



Project 4.6: Hybrid Optimization Schemes for Parameter Estimation Problems



✦ **TA4: Enabling Technologies and Advanced Algorithms**

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- *Lorenzo Ruiz*, BS Computer Science (Spring 30%)

✦ Objective #1

Provide an scalable high performance hybrid optimization code with application to problems of interest to ARL

✦ Objective #2

Enhance ARL computational predictive capabilities by developing high resolution parameter estimation solvers with a sensitivity analysis information

✦ Item #1

Reliable parameter estimation is a cornerstone to improving predictions and reducing the risk of decisions on several ARL applications.

✦ Item #2

Such applications require substantial computational resources and effort to solve nonlinear functions subject to constraints for different sets of parameters.

Therefore development of efficient and novel numerical solutions to key ARL nonlinear parameter estimation problems through the use of HPC is of high importance.

✦ Item #1

We are implementing a hybrid optimization scheme that is scalable for high-performance computing.

✦ Item #2

The HPC optimization procedure combines the capabilities of stochastic and deterministic methods via surrogate models in searching for a global solution.

Item #1

One major challenge in computational science and engineering is finding an optimal global solution for large-scale nonlinear parameter estimation problems.

Item #2

Finding a global optimal solution is a challenging task due to the fact that data and models are usually nonlinear, non-smooth, subject to different sources of errors, and multiple objective functions.

Deliverable #1

Formulate and document efficient and portable deterministic and stochastic optimization algorithms, (SPSA and IPM's methods)

Deliverable #2

Develop software package based on combining SPSA with NKIP, and perform preliminary testing on benchmark problems provided by ARL users.

- We present a hybrid optimization approach for solving global optimization problems, in particular automated parameter estimation models.
- The hybrid approach is based on the coupling of the Simultaneous Perturbation Stochastic Approximation (**SPSA**) and a Newton-Krylov Interior-Point method (**NKIP**) via a **surrogate model**.
- We implemented the hybrid approach on several test cases.

We consider the global optimization problem in the form:

$$\text{minimize } f(x) \quad f : \mathbb{R}^n \rightarrow \mathbb{R} \quad (1)$$

where the global solution x^* is such that

$$f(x^*) \leq f(x) \quad \text{for all } x \in \mathbb{R}^n$$

We are interested in problem (1) that have many local minima.

- Global Method: SPSA
- Surrogate Model
- Local Method: NKIP

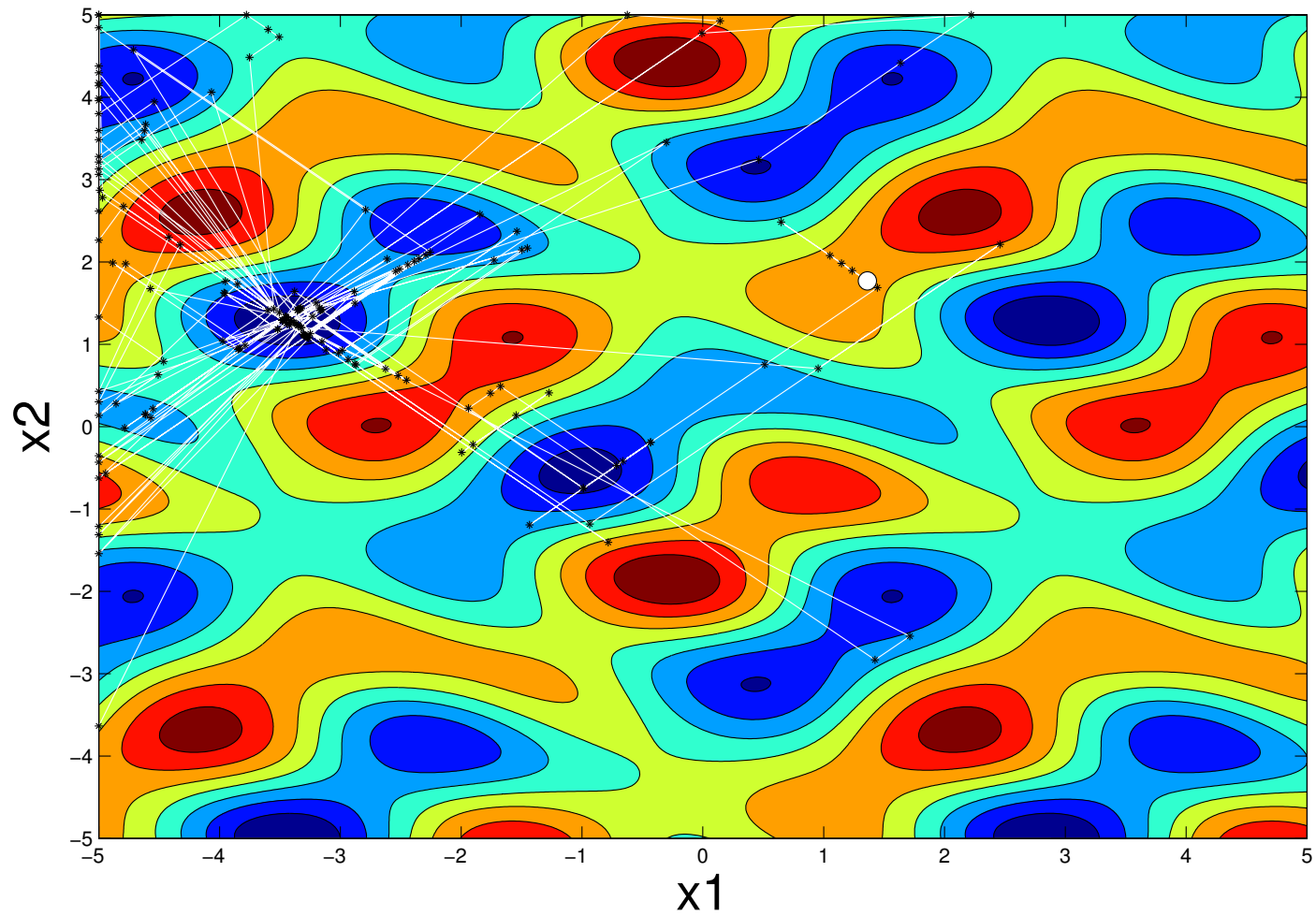
Stochastic steepest descent direction algorithm (James Spall, 1998)

- Advantage
 - SPSA gives region(s) where the function value is low, and this allows to conjecture in which region(s) is the global solution.
- Disadvantages
 - Slow method
 - Do not take into account equality/inequality constraints

```
function [x] = SPSA(x, a, A, c,  $\alpha$ ,  $\gamma$ )  
n = length(x);  
for k = 1 : iter_spsa  
     $a_k = a / (k + A)^\alpha$ ;  
     $c_k = c / k^\gamma$ ;  
     $\Delta = 2 * \text{round}(\text{rand}(n,1)) - 1$ ;  
     $x^+ = x + c_k \Delta$ ;  
     $x^- = x - c_k \Delta$ ;  
     $y^+ = f(x^+)$ ;  
     $y^- = f(x^-)$ ;  
     $\Delta x = (y^+ - y^-) ./ (2c_k \Delta)$ ;  
     $x = x - a_k \Delta x$ ;  
end
```

Note: $a \in (10^{-6}, 15)$, $c \in (10^{-3}, 10)$, $A \in (10, \text{iter_spsa}/10)$, $\alpha = 1.101$, $\gamma = 0.602$

SPSA ITERATIONS



- SPSA gives region(s) where the function value is low, and this allows to conjecture in which region(s) is the global solution.
- This give us a motivation to apply a local method in the region(s) found by SPSA.

- Advantages
 - Fast Rate of Convergence: Newton Type Methods
 - Interior-Point Methods: allow to add equality/inequality constraints
- Disadvantage
 - Needs first/second order information
- Solution
 - Construct a Surrogate Model using the SPSA function values inside the conjecture region(s)

A surrogate model $f_s(x_k)$ is created by using an interpolation method with the data, $(x_k, f(x_k))$, $k = 1, \dots, p$, provided by SPSA.

This can be performed in different ways, e.g., radial basis functions, kriging, regression analysis, or using artificial neural networks.

WHY SURROGATE MODELS?

Most real problems require thousands or millions of objective and constraint function evaluations, and often the associated high cost and time requirements render this infeasible.

RBF is typically parameterized by two sets of parameters: the center c which defines its position, and shape r that determines its width or form

An RBF interpolation algorithm (Orr,1996) characterizes the uncertainty parameters:

$$c_{ij}, r_{ij}, w_j, i = 1, \dots, n, j = 1, \dots, m.$$

Our goal is to optimize the surrogate function

$$f_s(x) = \sum_{j=1}^m w_j h_j(x),$$

where the RBF can be defined as:

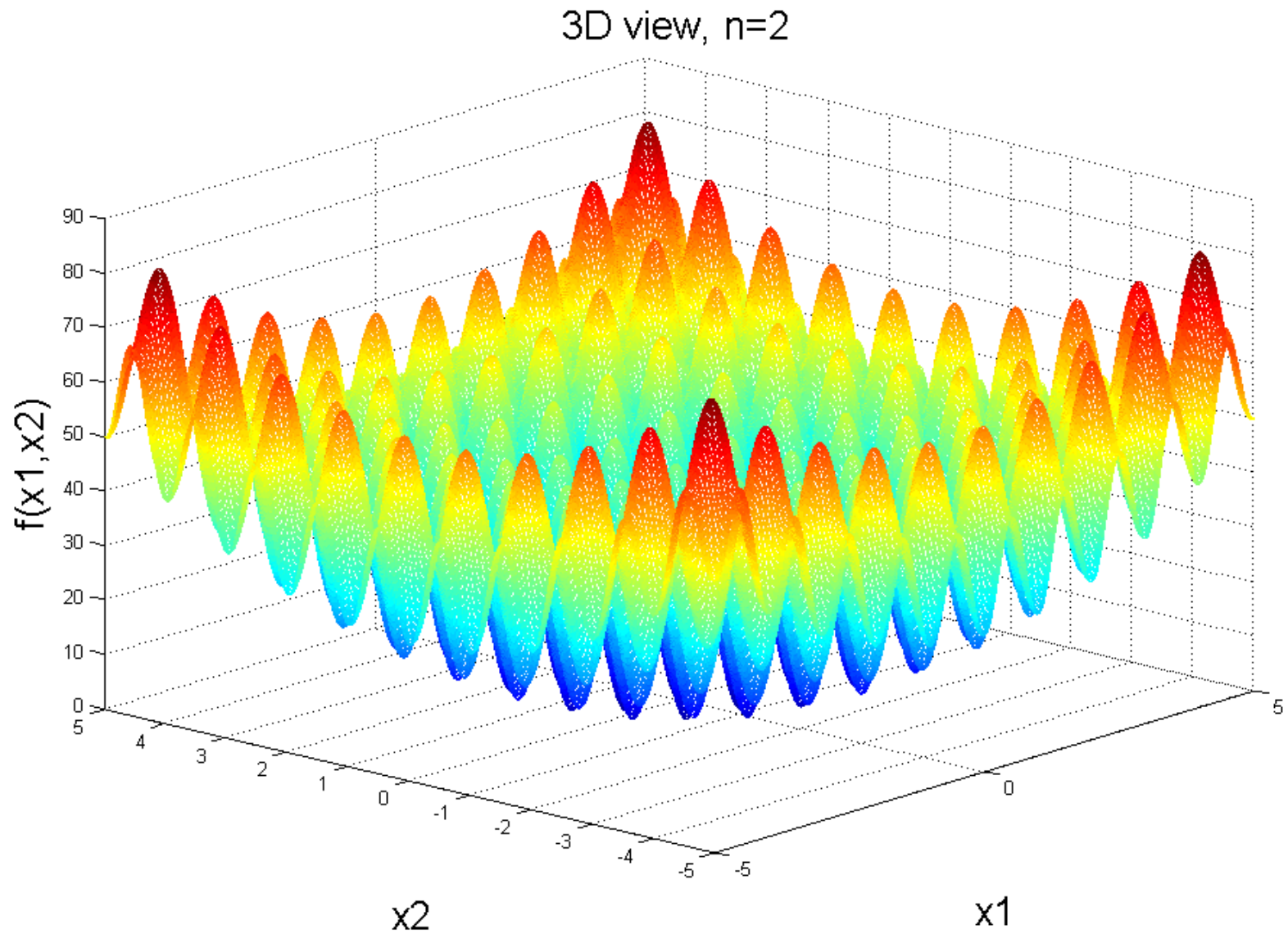
$$h_j(x) = \sqrt{1 + \sum_{i=1}^n \frac{(x_i - c_{ij})^2}{r_{ij}^2}} \quad \text{or} \quad h_j(x) = e^{-\left(\sum_{i=1}^n \frac{(x_i - c_{ij})^2}{r_{ij}} \right)}$$

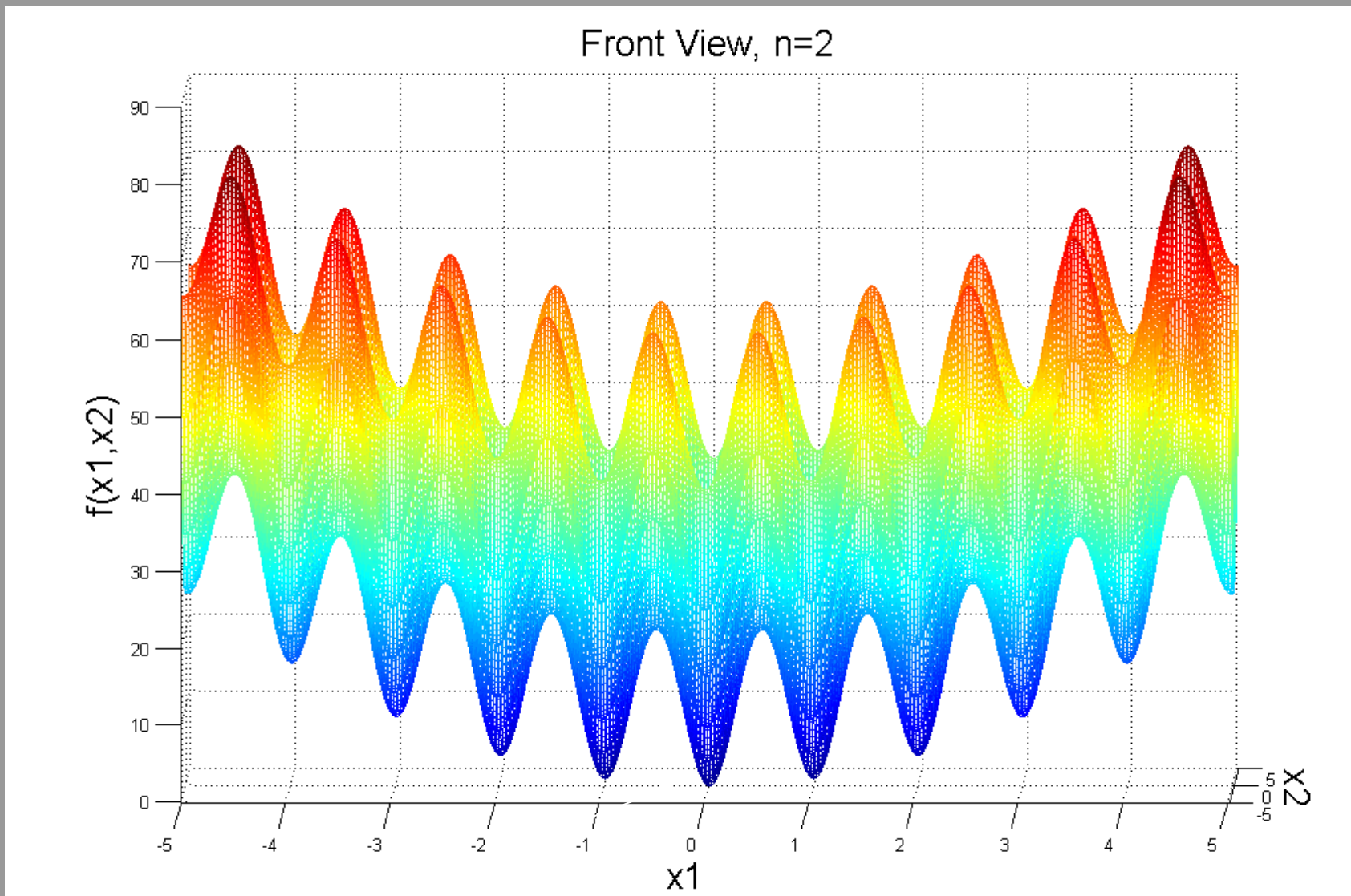
that are the multiquadric and the Gaussian basis functions, respectively

Rastrigin's Problem:

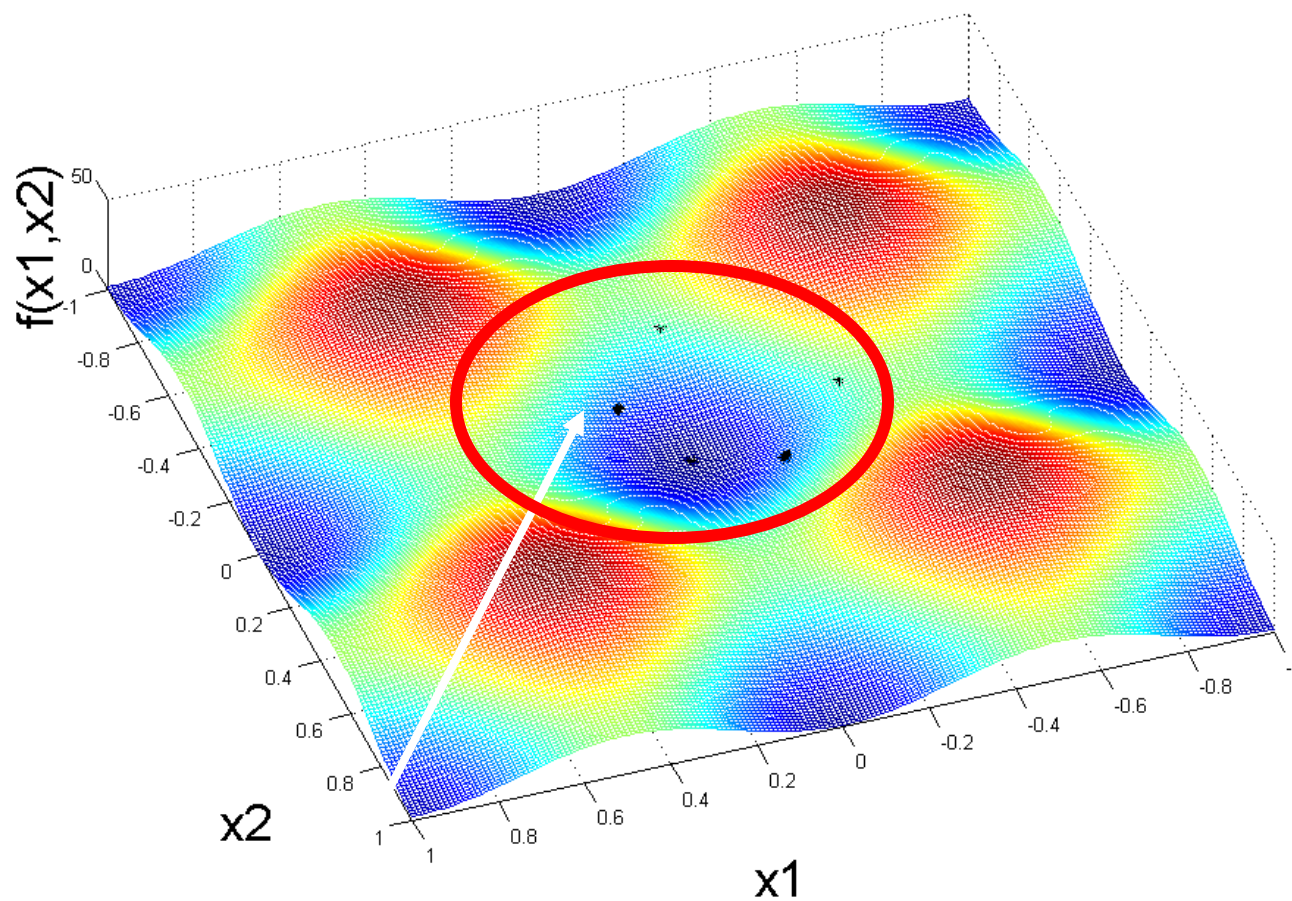
$$\begin{aligned} \min \quad & f(x_1, x_2, \dots, x_n) = 10n + \sum_{i=1}^n (x_i^2 - 10 \cos(2\pi x_i)), \\ \text{s.t.} \quad & -5.12 \leq x_i \leq 5.12 \end{aligned}$$

for $i = 1, 2, \dots, n$

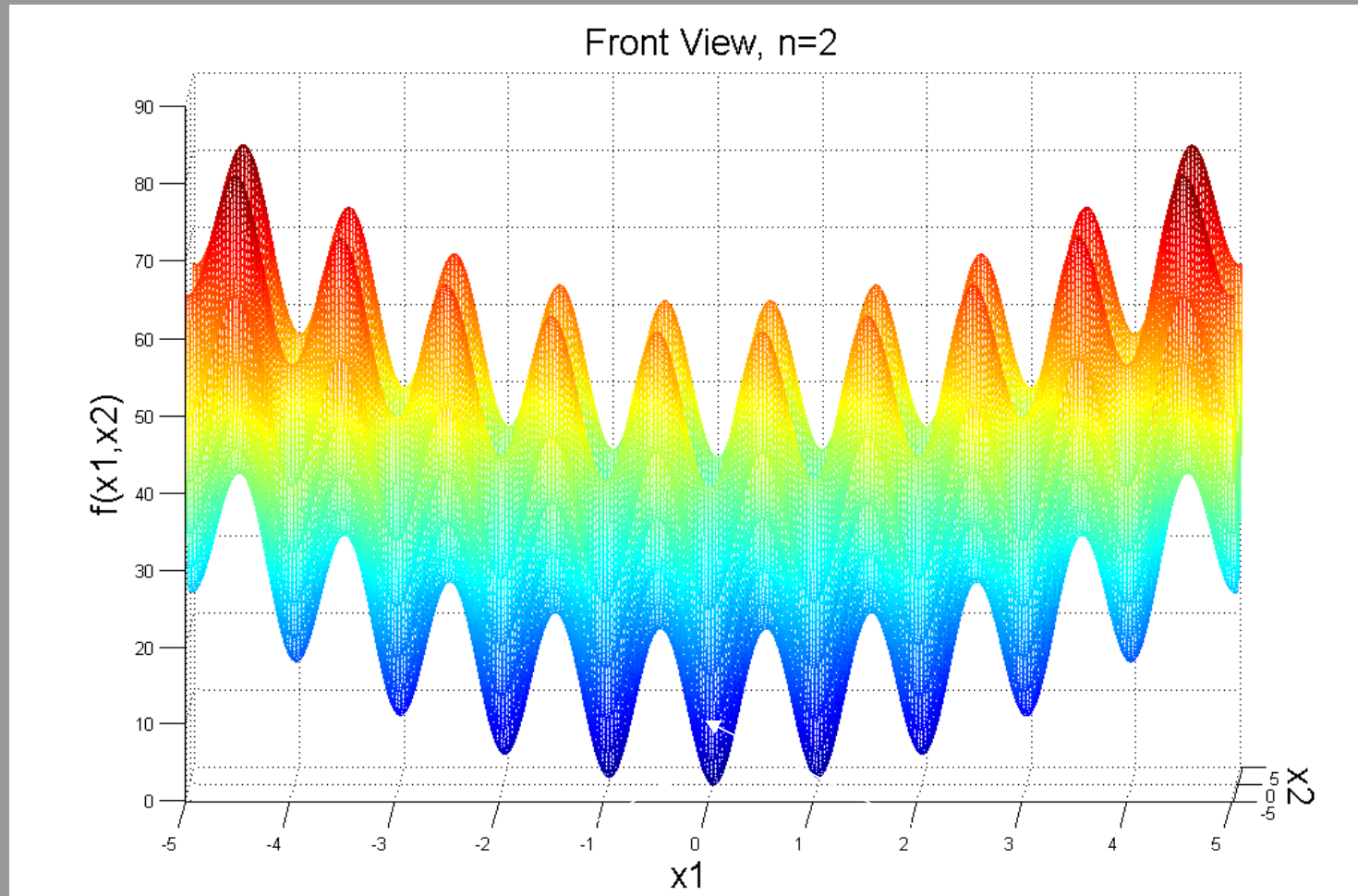




$$f(x^*)=0$$



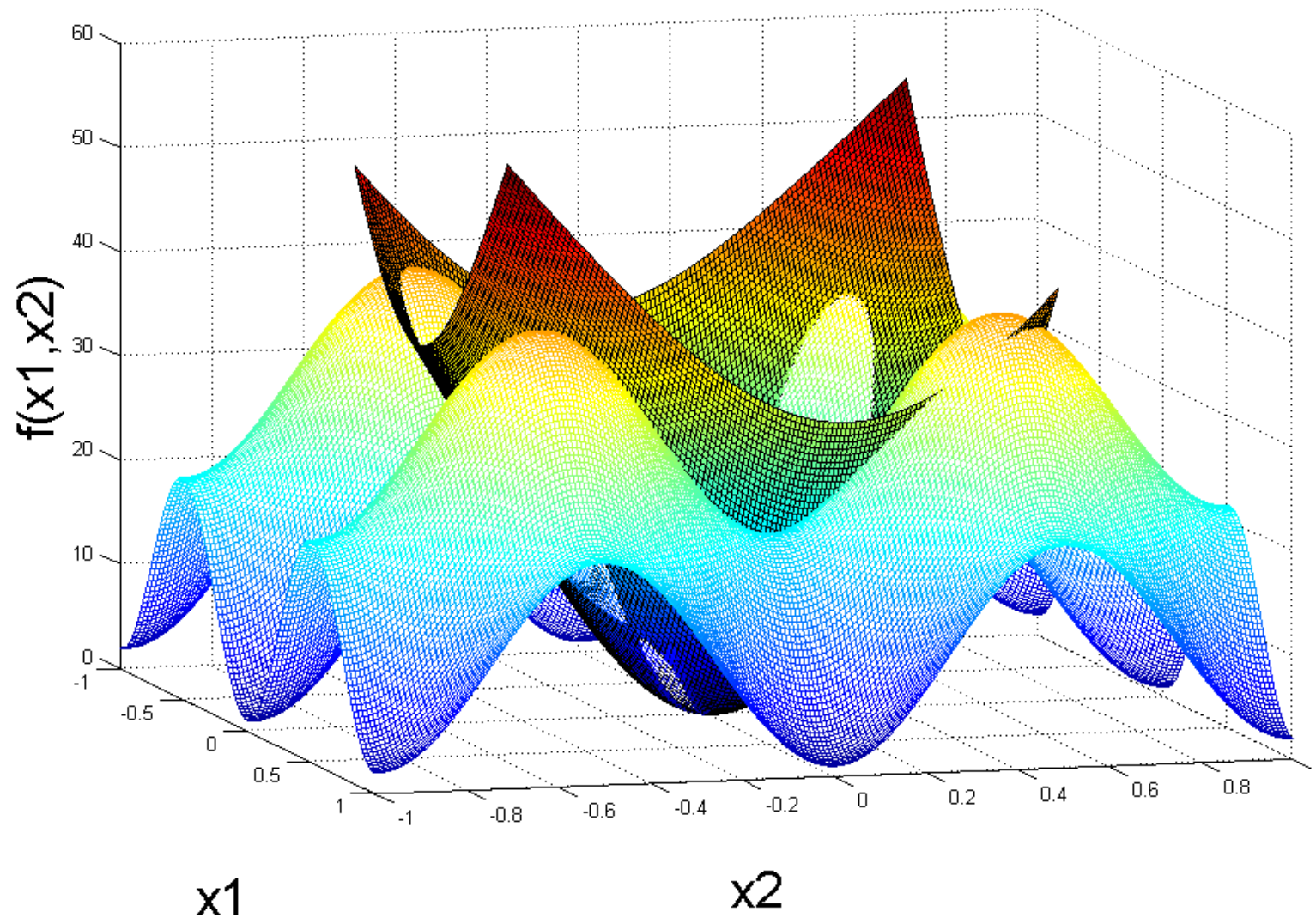
Sampling Data from SPSA

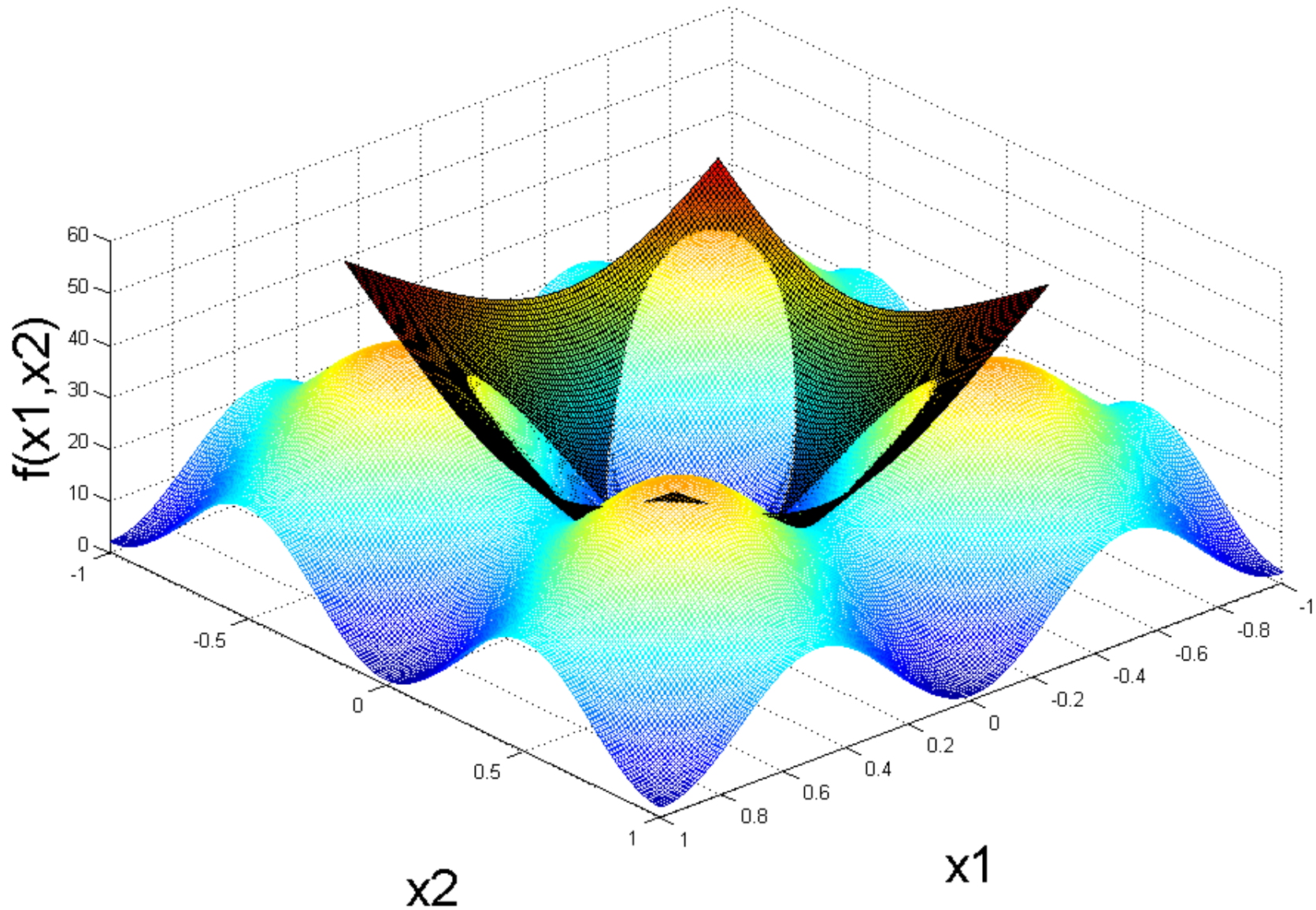


$x^*=(0,0)$ global solution
 $f(x^*)=0$

Sampling Data from SPSA

We plot the original model function and the surrogate function:



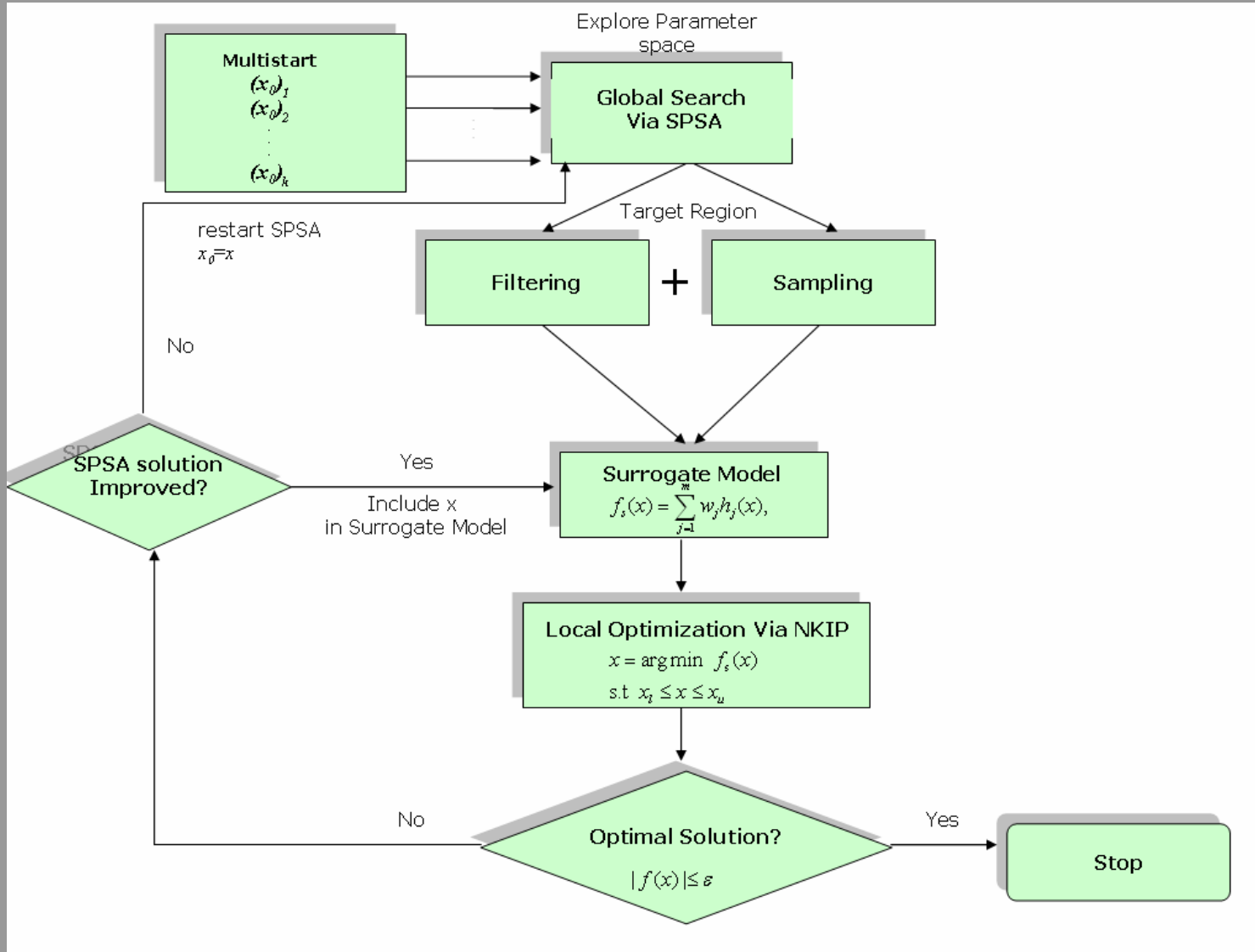


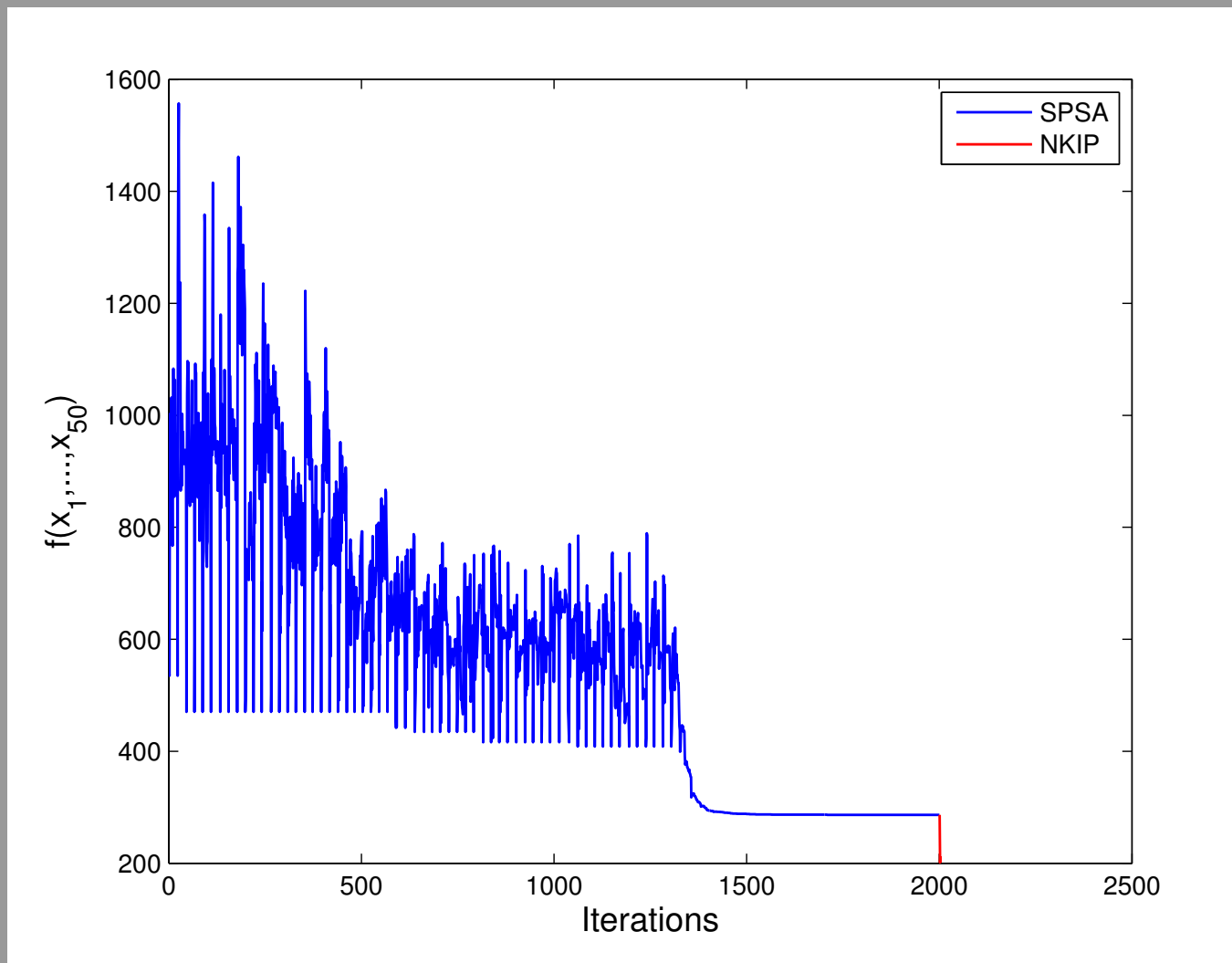
- NKIP is a Newton-Krylov Interior-Point method introduced by Miguel Argaéz and Richard Tapia in 2002.
- This method calculates the directions using the conjugate gradient algorithm, and a linesearch is implemented to guarantee a sufficient decrease of the objective function.
- This method was developed for obtaining an optimal solution for large scale and degenerate problems.

We consider the optimization problem in the form:

$$\begin{aligned} &\text{minimize } f_S(x) \\ &\text{subject to } a \leq x \leq b \end{aligned}$$

where a and b are determined by the sampled points given by SPSA.





Convergence history for $n=50$

The objective function can be written as a nonlinear least squares problem:

$$\underset{x \in R^n}{\text{minimize}} \quad \|G(x) - d_T\|_2^2$$

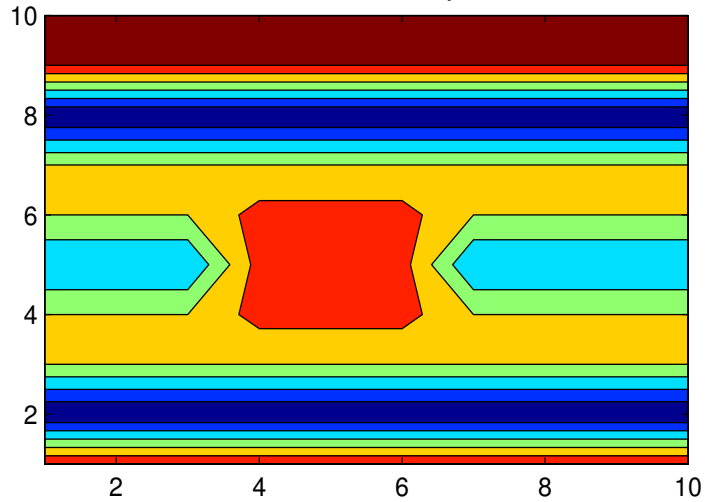
where $G(x) : R^n \rightarrow R^m$ is a nonlinear function
and $d_T \in R^m$ is a set of data observations

- Our goal is to estimate the permeability based on sensor pressure data for a small and sequential parameter estimation problem.
- Despite having full information of the pressure field, the inverse problem is highly ill-posed and has multiple local minima.

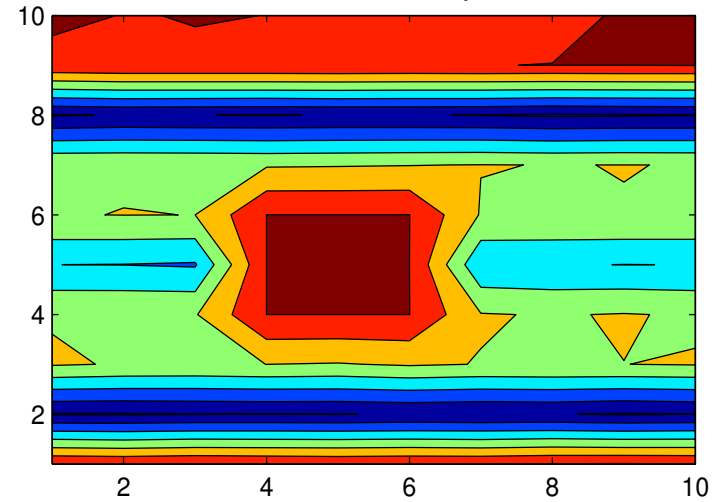
- We run a simulation for a permeability field of size 10×10 . The simulation returns 100 different pressure data points.
- We use 5 initial points and allow 2000 SPSA iterations. We obtain 10167 search points, and we filter these points to obtain 105 points for creating a surrogate model.
- Then we use NKIP to find a local solution in 103 iterations with an optimal function value of 0.00353.

PERMEABILITY RESULTS

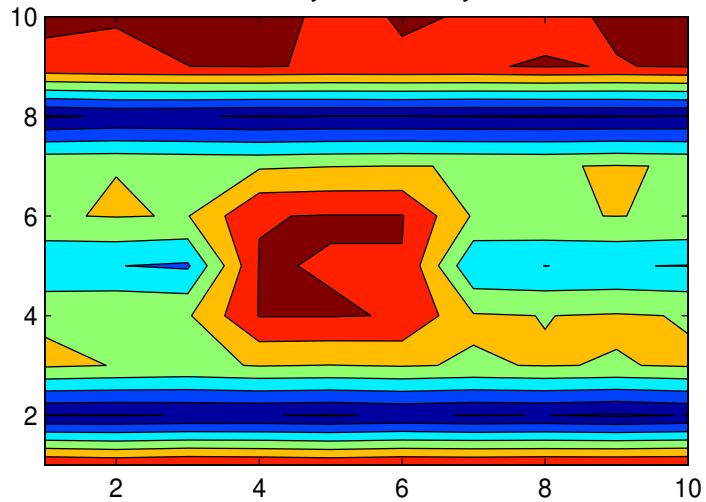
True Permeability



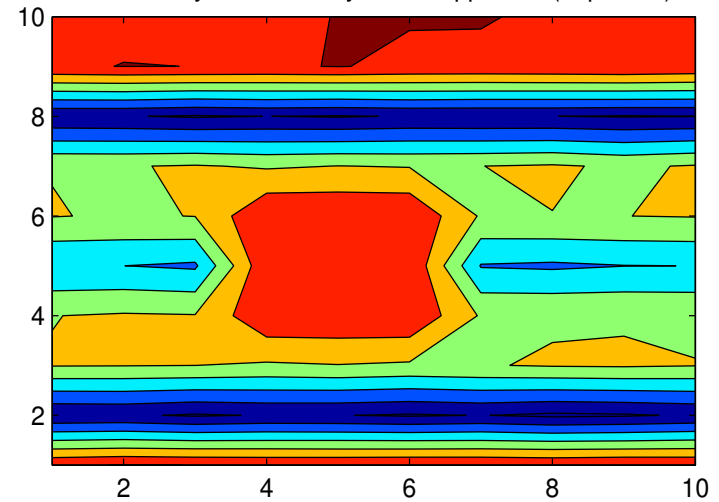
Initial Permeability



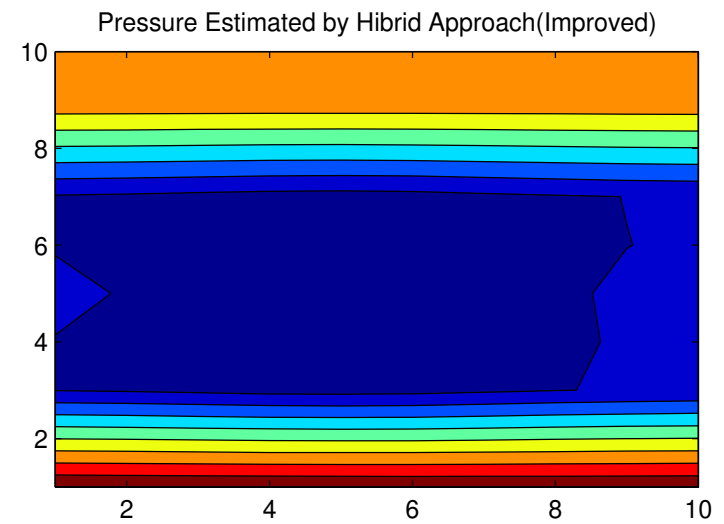
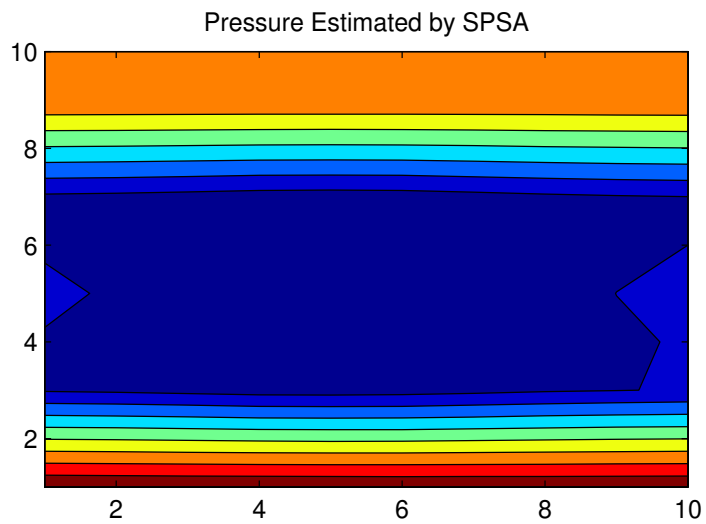
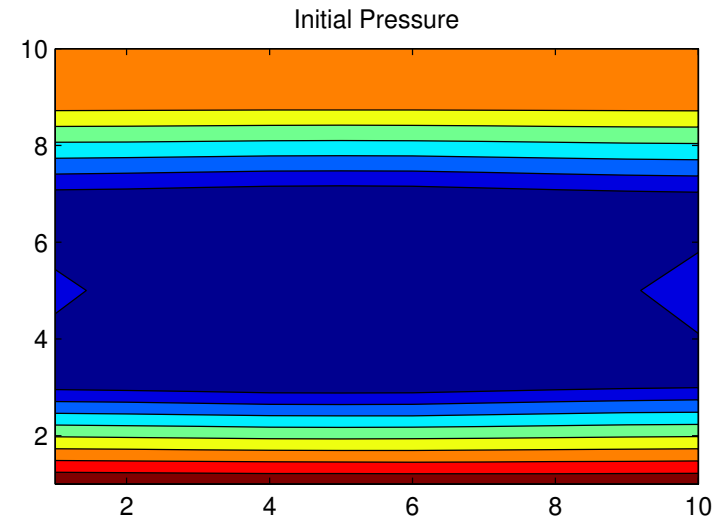
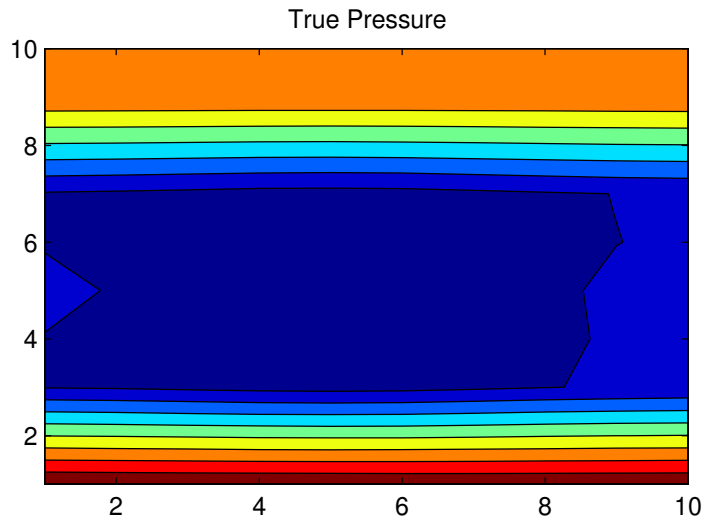
Permeability Estimated by SPSA



Permeability Estimated by Hibrid Approach (Improved)



PRESSURE RESULTS



- We run the simulator IPARS (Integrated Parallel Accurate Reservoir Simulator) on a Linux-based multicore network of workstations.
- Our goal is to estimate a permeability field that involves 2000 parameters. The field is parameterized by SVD reducing the parameter space to 20 (each parameter represents a scale resolution level).
- We choose several initial points by adding a percentage of noise to the true singular values: 5%, 10% and 15%

Number of Initial Points ran by SPSA	30
Total Iterations SPSA	3645
Function Evaluation SPSA	7290
Initial Objective Function Value	8 to 10
Final Objective Function Value given by SPSA	0.568 to 2.5
Best SPSA Iteration- Initial Objective Function Value	9.03
Best SPSA Iteration - Final Objective Function Value	0.568
Number of Function Values Used to create Surrogate Model	156
Iterations NKIP	94
Objective Function Hybrid	0.478
% Gain by Hybrid Approach	16%

Number of initial points ran by SPSA	20
Total Iterations SPSA	2248
Function Evaluation SPSA(2xTotal Iterations SPSA)	4496
Initial Objective Function Value	18.72 to 53.9
Final Objective Function Value given by SPSA	0.858 to 6.785
Best SPSA Iteration- Initial Objective Function Value	19.67
Best SPSA Iteration - Final Objective Function Value	0.858
Number of Function Values Used to create Surrogate Model	81
Iterations NKIP	67
Objective Function Hybrid	0.747
% Gain by Hybrid Approach	13%

Number of initial points ran by SPSA	20
Total Iterations SPSA	1647
Function Evaluation SPSA(2xTotal Iterations SPSA)	3294
Initial Objective Function Value	29.46 to 120.56
Final Objective Function Value given by SPSA	1.541 to 15.89
Best SPSA Iteration- Initial Objective Function Value	31.35
Best SPSA Iteration - Final Objective Function Value	1.541
Number of Function Values Used to create Surrogate Model	57
Iterations NKIP	110
Objective Function Hybrid	1.465
% Gain by Hybrid Approach	5%

- The hybrid approach finds a good estimate of the global solution for all the test cases.
- As the noise level was increased, the hybrid approach presented more difficulties in reproducing the true permeability field.
- However, the estimation is very accurate in all cases.

- To improve a parallel version of the hybrid scheme
- To add equality constraints to the minimization of the surrogate model
- To investigate parameterization schemes (SVD, Wavelet)
- To finish implementing Chris Kee's simulator (ERDC) with the help of Mark Potts (HPTi), and run HPC simulations

- Papers

- A Hybrid Optimization Approach for Automated Parameter Estimation Problems, ICIAM Proceedings, October 2007
- Numerical Testing of Parameterization Schemes for Solving Parameter Estimation Problems, The 26th Army Science Conference, December 2008

- Submitted 3 Papers

- Journal of Global Optimization, June 2008
- IEEE Transactions on Signal Processing, July 2008
- Transactions on Signal Processing, May 2008

- Invited Talks

- International Congress on Industrial and Applied Mathematics, Zurich, SW
- International Conference on Approximation and Optimization in the Caribbean, San Andres, CO

- Poster Presentations

- Supercomputing Conference, Reno Nevada, Nov. 2007
- Center of Subsurface Modeling Corporate Meeting, Austin, Feb. 2008
- SACNAS-UTEP Expo, May 2008

- Coastal and Hydraulics Laboratory, US Army Engineer Research and Development Center (ERDC), MS
 - Christopher Kees and Matthew Fulding
- Battlefield Environment Division (BED), Computational and Information Sciences Directorate (CISD), White Sands Missile Range, NM
 - James Cogan and Bob Dumais
- Stanford University
 - Michael Saunders

- Center for Subsurface Modeling, ICES, UT-Austin
 - Mary Wheeler, Hector Klie, and Eduardo Eldgin
- Leticia Velazquez, Director of the Computational Science Program, UTEP
Fall 2008: 4 Ph.D Students and 1 MS Student