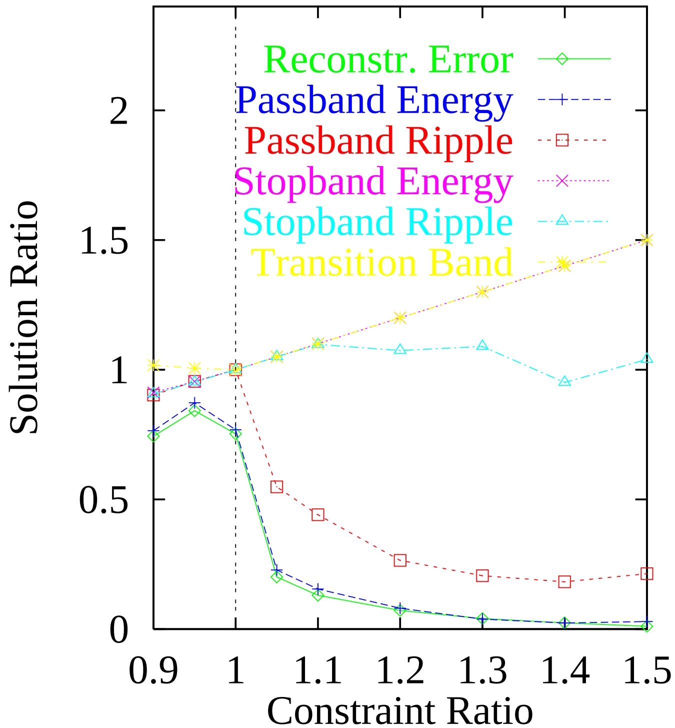


Reconstruction error

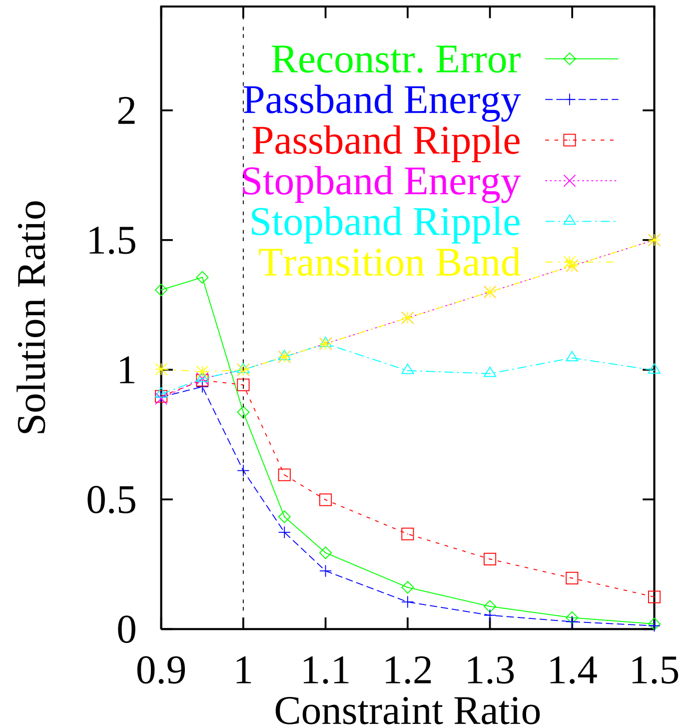
Initial Results: Better Designs

Performance	24D	32D	48D
E_r	0.75	0.87	0.95
E_p	0.77	0.80	0.76
E_s	1.00	1.00	1.00
δ_p	1.00	1.00	1.00
δ_s	1.00	1.00	1.00
$\Delta\omega$	1.00	1.00	1.00

Initial Results: Different Constraints



24D



32D

APPLICATION 3: DISCRETE SATISFIABILITY

Satisfiability (SAT) Problem

- Given
  - a set of m clauses $C_1, C_2, \cdots, C_m$ on n variables

$$X = (x_1, x_2, \cdots, x_n) \qquad x_i \in \{0, 1\}$$

  - Boolean formula in conjunctive normal form (CNF)

$$C_1 \cap C_2 \cap \cdots \cap C_m$$

- Find a truth assignment or derive infeasibility

Alternative Formulations

- Discrete constrained decision problem without objective

$$\text{Find } x \text{ such that} \quad U_i(X) = 0 \quad i = 1, \ldots, m$$

$$\text{where} \quad U_i(x) = \begin{cases} 0 & \text{assignment } x \text{ satisfies } C_i, \\ 1 & \text{otherwise.} \end{cases}$$

  – Examples: Resolution, backtracking, constraint satisfaction, Davis-Putnam's algorithm

  – High computational complexity

Alternative Formulations (cont'd)

- Discrete unconstrained formulation

$$\min N(x) = \sum_{i=1}^{m} U_i(x)$$

  - Local search methods
    - GSAT
    - WSAT
    - Gu's methods
    - Simulated annealing
    - Genetic algorithm
  - Can solve many large SAT problems efficiently
  - May not work well when there are very few local minima
  - Restarts may bring the search to a completely new terrain

Alternative Formulations (cont'd)

- Continuous unconstrained formulation

$$
\begin{aligned}
c_i(x) &= \prod_{j=1}^{m} a_{i,j}(x_j) \\
a_{i,j}(x_j) &= \begin{cases} (1 - x_j)^2 & \text{if } x_j \text{ in } C_i \\ x_j^2 & \text{if } \bar{x}_j \text{ in } C_i \\ 1 & \text{otherwise} \end{cases} \\
\text{Objective} &: \ min \ \sum_i c_i(x)
\end{aligned}
$$

  - Gu's UniSAT model
  - Local search methods: gradient descent, conjugate gradient, Quasi-Newton
  - Computationally expensive

Alternative Formulations (cont'd)

- Continuous constrained formulation

$$\begin{array}{ll} \min\limits_{x \in E^m} & f(x) = \sum\limits_{i=1}^{n} c_i(x) \\ \text{subject to} & c_i(x) = 0 \quad \forall i \in \{1, 2, \ldots, n\} \end{array}$$

  - Smooth out local minima in discrete space
  - Lagrangian methods
  - Very expensive

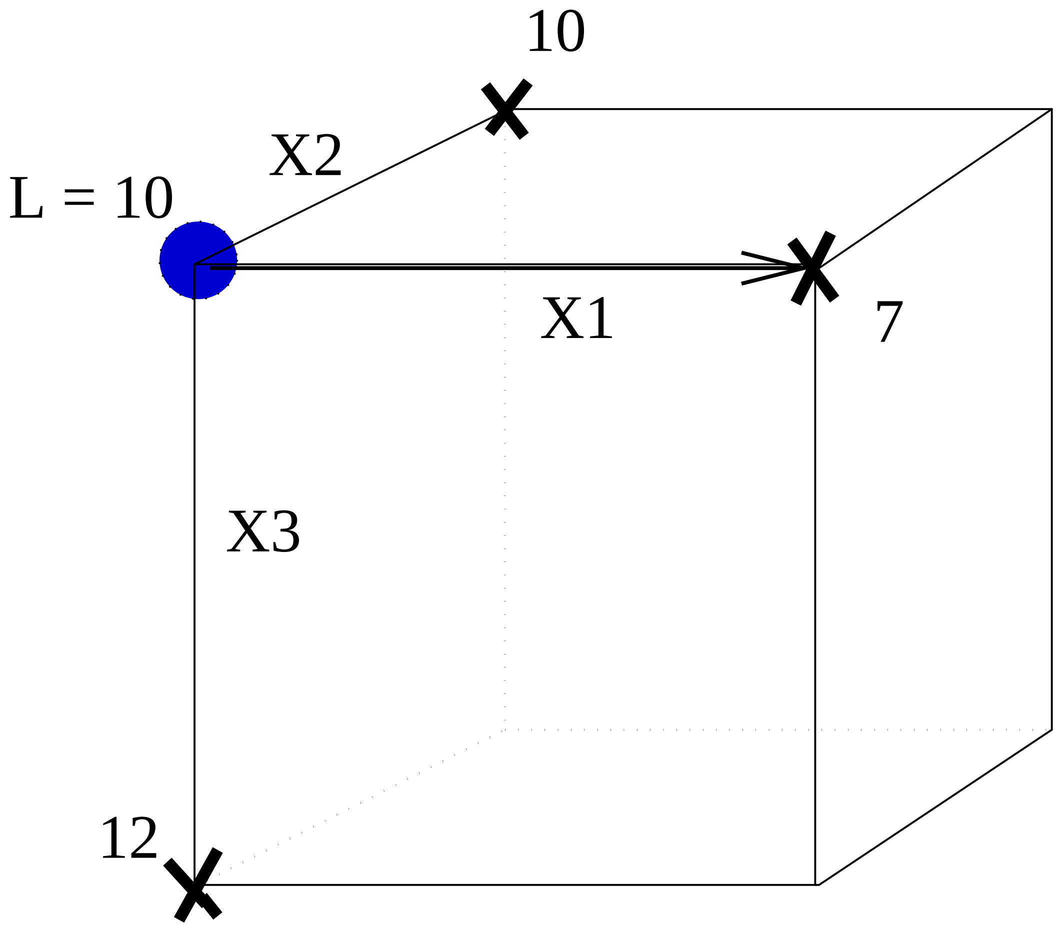
Our SAT Formulation

- Constrained optimization with artificial (discrete) objective

$$\begin{aligned} \min \quad & N(X) = \sum_{i=1}^{m} U_i(X) \\ \text{subject to} \quad & U_i(X) = 0 \quad i = 1, \ldots, m \end{aligned}$$

  - Local minima satisfying constraints are also global minima
  - Use objective to guide search
  - Use constraints to bring search out of local minima without restarts

Gradient Operator $\Delta_X L(X, \lambda)$



An Implementation to solve SAT Problems

Set initial point x
while x is not a solution, *i.e.*, $N(x) > 0$
    while $\Delta_x L(x, \lambda) \neq 0$
        update x: $x \longleftarrow x - \Delta_x L(x, \lambda)$
    end while
    update λ: $\lambda \longleftarrow \lambda + c \times U(x)$
end while

Comparing DLM with GSAT, WSAT, DP, IP and SA

Problem Id	No. of Var.	No. of Clauses	DLM Version 2			WSAT	GSAT	DP
			SS 10/51	Challenge	# Iter.			
ssa7552-038	1501	3575	0.228	0.3	7970	2.3	129	7
ssa7552-158	1363	3034	0.088	0.1	2169	2	90	*
ssa7552-159	1363	3032	0.085	0.1	2154	0.8	14	*
ssa7552-160	1391	3126	0.097	0.1	3116	1.5	18	*

Problem Id.	No. of Var.	No. of Clauses	DLM Version 2			GSAT	Integer Prog.	SA
			SS 10/51	Challenge	# Iter.			
ii16a1	1650	19368	0.122	0.128	819	2	2039	12
ii16b1	1728	24792	0.265	0.310	1546	12	78	11
ii16c1	1580	16467	0.163	0.173	797	1	758	5
ii16d1	1230	15901	0.188	0.233	908	3	1547	4
ii16e1	1245	14766	0.297	0.302	861	1	2156	3

Problem Identification	No. of Var.	No. of Clauses	DLM Version 3		GSAT	
			Time	Success	Time	Success
g125.17	2125	66272	1390.32	10/10	264.07	7/10
g125.18	2250	70163	3.197	10/10	1.9	10/10
g250.15	3750	233965	2.798	10/10	4.41	10/10
g250.29	7250	454622	1219.56	9/10	1219.88	9/10

Results On Difficult But Satisfiable DIMACS Benchmarks

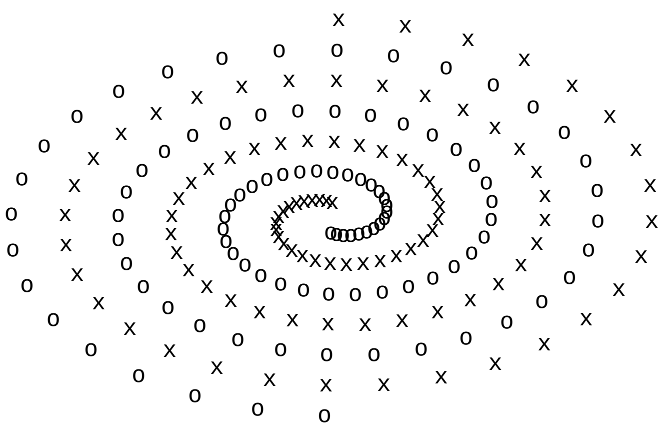
Prob. Id.	Succ. Ratio	Time in CPU seconds			Prob. Id.	Succ. Ratio	Time in CPU seconds		
		Avg.	Min.	Max.			Avg.	Min.	Max.
par8-1	10/10	4.780	0.133	14.383	par16-1-c	10/10	398.1	11.7	1011.9
par8-2	10/10	5.058	0.100	13.067	par16-2-c	10/10	1324.3	191.0	4232.3
par8-3	10/10	9.903	0.350	21.150	par16-3-c	10/10	987.2	139.8	3705.2
par8-4	10/10	5.842	0.850	16.433	par16-4-c	10/10	316.7	5.7	692.66
par8-5	10/10	14.628	1.167	34.900	par16-5-c	10/10	1584.2	414.5	3313.2
hanoi4	1/10	682.6	682.6	682.6	f1000	10/10	126.8	4.4	280.7
f600	10/10	16.9	2.1	37.2	f2000	10/10	1808.6	174.3	8244.7

- Still cannot solve 16 satisfiable DIMACS benchmark problems
  - *par16-1* thru *par16-5*
  - *par32-1* thru *par32-5*
  - *par32-1-c* thru *par32-5-c*
  - *hanoi5*

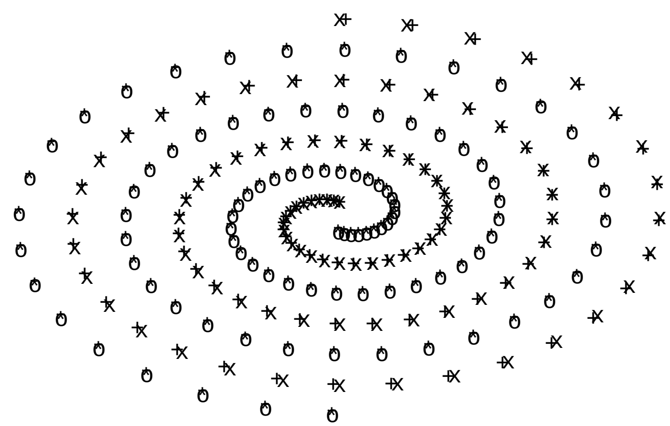
APPLICATION 4: FEEDFORWARD NEURAL-NETWORK LEARNING

Two-spiral problem

- Discriminate between two sets of points that lie on two distinct spirals in the x-y plane
- Best known network: 9 hidden units with 75 weights
- Training and test data set



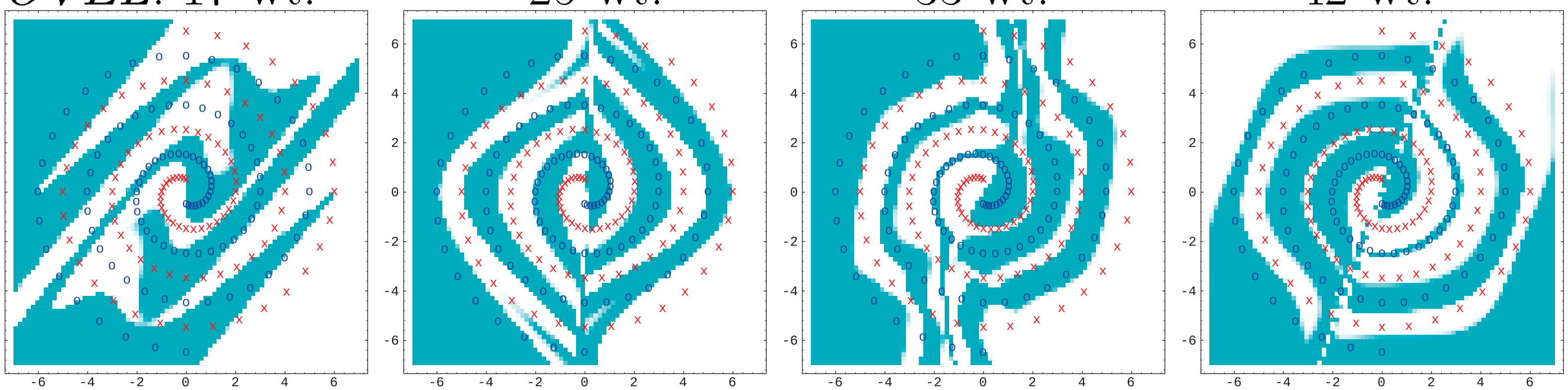
194 training patterns



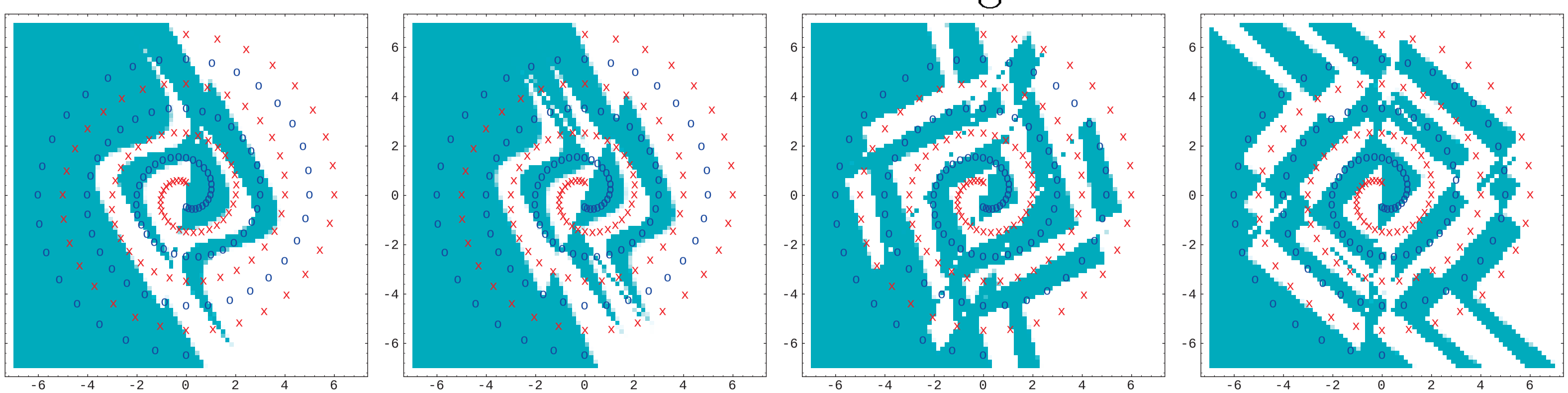
194 testing patterns

2-D Classification Graphs for 3, 4, 5, 6 Hidden Units

NOVEL: 17 wt. 25 wt. 33 wt. 42 wt.



Simulated Annealing



Best 4 hidden unit network: 77.5 hours – 99% correct, 89.4 hours – 100%

Experimental Results

Problems	# of H.U.	# of Wts.	*TN-MS* Correct % training	*TN-MS* Correct % test	*TN-MS* # of restarts	*NOVEL* Correct % training	*NOVEL* Correct % test	*NOVEL* # time units	*TN-MS + NOVEL* Correct % training	*TN-MS + NOVEL* Correct % test	*TN-MS + NOVEL* # time units	CPU time limits
Sonar	2	125	98.1	90.4	454	0%	**+3.8%**	191	0%	**+1.9%**	226	1000 sec
	3	187	100	91.3	485	0%	**+1%**	291	0%	**+1%**	315	2000 sec
Vowel	2	55	72.2	50.9	298	**+0.3%**	-1.8%	131	**+1.3%**	-0.3%	203	2 hours
	4	99	80.7	56.5	152	**+1.9%**	**+1.3%**	41	**+0.5%**	**+0.6%**	168	2 hours
10-parity	5	61	97.2	—	148	**+1.7%**	—	51	0%	—	49	2000 sec
	6	73	97.6	—	108	**+2.2%**	—	62	0%	—	44	3000 sec
NetTalk			*Pattern-wise BP*			*NOVEL*			*Pattern-wise BP + NOVEL*			
	15	3,476	86.3	70.5	13	**+1.1%**	**+2.2%**	11	**+2.7%**	-0.1%	11	3 hours
	30	6,926	92.9	73.1	9	**+0.3%**	-0.6%	4	**+1.8%**	-0.8%	7	4 hours

Conclusions

- Escaping from local minima – Trace
  - Generate information bearing trajectory
  - Identify good starting points for local search
- Constraint satisfaction
  - Lagrangian formulation
  - Discrete Lagrangian formulation

Publications

- Constrained Problems
  - "Trace-Based Methods for Solving Nonlinear Global Optimization and Satisfiability Problems," B. W. Wah and Y. J. Chang, *J. of Global Optimization*, (to appear) 1996.
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- Unconstrained Problems
  - "Global Optimization for Neural Network Training," Y. Shang and B. W. Wah, *IEEE Computer*, vol. 29, No. 3, March 1996, pp. 45-54.
  - Neural-Network Training Software: Sun Sparc object code, Y. Shang and B. W. Wah, Released: May 27, 1996.
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- Non-Linear Discrete Optimization
  - "A Discrete Lagrangian-Based Global-Search Method for Solving Satisfiability Problems," B. W. Wah and Y. Shang *Proc. DIMACS Workshop on Satisfiability Problem: Theory and Applications*, Ed: Ding-Zhu Du, Jun Gu, and Panos Pardalos, American Mathematical Society, March 1996.