Advances in Inverse Transport Methods and Applications to Tomography

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Outline

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- Former Work
- Advances Introduced
- Procedures Proposed
- Present Status

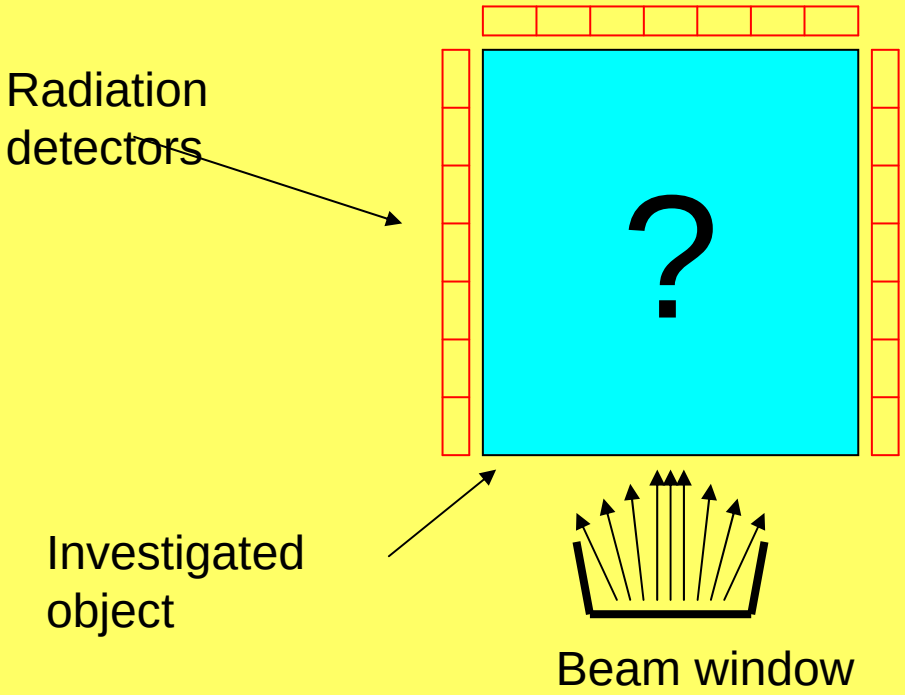
Project Overview

- Problem Statement
- Scattering Blur
- Minimization Based Approach

Problem Statement

We define the "inverse problem" as the inference of material properties inside an object under investigated.

The purpose of our project is to find out the material distribution inside an object based upon detection and analysis of radiation emerging from the object.



Scattering Blur Issue

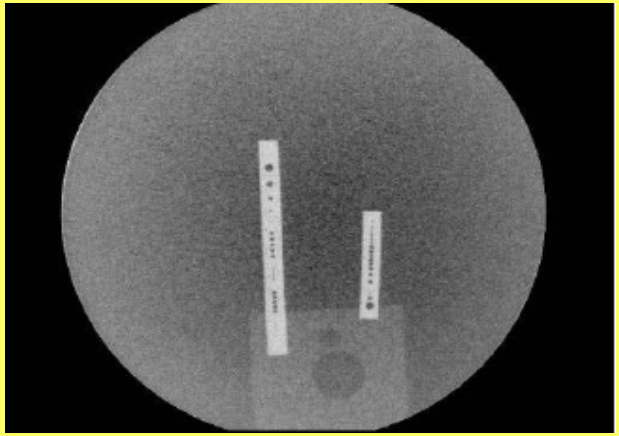
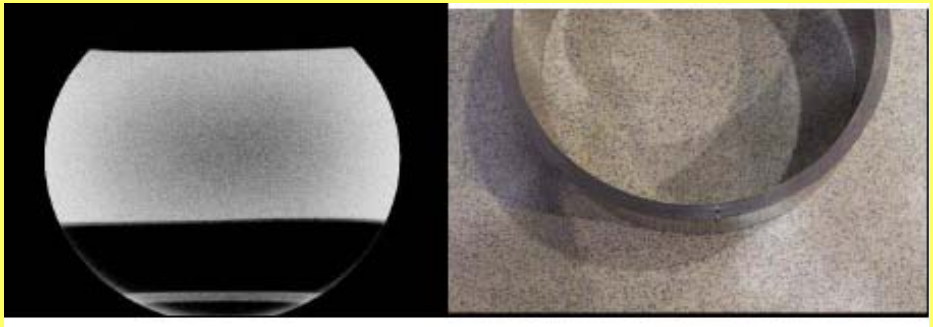


Fig 1. Neutron radiograph of two cadmium strips displaying good image resolution for highly absorbing, low scattering materials.

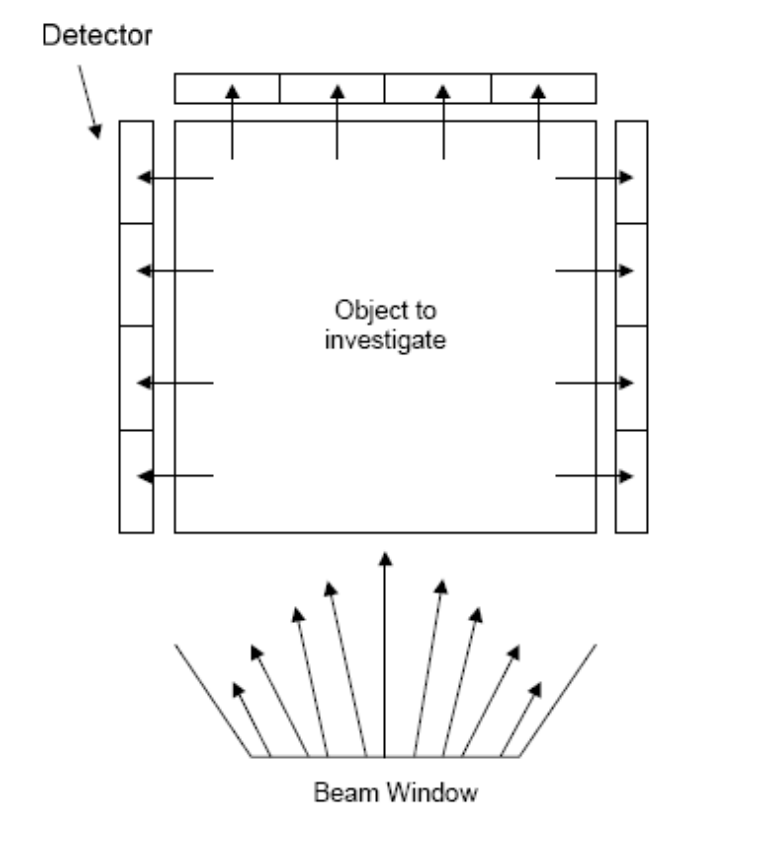


(a) (b)

Fig 2. Image on the left (a) is a neutron radiograph of a thick carbon fiber composite object with 1/8 inch hole present. Image on the right (b) shows the object and the hole.

(Pictures are from W.S. Charlton's DOE NEER proposal.)

Beam-Object-Detector System



A schematic diagram of the beam-object-detector system

Minimization Based Approaches

- Objective function

$$\Phi = \frac{1}{2}\sum_{n=1}^{N}\left(M_n - P_n\right)^2$$

- Here ‘P’ is treated as a function of properties of the unknown object

$$P = P\left(\sigma_t, \sigma_s, \sigma_{s1}, \cdots\right) \Rightarrow \Phi = \Phi\left(\sigma_t, \sigma_s, \sigma_{s1}, \cdots\right)$$

Former Work

Continued with V. Scipolo's Master Work. His work could be summarized as the following three parts:

1. Computational simulation. (MCNP)
2. X-Y 2D neutron transport forward model development.
3. Gradient calculation with Adjoint method.

$$\Rightarrow \left.\frac{\partial \Phi}{\partial \sigma_{x,i}}\right|_{\left\{\sigma_{t,1},\sigma_{s,1},\sigma_{s1,1},\ldots,\sigma_{s1,I}\right\}}$$

Drawbacks Associated with Minimization Methods

- Deterministic search method could be trapped into local minima
- Stochastic search method is not stable and is time consuming
- Cross-section sets obtained are not constrained to be realistic
- Dimension of unknowns grows fast as the case becomes more realistic

Notes: Number of possible variables (only thinking of scattering cross sections) in continuous searching scheme:

$$\underbrace{16}_{\text{number of cells}} \times \underbrace{100 \times 100}_{\text{100 groups}} \times \underbrace{4}_{P_3 \text{ method}} = 640000$$

Advances Introduced

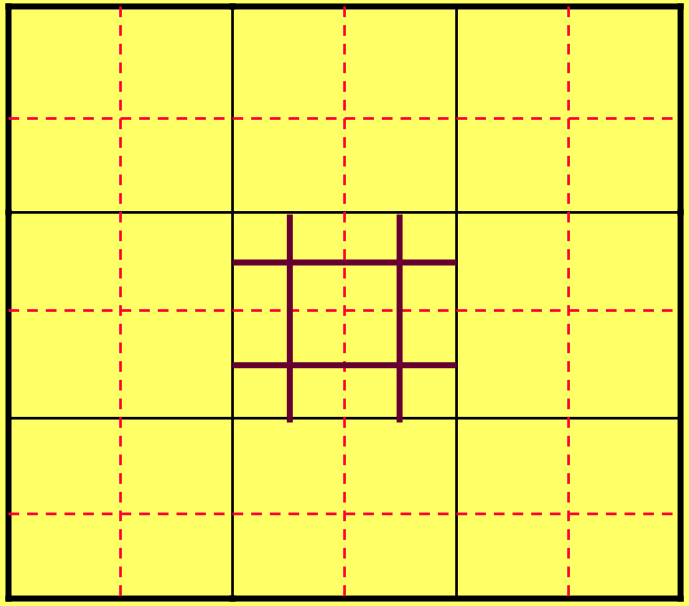
- Treat unknowns as materials instead of cross sections

  This is an important improvement!

- Both Continuous and Stochastic optimization method involved.
- Hierarchical Approach

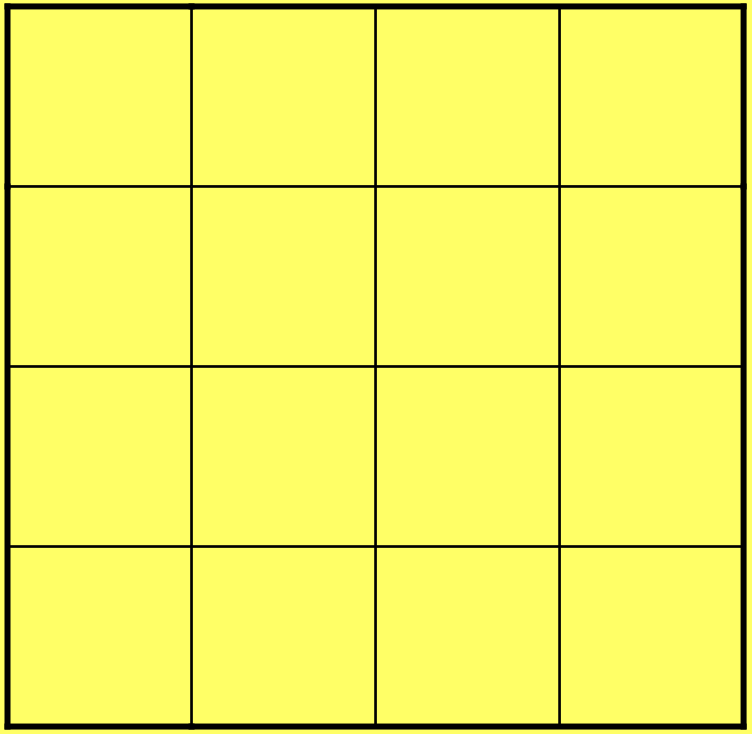
  Adaptive Mesh Refinement (AMR)

- Advanced tabu-search techniques
- Intelligent Sampling (LHS)



Combinatorial Optimization Problem

- Suppose we divide an object into have a 4x4 cells in a 2-D view and we have 10 material candidates in our material library.
- In each cell, the material in it has 10 possibilities, so over all there're totally $\underbrace{10 \times 10 \times \cdots \times 10}_{16 \text{ times}} = 10^{16}$ possibilities (solutions) to construct the object.
- Call one solution as one combination, it has a limited but discrete space.



Procedures Proposed

- Step I:

  Gradient-based linear search for cross sections, using crude forward model (e.g. coarse-mesh one-group diffusion).
  - unknowns are cross sections; use hierarchy of spatial grids; must address local-minimum problem
- Step II:

  Use results from Step 1 to restrict *material* search space for following step.
  - For each region, eliminate materials that are inconsistent with findings from Step 1. Must address collapse-spectrum issue.
- Step III:

  Stochastic-based optimization with realistic transport forward model, fine meshes and multi-group.
  - unknowns are materials; fewer possibilities because of step 2; use advanced sampling techniques to generate iterates

Present Status

- Some completed work
- Some work in progress
- Difficulties and problems
- Possible solutions

MCNP Simulation

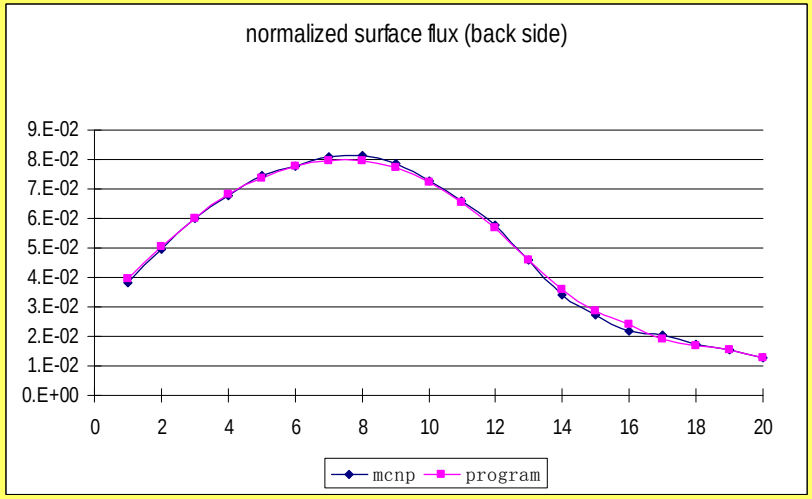


Fig 1. Comparison of MCNP "experiment" vs. S_N forward model.

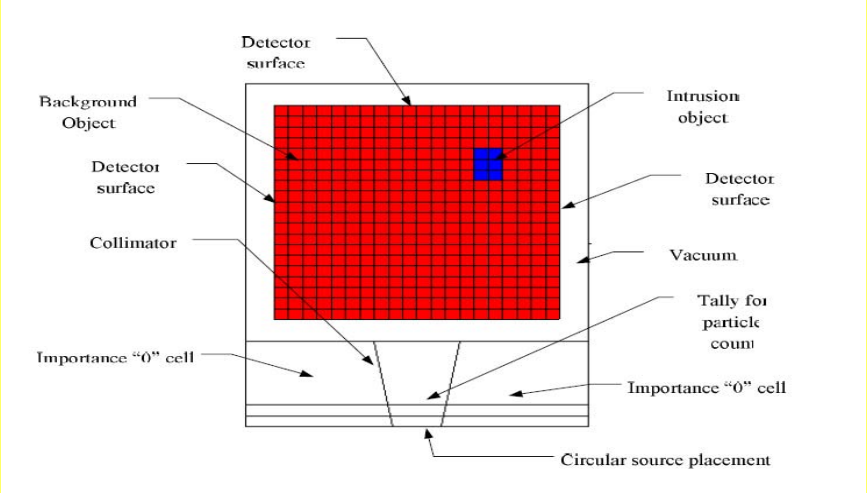


Fig 2. X-Y view of the object that produced Fig. 1.

These figures show that our S_N transport model can reproduce MCNP results for a simple problem (Maxwellian incident energy distribution in MCNP; one energy group S_8 in model).

Gradient Verification

In a 2-cell problem, we use finite difference (FD) method to check the accuracy of derivatives calculated by adjoint method, there's two derivatives actually calculated in each cell:

$$\left.\frac{\partial \Phi}{\partial \sigma_t}\right|_{\sigma_s = cont.} = \left.\frac{\partial \Phi}{\partial \sigma_a}\right|_{\sigma_s = cont.} \quad \text{and} \quad \left.\frac{\partial \Phi}{\partial \sigma_s}\right|_{\sigma_t = cont}.$$

Mat. Pro.	Cell #1	Cell # 2
σ_s (1/cm)	0.01	10
σ_a (1/cm)	0.5	1.2
σ_t (1/cm)	0.51	11.2

Table 1. Material properties in each cell.

	Cell #1		Cell #2	
	Adjoint	FD	Adjont	FD
$\frac{\partial \Phi}{\partial \sigma_s}$	2.1334311E-5	2.1334328E-5	1.2433677E-5	1.2433749E-5
$\frac{\partial \Phi}{\partial \sigma_a}$	-6.2106049E-5	-6.2107084E-5	-6.2834296E-5	-6.2835641E-5

Table 2. Comparison of the derivatives calculation results by adjoint and FD method.

One-group Cross Sections

Using MCNP to generate energy collapsed cross sections for different materials. These information will be used to make a material candidate library for discrete optimization.

material	sigma_t(1/cm)	sigma_s(1/cm)	sigma_a(1/cm)
paraffin	0.566949637	0.566575454	0.000374060
B-10	554.068773212	0.319697120	553.749645166
water	0.743519835	0.736203099	0.007317882
Si	0.110164975	0.102154305	0.008010556
Fe	1.178827056	0.967152960	0.211677974
Nitrogen	0.000654006	0.000554943	0.000099062
Uranium	0.812264369	0.453973014	0.160693259
Cadmium(Cd)	0.300568600	0.247206364	0.053361707
Aluminum(Al)	0.096671505	0.083069958	0.013601340

Conjugate Gradient Iteration

- First invented to solve linear equations problem, and later introduced to non-constrained optimization problem.
- Unlike the steepest descent (SD) method , in each iteration step conjugate gradient (CG) method moves along a so-called conjugate direction instead of moving along a direction only orthogonal the previous direction.
- A more understandable point of view, the CG method tries to minimize the residual rather than the objective function itself.
- In order to do that, the new search direction in every iteration step is produced by a linear interpolation between the old direction and the new gradient direction.

$$d_{k+1} = r_{k+1} + \beta_k d_k$$

Line Search

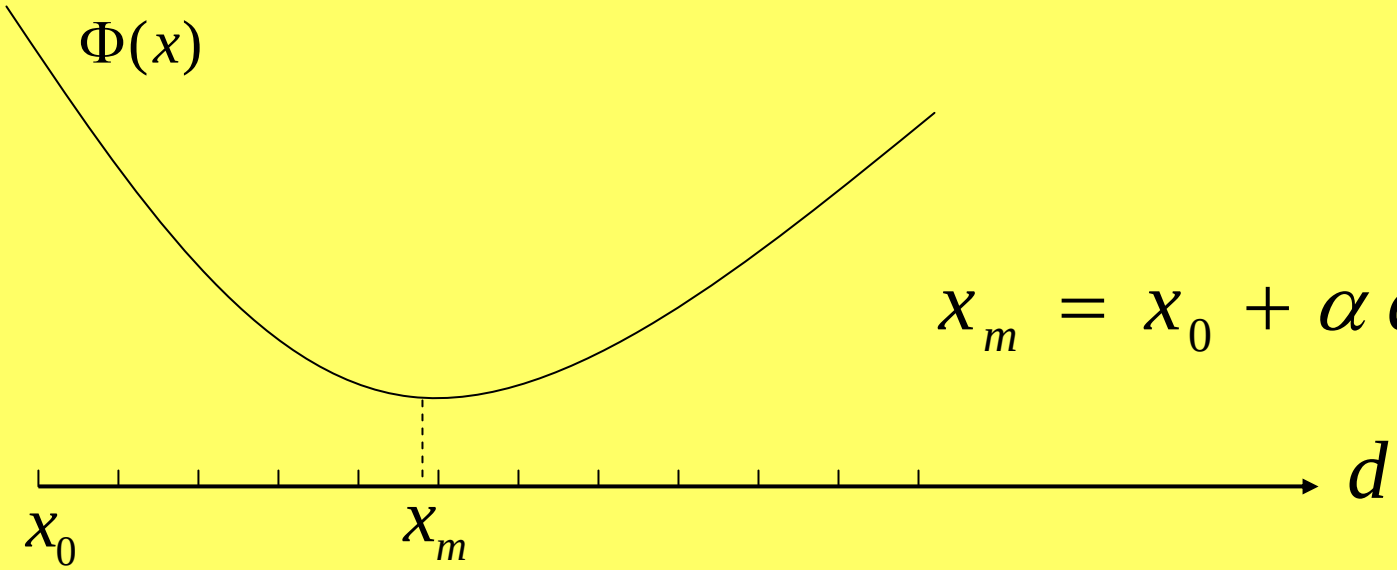
- Once the search direction is set, you have to know how far to move along this direction to make the objective function minimum. This is the basic conception of line search (1D search).

$$x_{k+1} = x_k + \alpha_k d_k$$

- The importance of line search is that the accuracy of its result is usually vital to the efficiency of the whole CG method.
- If the objective function could be written as a quadratic function to the unknown variables, it would be easy to find the minimum. Unfortunately our objective doesn't have such a good quality.

$$f(x) = \frac{1}{2} x^T A x - b^T + c = \frac{1}{2}(Ax, x) - (b, x) + c$$

Line Search (cont.)



$$x_m = x_0 + \alpha d$$

A variant of line search methods was applied and tested here, either utilizing trial method such as the golden section search or using only function evaluations such as the quadratic fit method.

Difficulties in Line Search

- Computationally expensive

  lots of forward model calculation required.

- Cross sections must be positive!

  unconstrained optimization

→ constrained optimization

- Easy to get stuck!

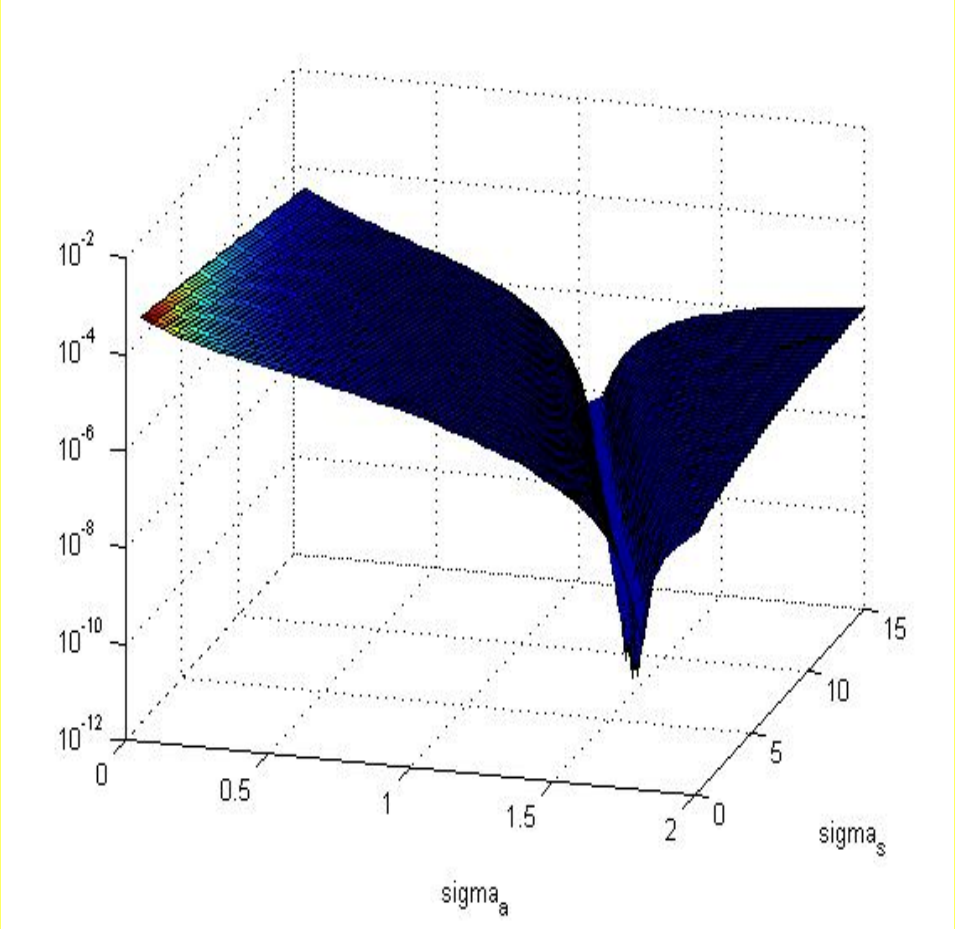
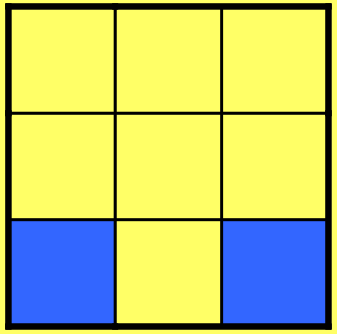
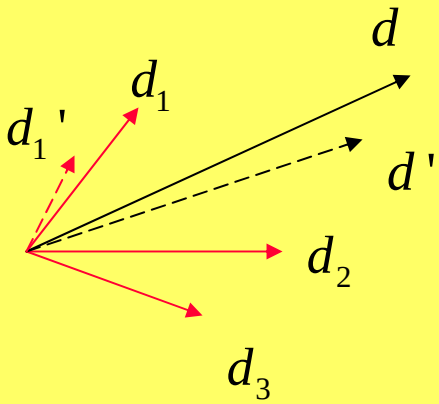


Fig. Surface plot of objective in one cell problems (only two variables).

Some ways to overcome the difficulties

- Fix some cells properties





- Smooth inversion (Regularized optimization)

  Add more constraints to objective function

  e.g. Objective = misfit + roughness

Stochastic Methods

- Approaches to combinatorial optimization
- Avoid local minimum
- Investigate two methods
  1. *Simulated annealing (SA) method*
  2. *Tabu search (TS) method*
- Investigate intelligent sampling techniques

End

Thank you & Questions?