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Laboratorij za sisteme z naprednimi materiali (Laboratorij za krmilne sisteme)

DELO v LABORATORIJU V LETIH 2010/2011

Vodja laboratorija: Prof. dr. Božidar Šarler

Namestnik vodje laboratorija: Zoran Pajcur

Sodelujoči partnerji: Systec d.o.o.

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Okolje za simulacije in optimiranje
Modelling & Optimization Environment

Igor Grešovnik

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Outline

1. Envisaged optimization procedures to be developed
2. Outline of planned optimization environment
3. Approximation of process response by neural networks
4. Idea of unified simulation framework
5. Discussion of further steps

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Optimization Problems – Formulation

minimise	$f(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^n$
subject to	$c_i(\mathbf{x}) \le 0, \; i \in I$
and	$c_j(\mathbf{x}) = 0, \; j \in E,$
where	$l_k \le x_k \le u_k, \; k = 1, 2, \ldots, n$

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Use of optimization

Numerical simulations in industry:

- Improvement of Current Processes & Designs
- Virtual Prototyping

Development of numerical models:

- Experimental Validation
  - Inverse identification of model parameters

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Inverse identification of model parameters

Concept

- Perform laboratory or industrial measurements
- Prepare numerical models of these tests, some parameters unspecified
- Minimization of discrepancies between measurements and model results -> parameter estimates

Numerical difficulties

- Long computational times
- Noise in model results
- Non-availability of derivatives w.r. parameters

In industrial environment

- Complexity of industrial systems (variability of process conditions, complex interactions)
- Limited set of affordable measurements
- Insufficiency of data for solution of identification problem

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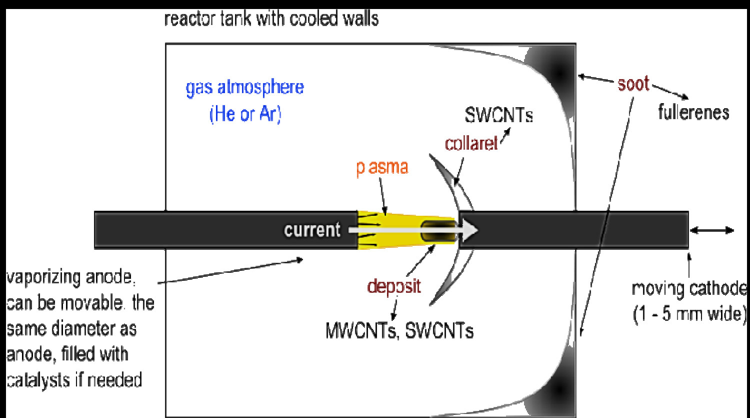
Example: Use within fullerene production cell

- Find values of process parameters:
  - Pressure within the cell
  - Temperature of cell walls
  - Electric current
  - Gap between electrodes
- that give maximal yield of different types of carbon nanostructures



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Input and output parameters of the model

Input parameters:

anode diameter
cathode diameter
anode length
anode hole diameter
anode hole depth
catode length
reactor dimensions (length and diameter)
current and current intensity
presure
anode cathode distance
anode temperature (side and tip)
cathode temperatute (side and tip)
wall temperature
mass density of the inert gas
anode surface area
pre-exponential factor
carbon mass fraction
initial C, C2, C3, Ni mole fraction

Output parameters:

deposit rate
anode gas velocity
electric power dissipation
dilution factor at the anode
erosion rate
estimated electron density
temperature
He, Ni, Y ... number density
growth rate

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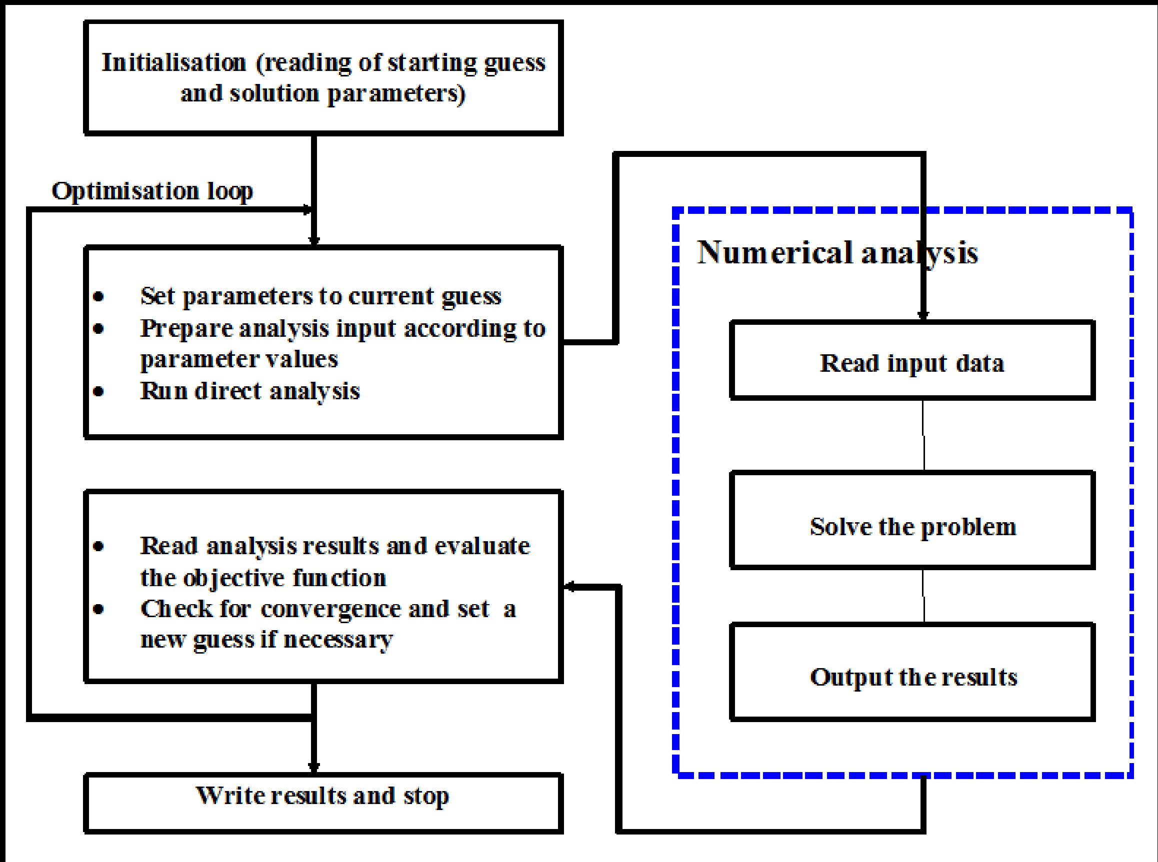
Optimization Problems – Solution Scheme



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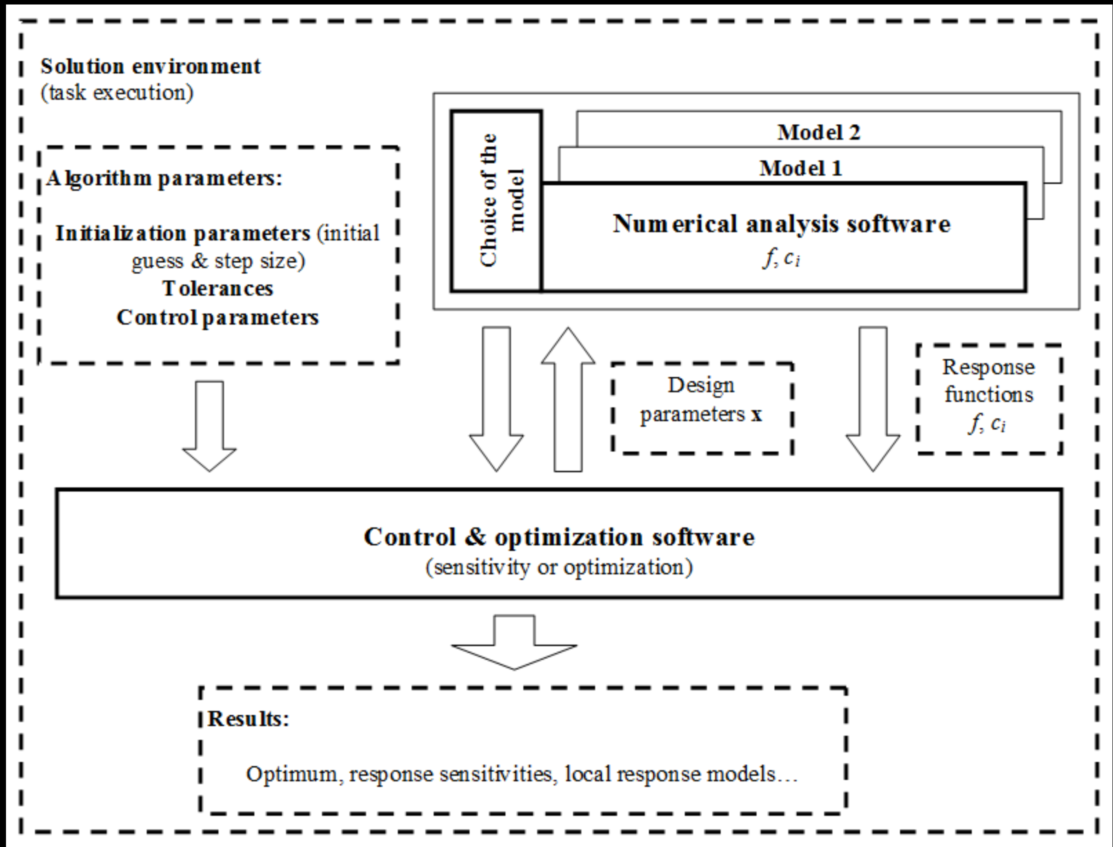
Optimization Problems – Solution Scheme

1. Take current optimization parameters
2. Prepare numerical model according to parameters
3. Run numerical simulation of the process
4. Extract the relevant quantities from simulation results
5. From measured data
- Read result file
- Extract relevant data
6. Calculate the response functions and eventually their gradients (in our case the discrepancy function f)
7. Store the response functions in output arguments and return

Integrated Optimization Platform



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Popular Constrained Optimization Algorithms

- Transformation to unconstrained problems
  - Penalty methods
  - Lagrangean methods (eliminate constraints by Lagrange multipliers)
  - Projection methods (feasible set)
- SQP
  - Newton method for 1st order conditions for a local minimum
  - QP subproblem
  - Feasible set method
  - Sequentially solve unconstrained problems by BFGS
  - Superilinear convergence

Very efficient, but depend crucially on derivative information

Sensitive to numerical noise

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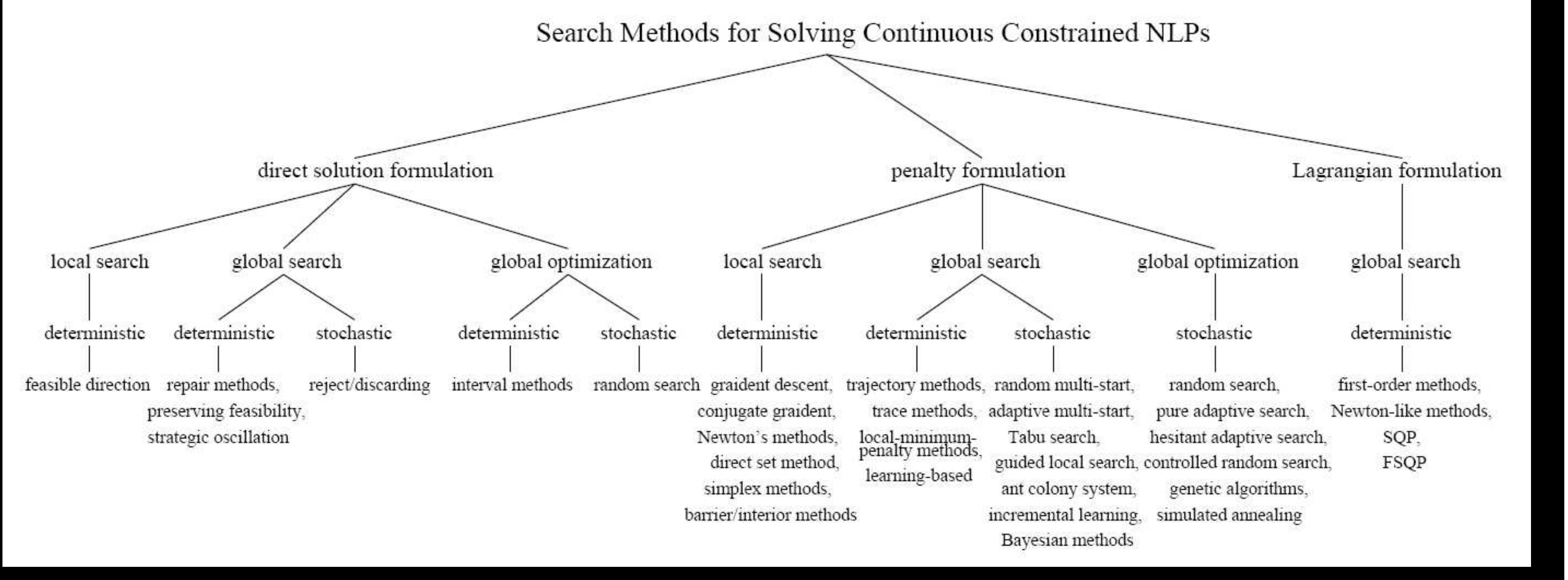
Popular Optimization Algorithms: Global Optimisation

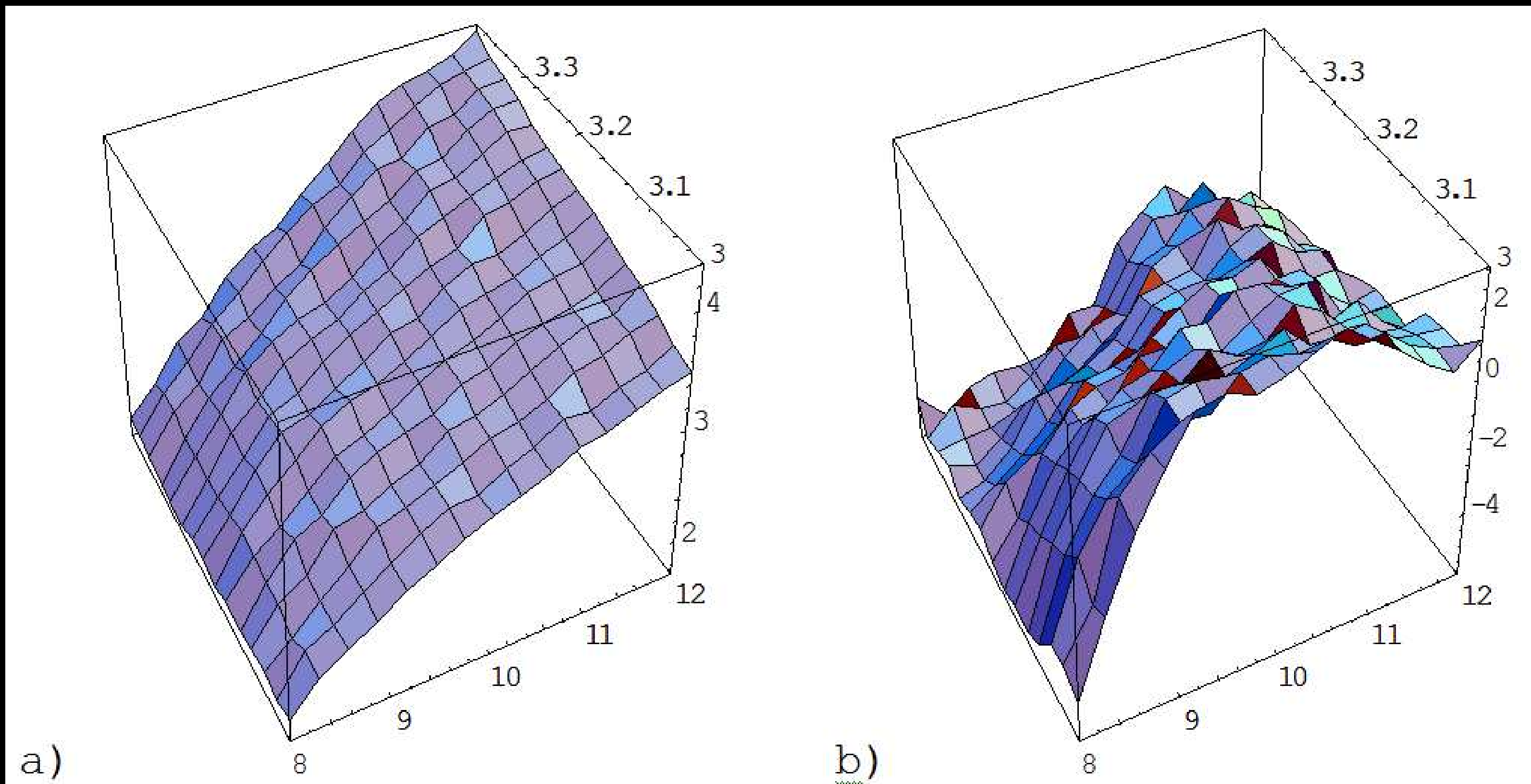
- Predominantly stochastic approaches
  - Simulated annealing, genetic algorithms, particle swarm method, differential evolution
- <u>Robust in terms of response requirements</u>
- Perform on discontinuous, multimodal functions
- <u>Inefficient in terms of required number of function evaluations</u>
- Notion of “global algorithm” is asymptotic
  - Even if not “global” in practical sense, these methods less easily get stuck in a local minimum
  - Notion of local convergence is difficult to define
  - Performance typically increased by tuning a number of control parameters (case dependent)

Classification of Optimization Algorithms



Response functions with noise

a) Objective function; b) Constraint function



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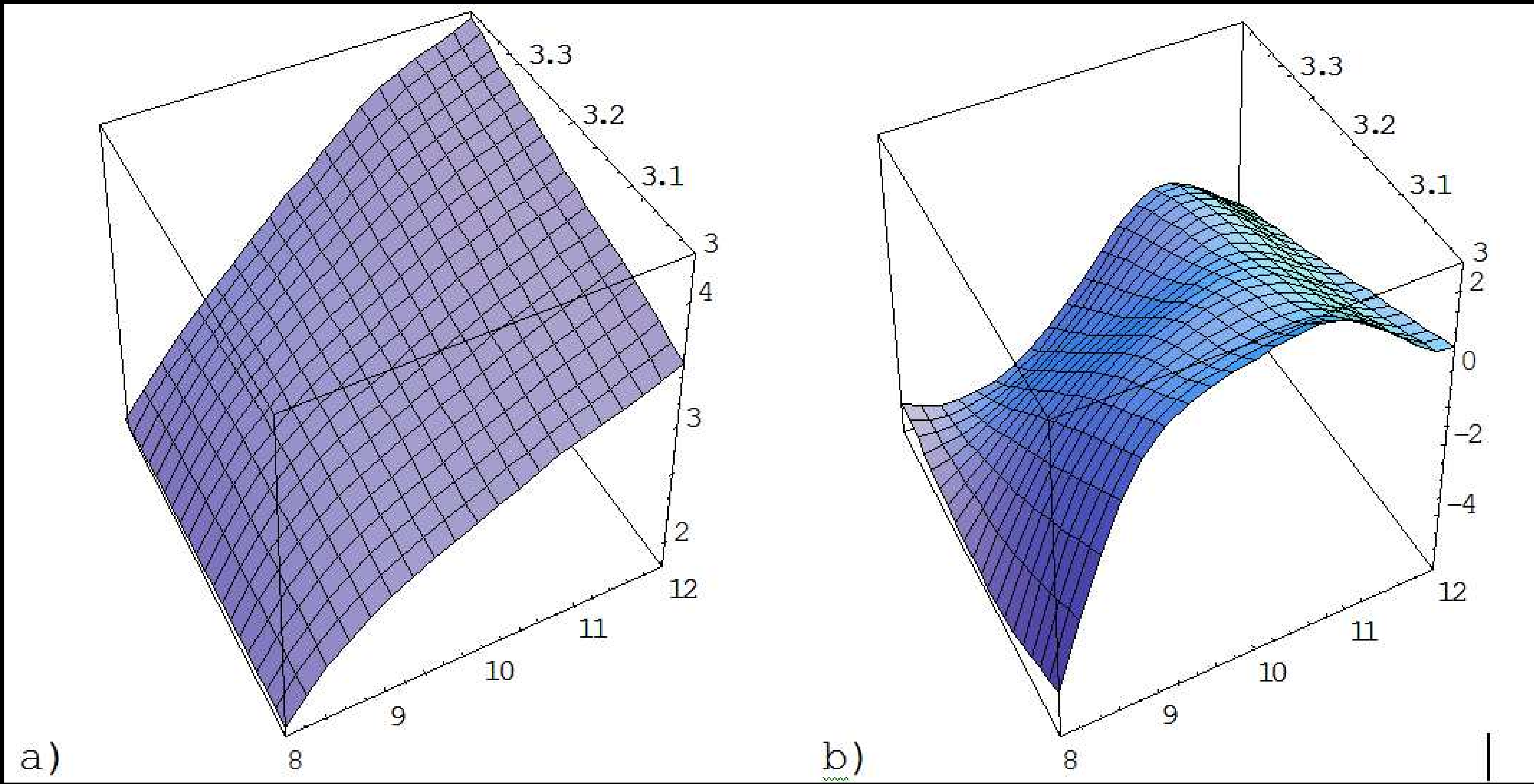
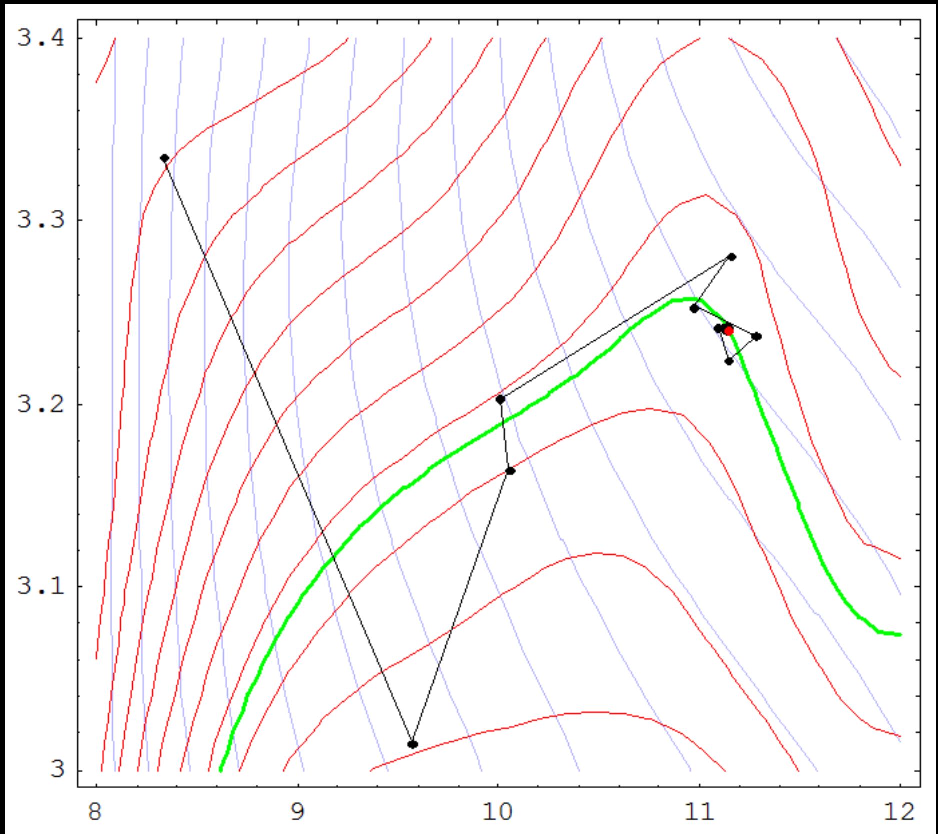
Response Smoothing (Global, MLS Approximation)



Optimization of Approximated Response (SQP)



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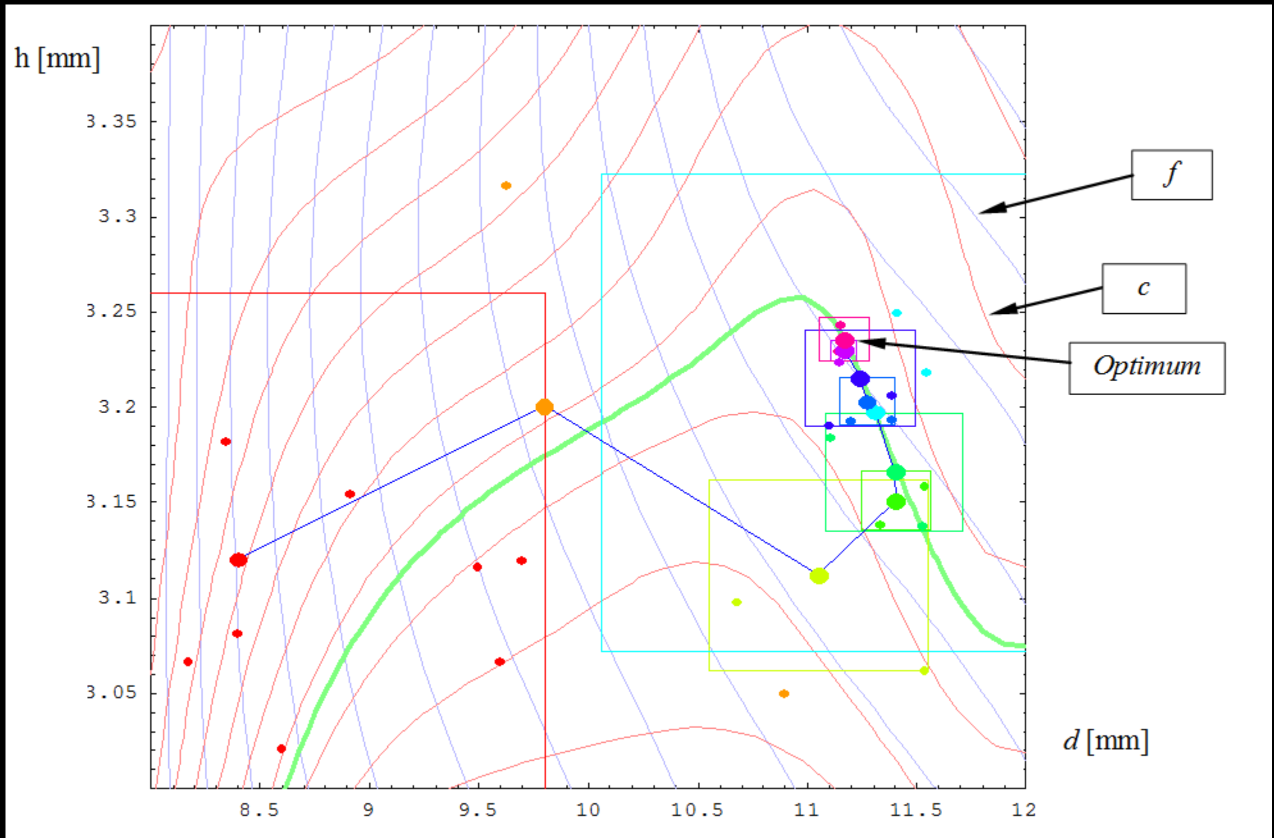
Feasible Alternative: Successive MLS Approximations with Restricted Step



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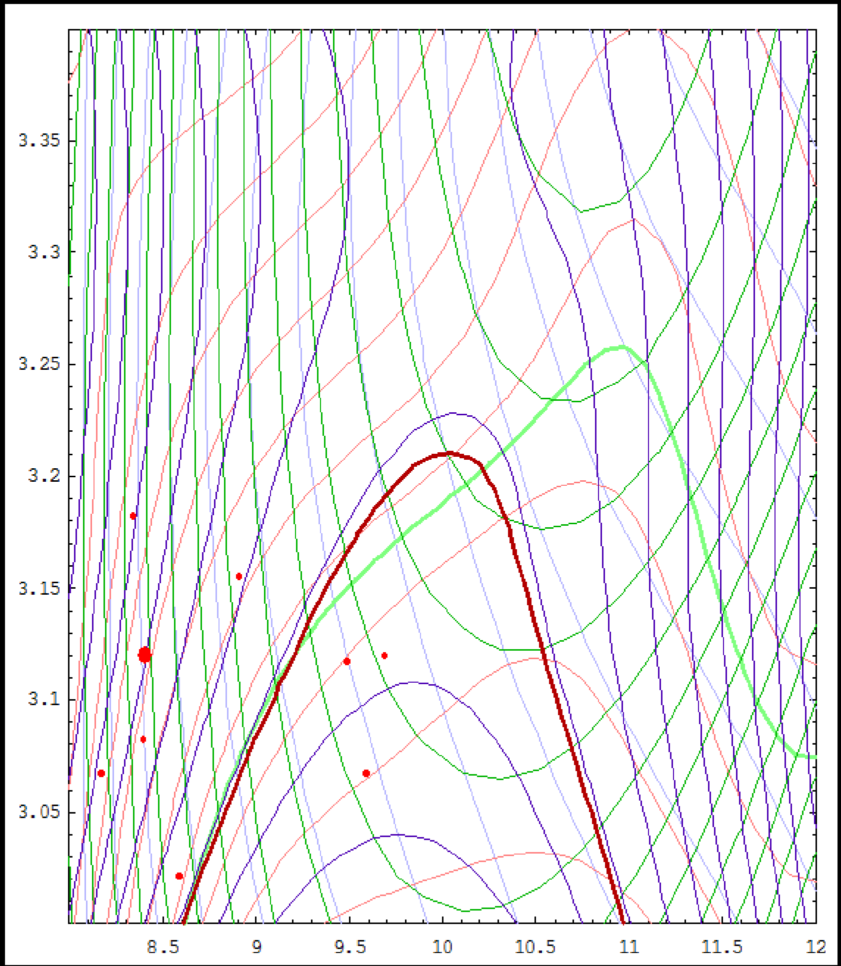
Approximated response for iteration 1



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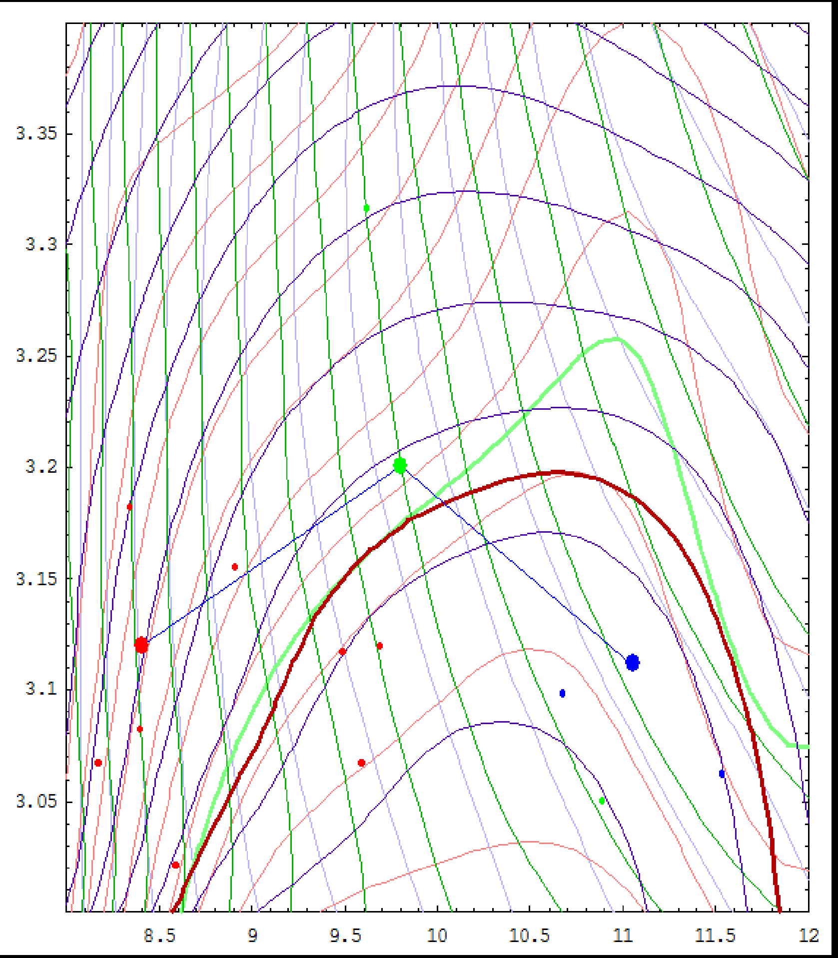
Approximated response for iteration 3



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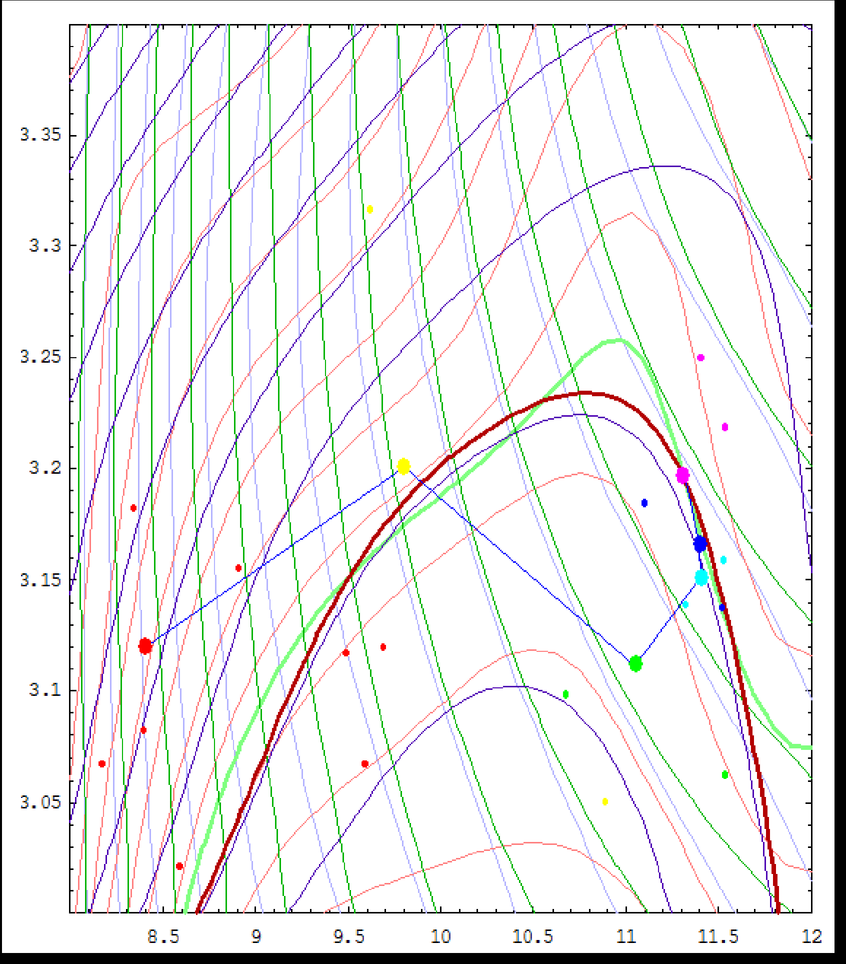
Approximated response for iteration 6



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Building Blocks: Restricted Step Constraint

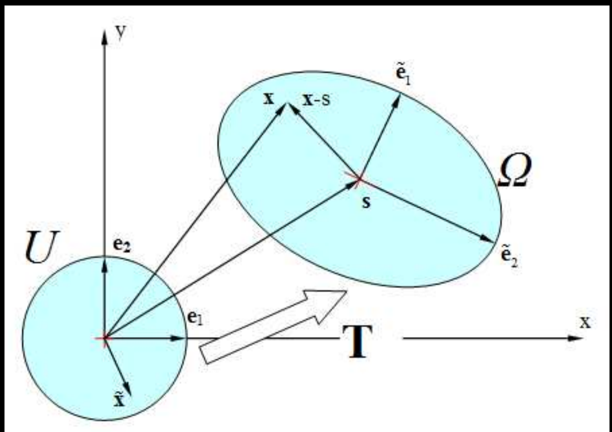
Restricts the feasible region to a neighborhood of the current guess

- Unit ball constraint:

$$c_U(\tilde{\mathbf{x}}) = \|\mathbf{x}\|_2 - 1 \le 0$$

- General form:
  - Obtained from unit ball constraint by affine transformation of co-ordinates

$$c_{rs}(\mathbf{x}) = \left\|\tilde{\mathbf{A}}^{-1}(\mathbf{x} - \mathbf{x}_0)\right\|_2 - 1 \le 0$$



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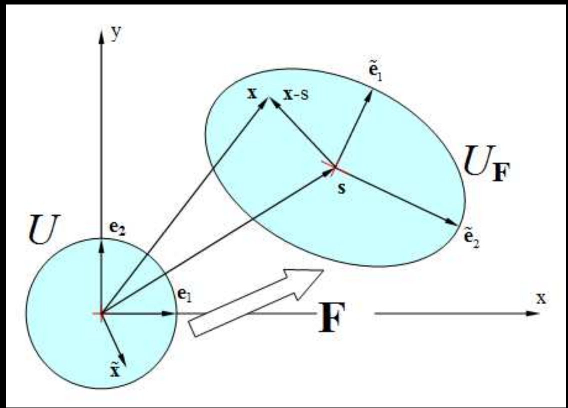
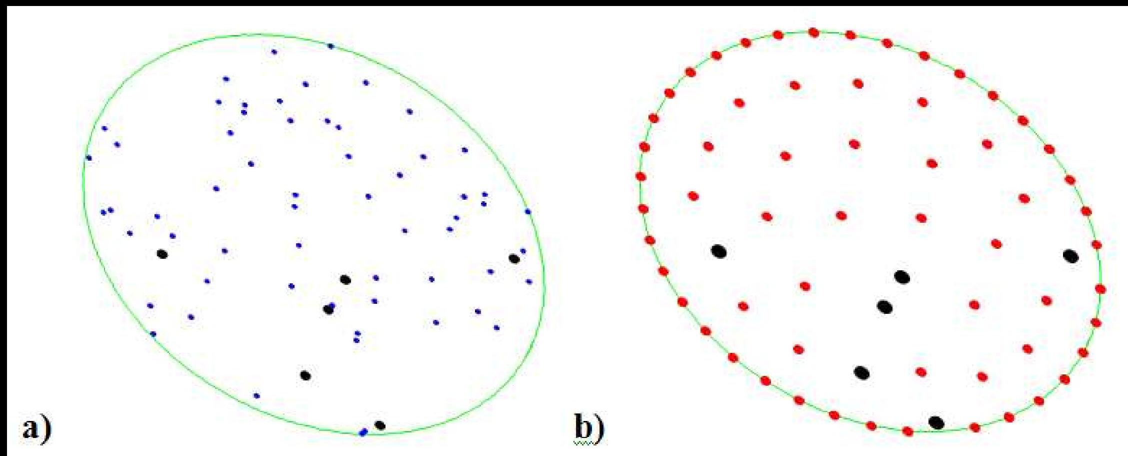
Design of Experiments





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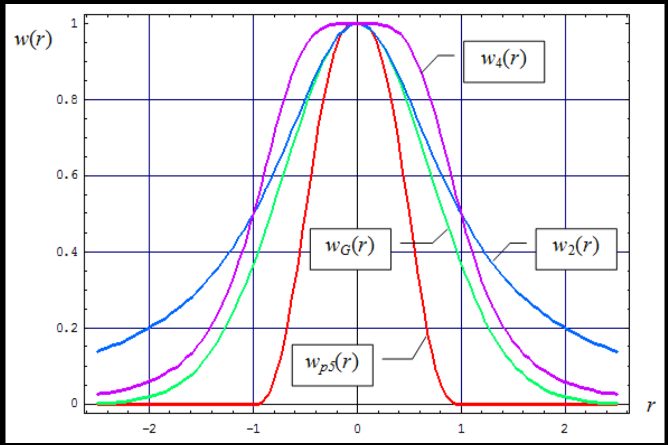
Weighting Functions for Approximations

- Different forms of 1D weighting functions $w(r)$

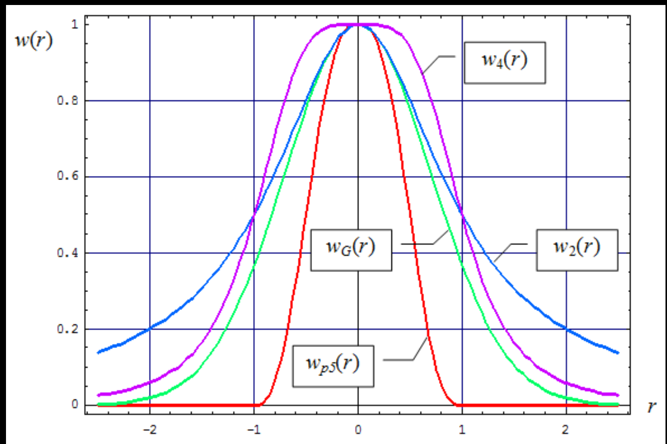


Integration in algorithm scheme

- To build **adaptive** approximations of response functions
- To solve approximated sub-problem with restricted step constraint

Weighting Functions for Approximations

- Different forms of 1D weighting functions *w*(*r*)



Integration in algorithm scheme

- To build **adaptive** approximations of response functions
- To solve approximated sub-problem with restricted step constraint
- Target as small number of function evaluations as possible

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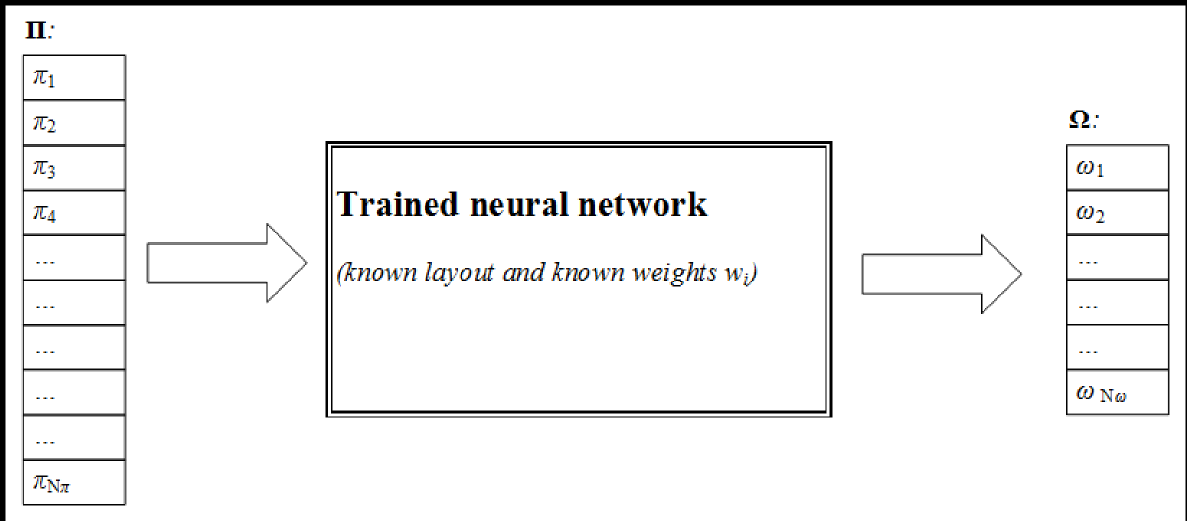
Part II: Overview of accomplished

Response approximation with neural networks

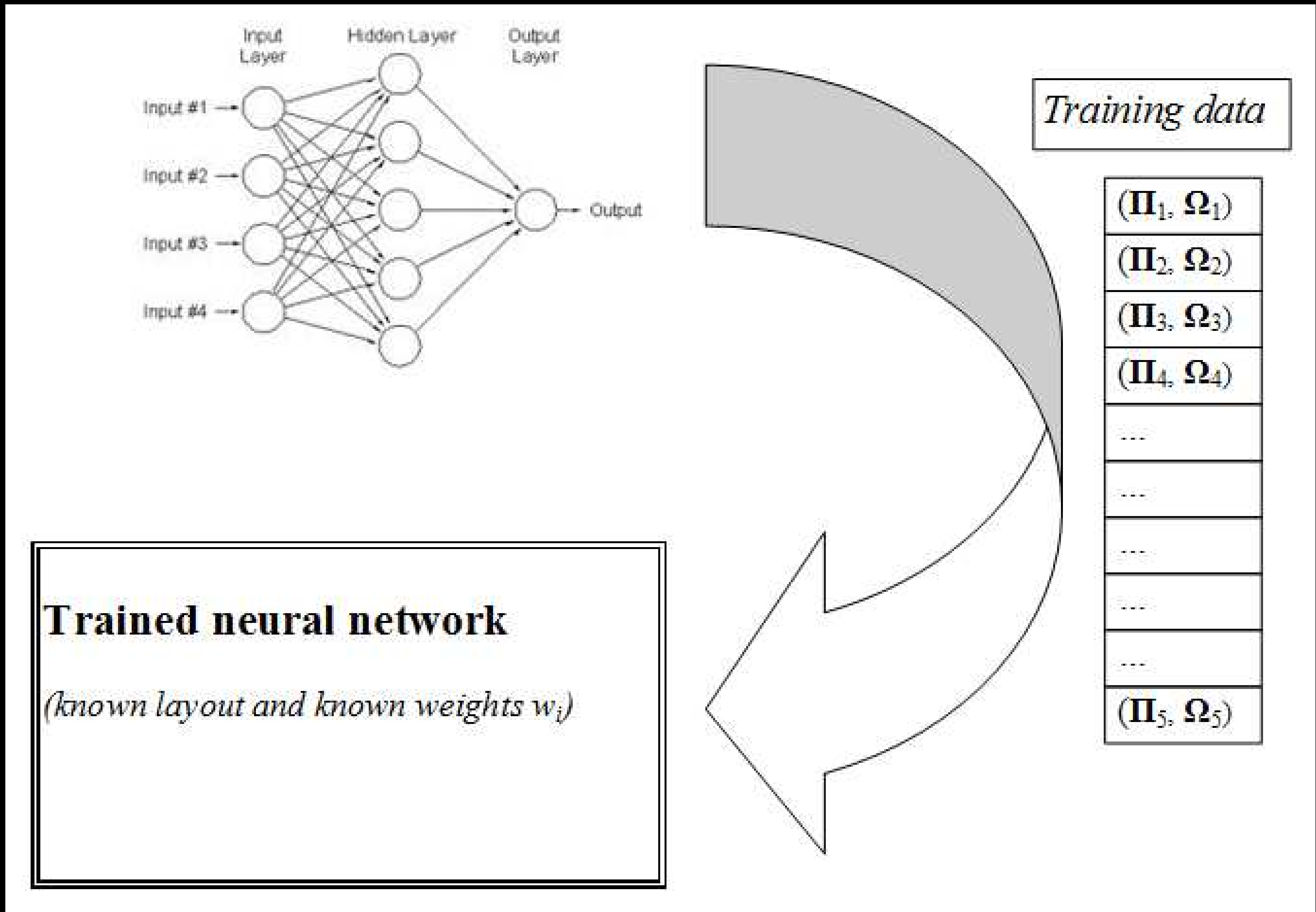
- Popular use as general black box approximator
- Global approximations over domain of interest
- Convenient separation of training and evaluation stage
  - Evaluation stage very efficient
- As global approximator, best practical value where:
  - … either large number of training samples with good space coverage
  - … or simple (e.g. close to linear) response

Software module: NN response approximation

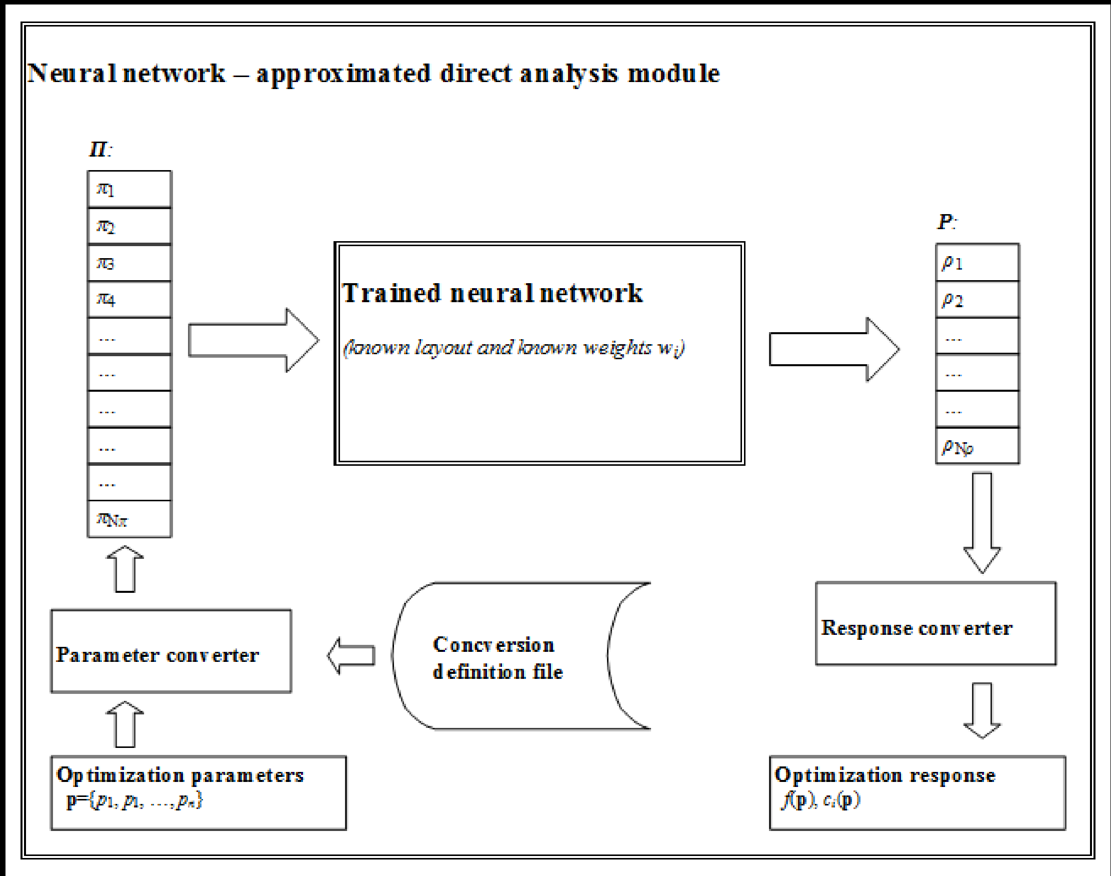
- Based on Aforge.NET open source library
- Provides approximate relation between process parameters and outcomes
  - Flexible training and verification procedure
  - Easily integrated with other software
  - Simple use of other NN libraries



Training with measured or simulated data



Use of trained network: Simulation surrogate in optimization



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Further info:

Tadej Kodelja:

- Use of the module
- Training on real industrial & simulation data
- Format conversions for interaction with other software through files

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Unified simulation framework

Idea:

- Unification of development of different simulation codes
- Joint development between COBIK and UNG groups

Expected benefits:

- Less duplication of work
- Aggregation of development potential
- Systematic and directed development of common libraries and other tools
- Various synergetic effects:
    - Increased exchange of ideas
    - Easier introduction of new developers
    - Gradual accumulation of advanced tools important for industrial application
        - Mesh adaptivity, geometry definition, multibody problems, processing of results…

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Simulation framework – results

Detailed plan for launching framework development

- Startup, organization of team work, gradual switch form old codes
- Detailed consideration of development platform
- Order of development
- Proposal of software development concept suitable for industrial needs
- Suitable for academic and industrial needs
- Can fit industrial requirements with respect to non-disclosure of technology, licensing, etc.
- Designed to reduce the time between development and practical use of new concepts
- Development environment established
- SVN server, bugzilla
- Outline of base libraries for optimization and eventually for simulation
- Example class library structure for simulation framework