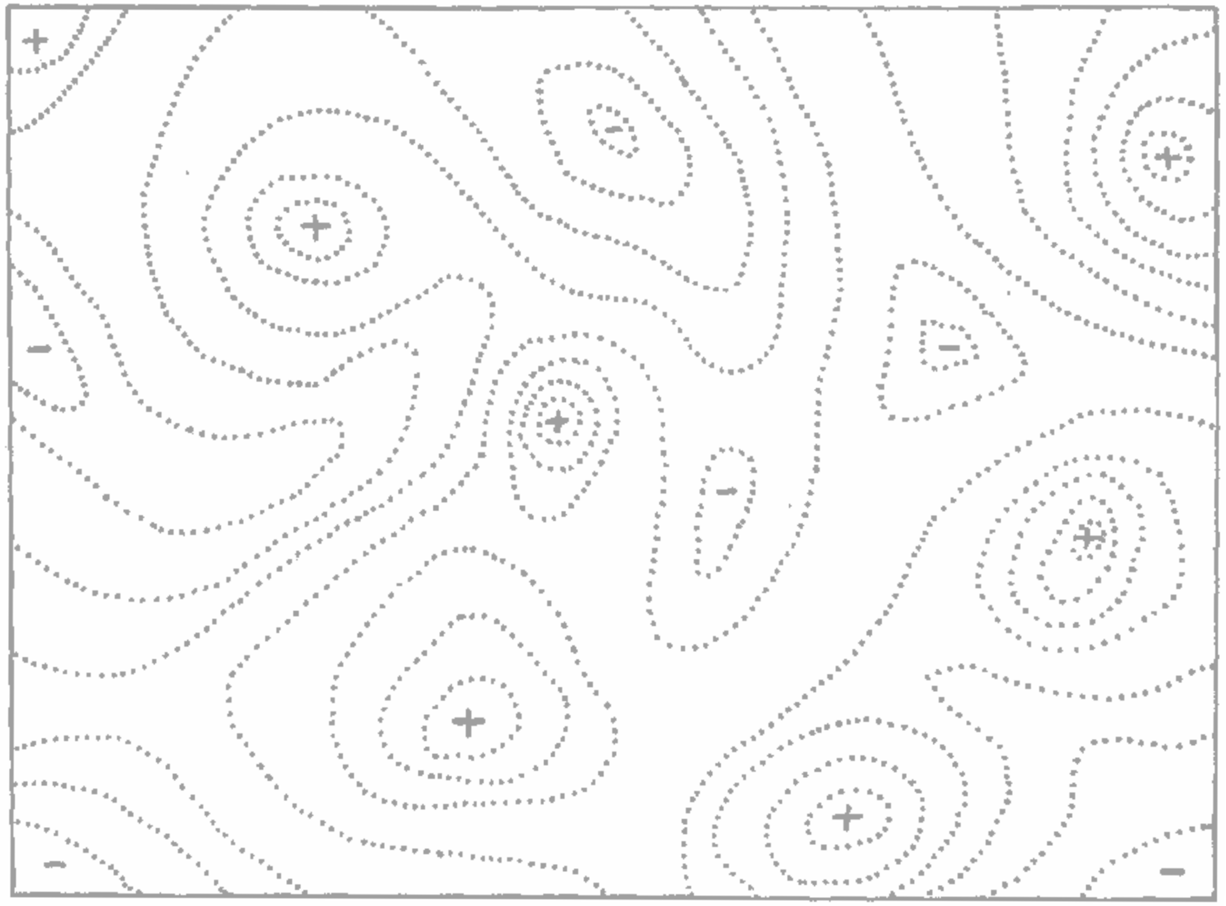
OPTIMIZATION LANDSCAPES



CHRISTIAN L. MÜLLER
CENTER FOR COMPUTATIONAL MATHEMATICS, FLATIRON INSTITUTE, NEW YORK
INSTITUTE FOR STATISTICS, LUDWIG-MAXIMILIANS-UNIVERSITÄT &
INSTITUTE OF COMPUTATIONAL BIOLOGY, HELMHOLTZ ZENTRUM, MUNICH

FWAM Flatiron Conference 10/30/2019

CONGRATULATIONS

SIMONS FOUNDATION 25
1994–2019

CONGRATULATIONS

FLATIRON INSTITUTE
Center for Computational Mathematics

5 YEARS OF SIMONS CENTER FOR DATA ANALYSIS (SCDA)/ FLATIRON INSTITUTE

CONGRATULATIONS

FLATIRON INSTITUTE
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SIMONS FOUNDATION
1994–2019
25

5 YEARS OF SIMONS CENTER FOR DATA ANALYSIS (SCDA)/ FLATIRON INSTITUTE

OPTIMIZATION

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Center for Computational Mathematics

OPTIMIZATION

op·ti·mi·za·tion

/ˌäptəməˈzāSHən,ˌäptəˌmīˈzāSHən/

noun

noun: **optimization**; plural noun: **optimizations**; noun: **optimisation**; plural noun: **optimisations**

1. the action of making the best or most effective use of a situation or resource.

google dictionary

OPTIMIZATION

op·ti·mi·za·tion

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noun: **optimization**; plural noun: **optimizations**; noun: **optimisation**; plural noun: **optimisations**

1. the action of making the best or most effective use of a situation or resource.

google dictionary

Mathematical optimization

Discipline

Description

Mathematical optimization or mathematical programming is the selection of a best element from some set of available alternatives. Wikipedia

wikipedia

OPTIMIZATION

Mathematical optimization (alternatively spelled *optimisation*) or **mathematical programming** is the selection of a best element (with regard to some criterion) from some set of available alternatives.[1]

Optimization problems of sorts arise in all quantitative disciplines from computer science and engineering to operations research and economics, and the development of solution methods has been of interest in mathematics for centuries.[2]

wikipedia

1. "The Nature of Mathematical Programming Archived 2014-03-05 at the Wayback Machine," *Mathematical Programming Glossary*, INFORMS Computing Society.
2. ^ Du, D. Z.; Pardalos, P. M.; Wu, W. (2008). "History of Optimization". In Floudas, C.; Pardalos, P. (eds.). *Encyclopedia of Optimization*. Boston: Springer. pp. 1538–1542.

OPTIMIZING A BLACK-BOX

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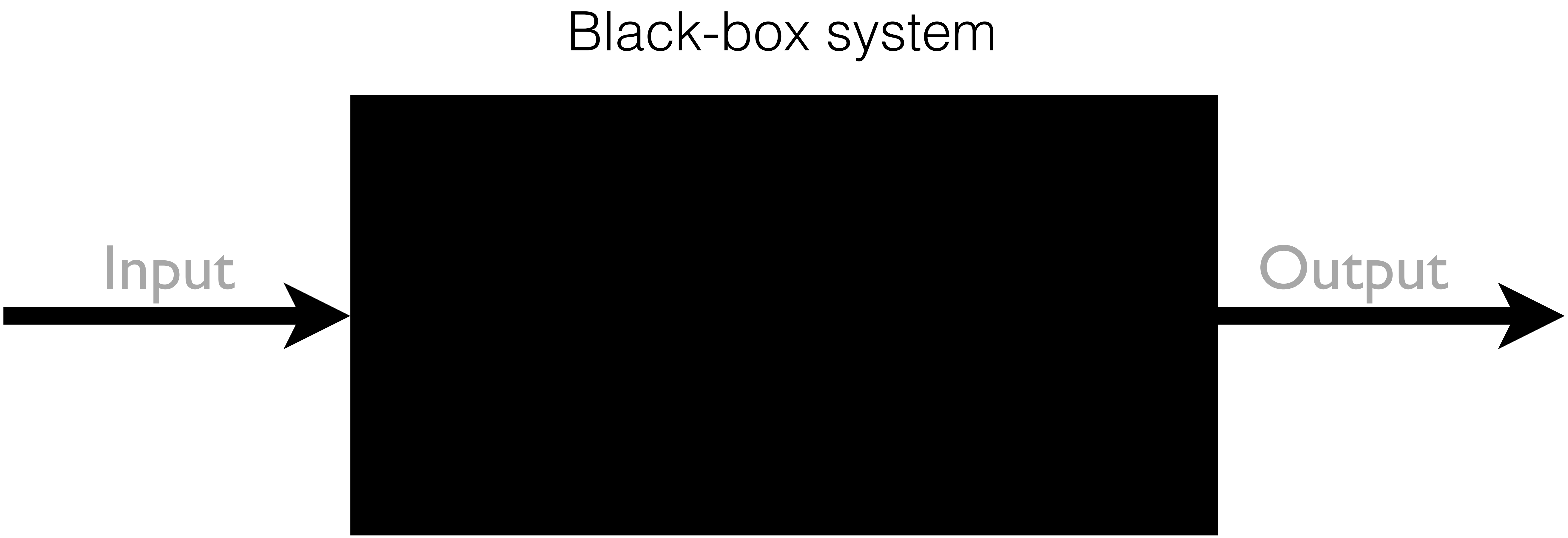
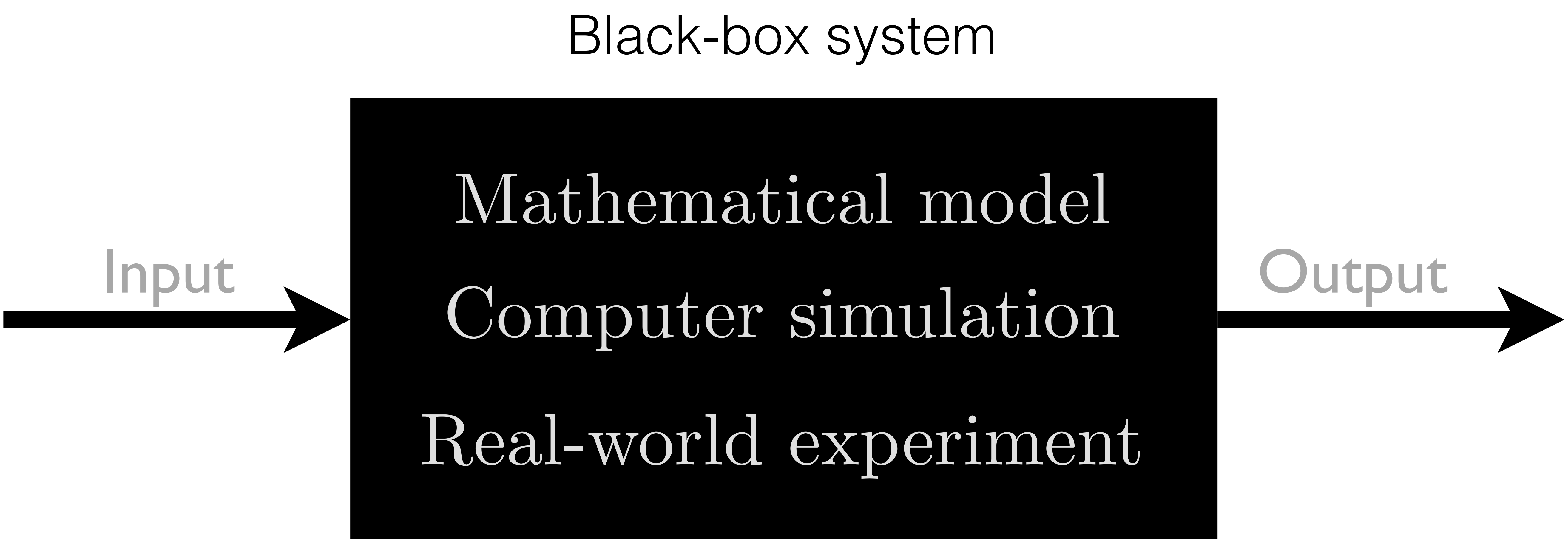


OPTIMIZING A BLACK-BOX



BLACK-BOX OPTIMIZATION

Input

$\mathbf{x} \in \mathbb{R}^n$

Black-box system

Output

$f(\mathbf{x}) \in \mathbb{R}$

BLACK-BOX OPTIMIZATION

Input

$\mathbf{x} \in \mathbb{R}^n$

Black-box system

Output

$f(\mathbf{x}) \in \mathbb{R}$

x_1

x_2

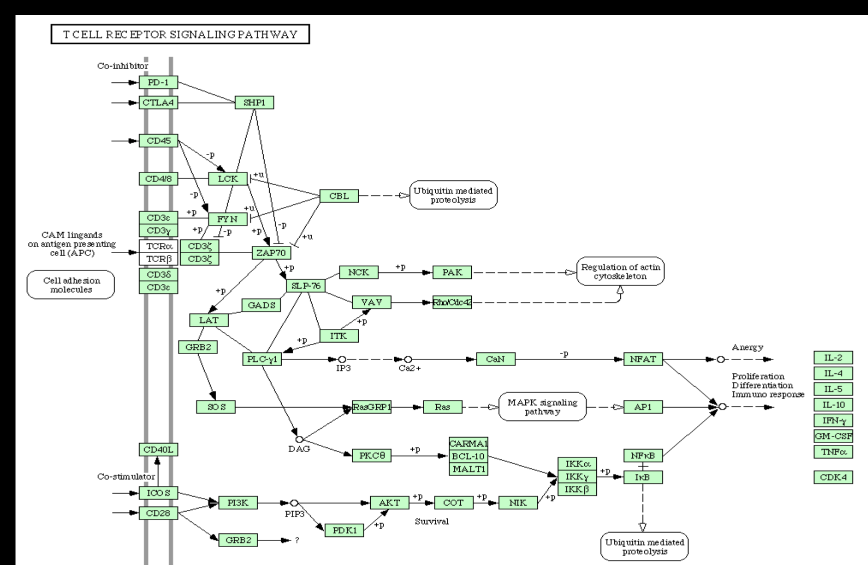
...

x_i

...

x_n

Systems biology models



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Center for Computational Mathematics

Input

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Black-box system

Output

$f(\mathbf{x}) \in \mathbb{R}$

x_1

x_2

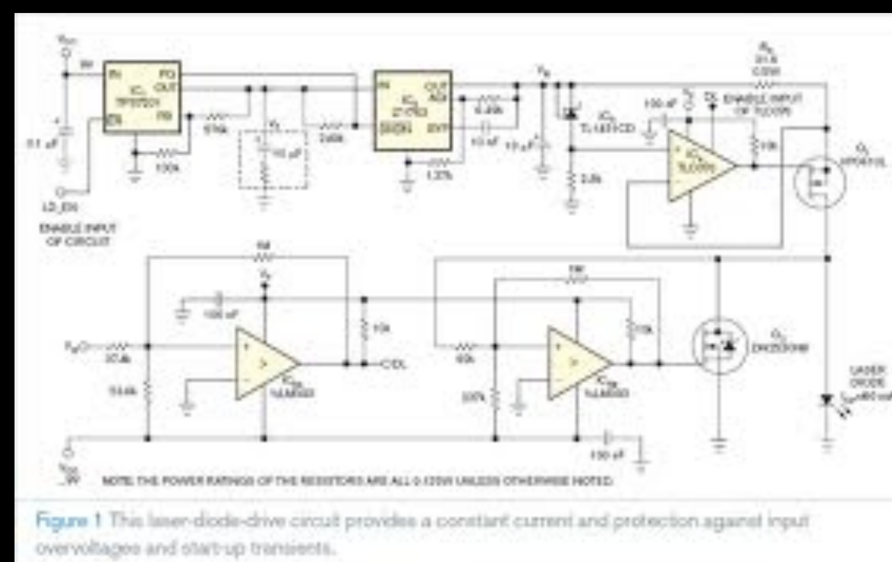
...

x_i

...

x_n

Analog circuit design



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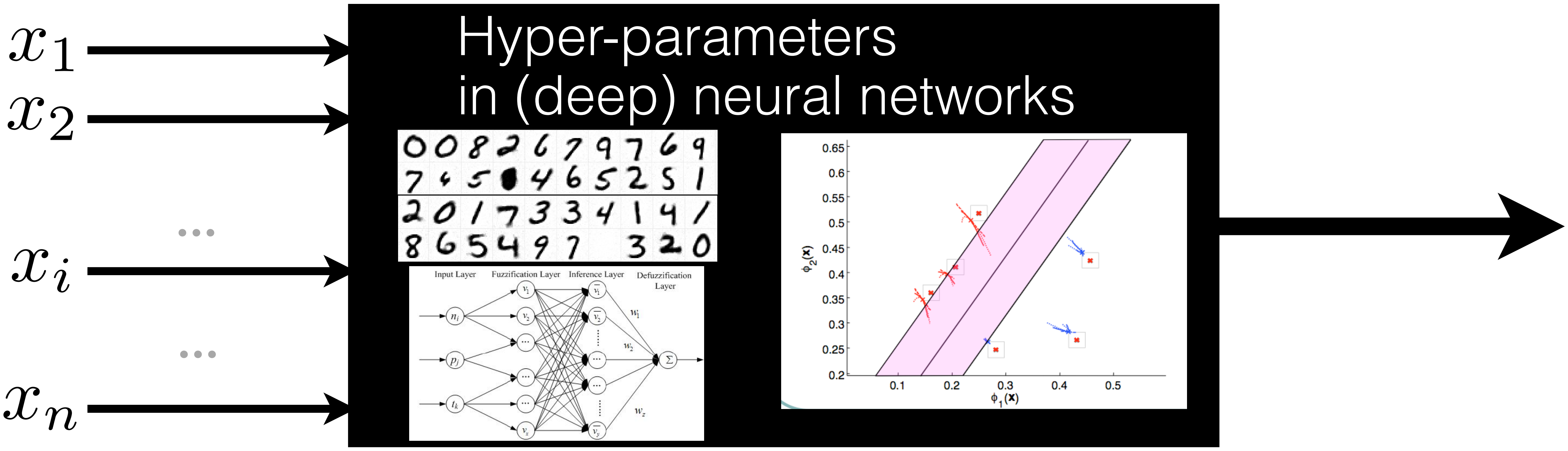

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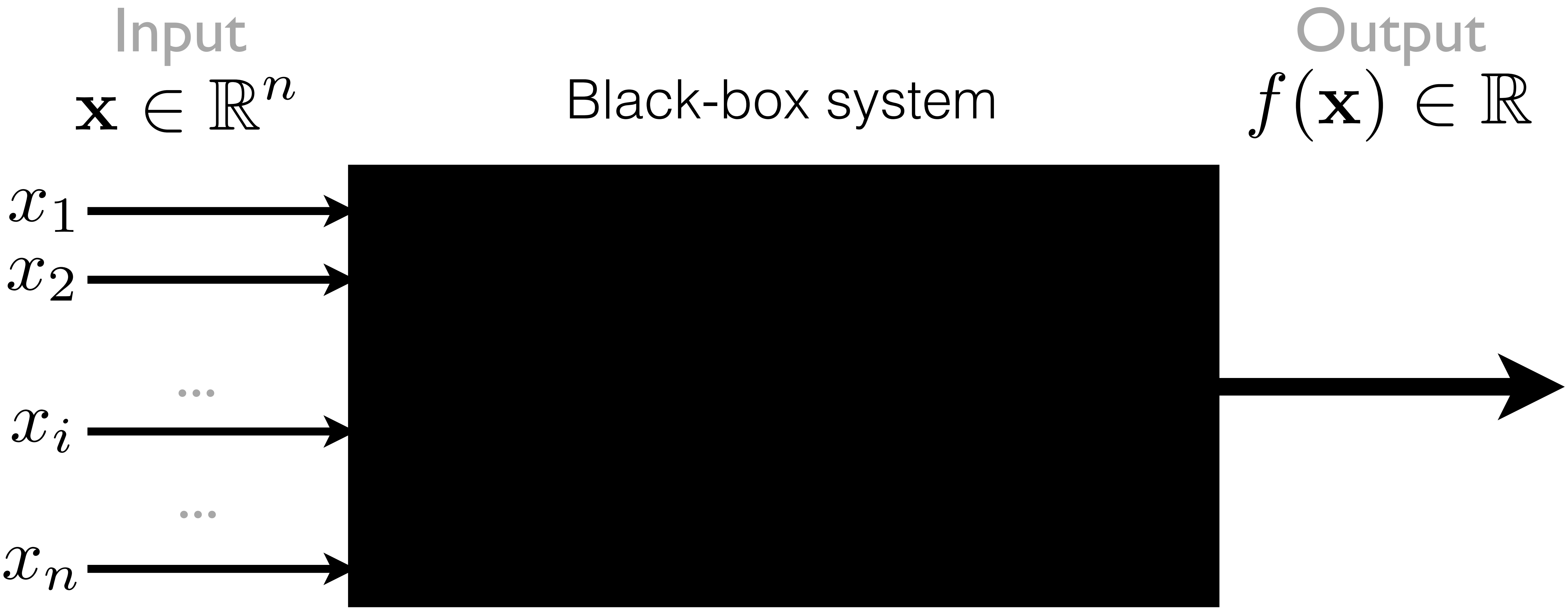

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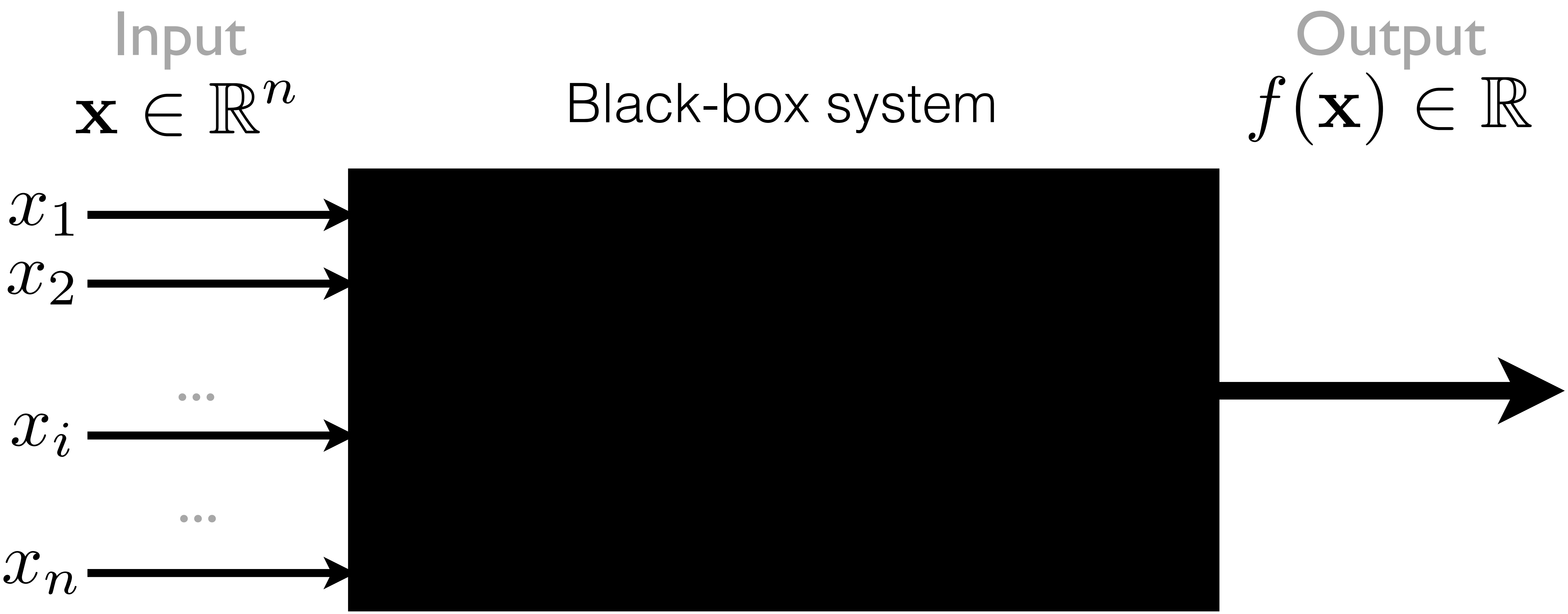


- Variables
- Parameters
- Configuration
- Factors

BLACK-BOX OPTIMIZATION

Input

$\mathbf{x} \in \mathbb{R}^n$

Black-box system

Output

$f(\mathbf{x}) \in \mathbb{R}$

- Variables
- Parameters
- Configuration
- Factors

- Cost
- Criterion
- Objective
- Energy
- Fitness

BLACK-BOX OPTIMIZATION

FLATIRON INSTITUTE
Center for Computational Mathematics

Input

$\mathbf{x} \in \mathbb{R}^n$

Black-box system

Output

$f(\mathbf{x}) \in \mathbb{R}$

- Variables
- Parameters
- Configuration
- Factors

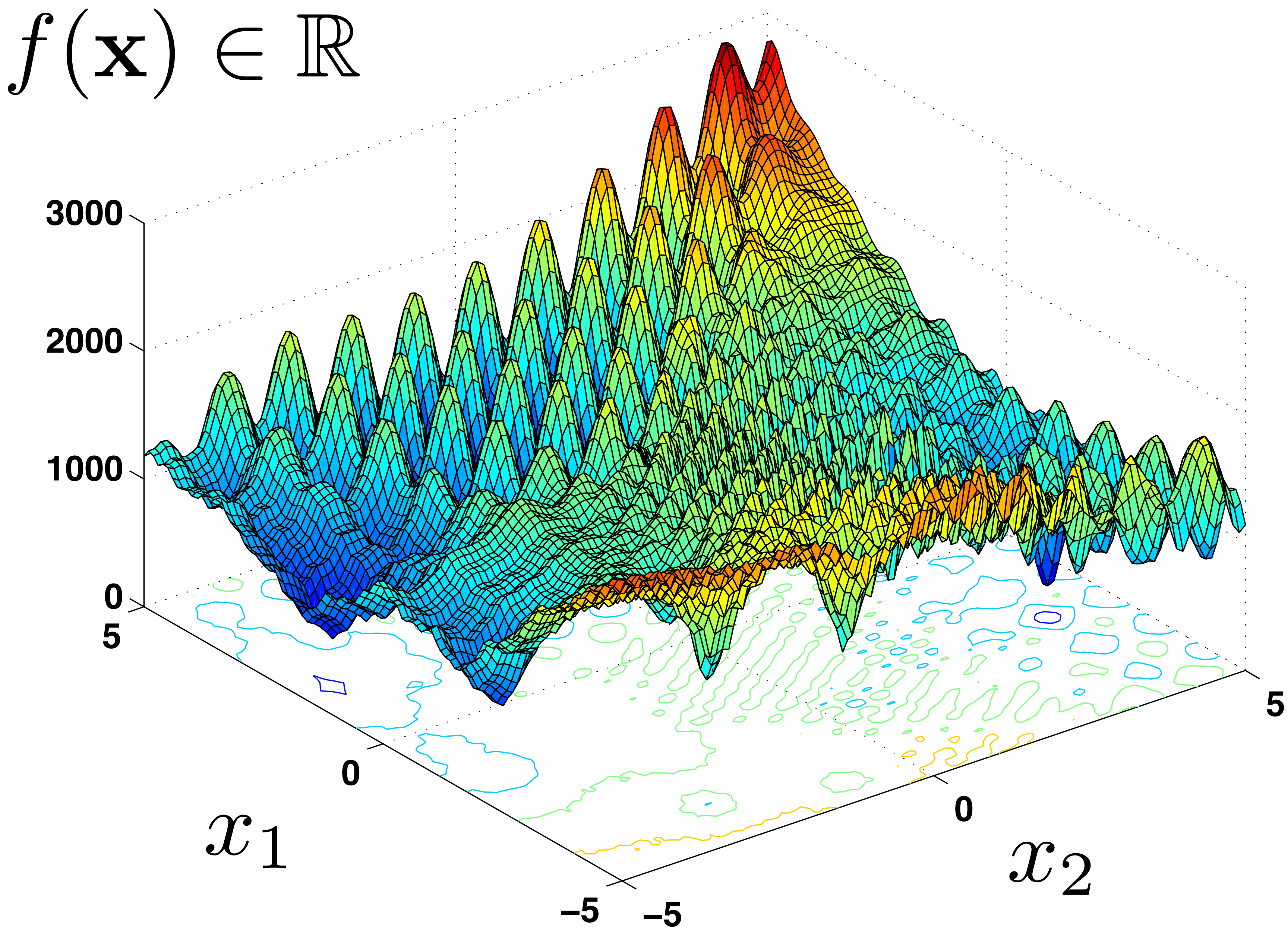
Find x* such that f(x*)≤f(x) ∀x

- Cost
- Criterion
- Objective
- Energy
- Fitness

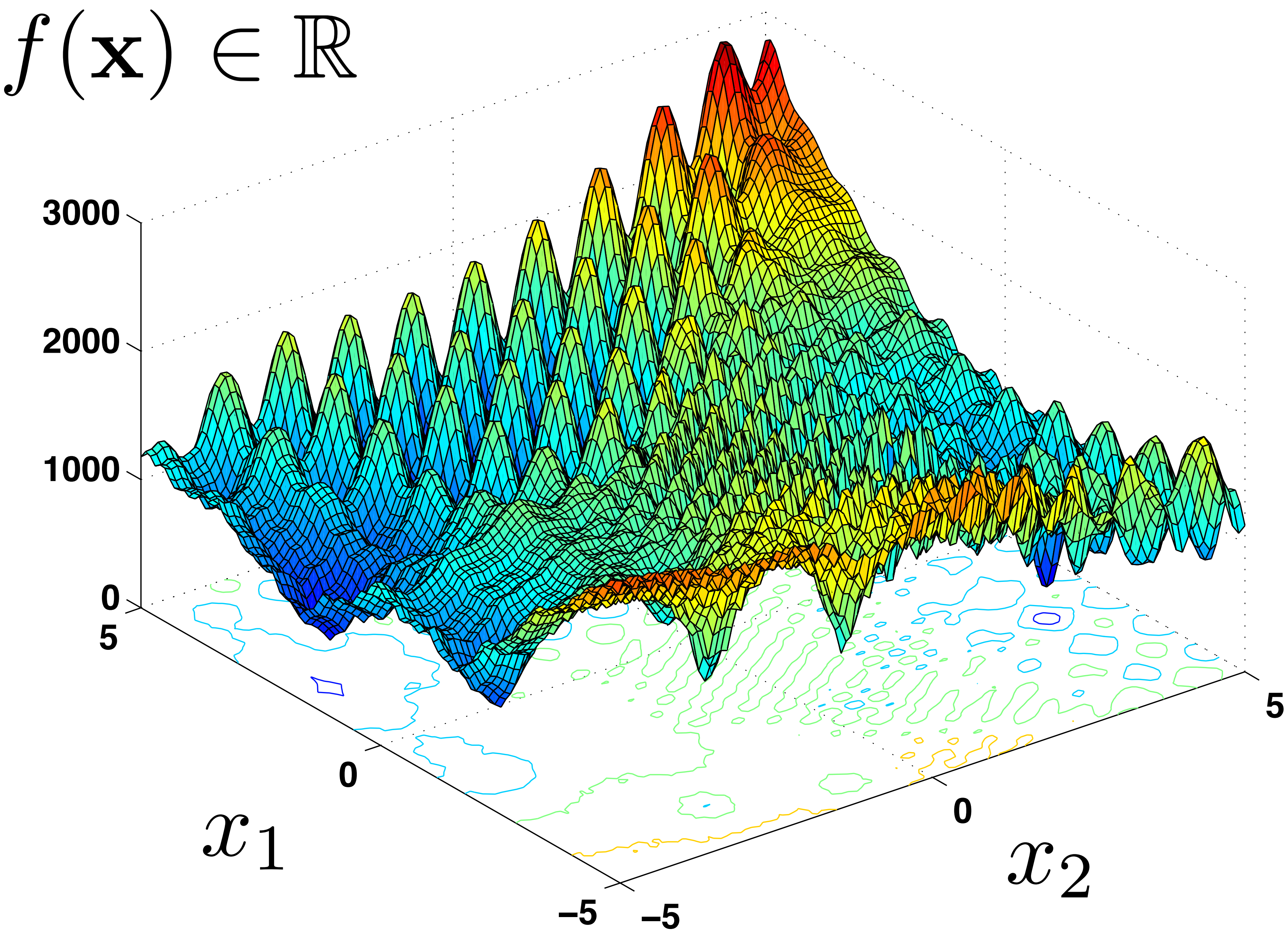
OPTIMIZATION LANDSCAPES

OPTIMIZATION LANDSCAPES

FLATIRON INSTITUTE
Center for Computational Mathematics



BLACK-BOX LANDSCAPES $\mathcal{L}_{\mathrm{B}}$



BLACK-BOX LANDSCAPES $\mathcal{L}_{\mathrm{B}}$

FLATIRON INSTITUTE
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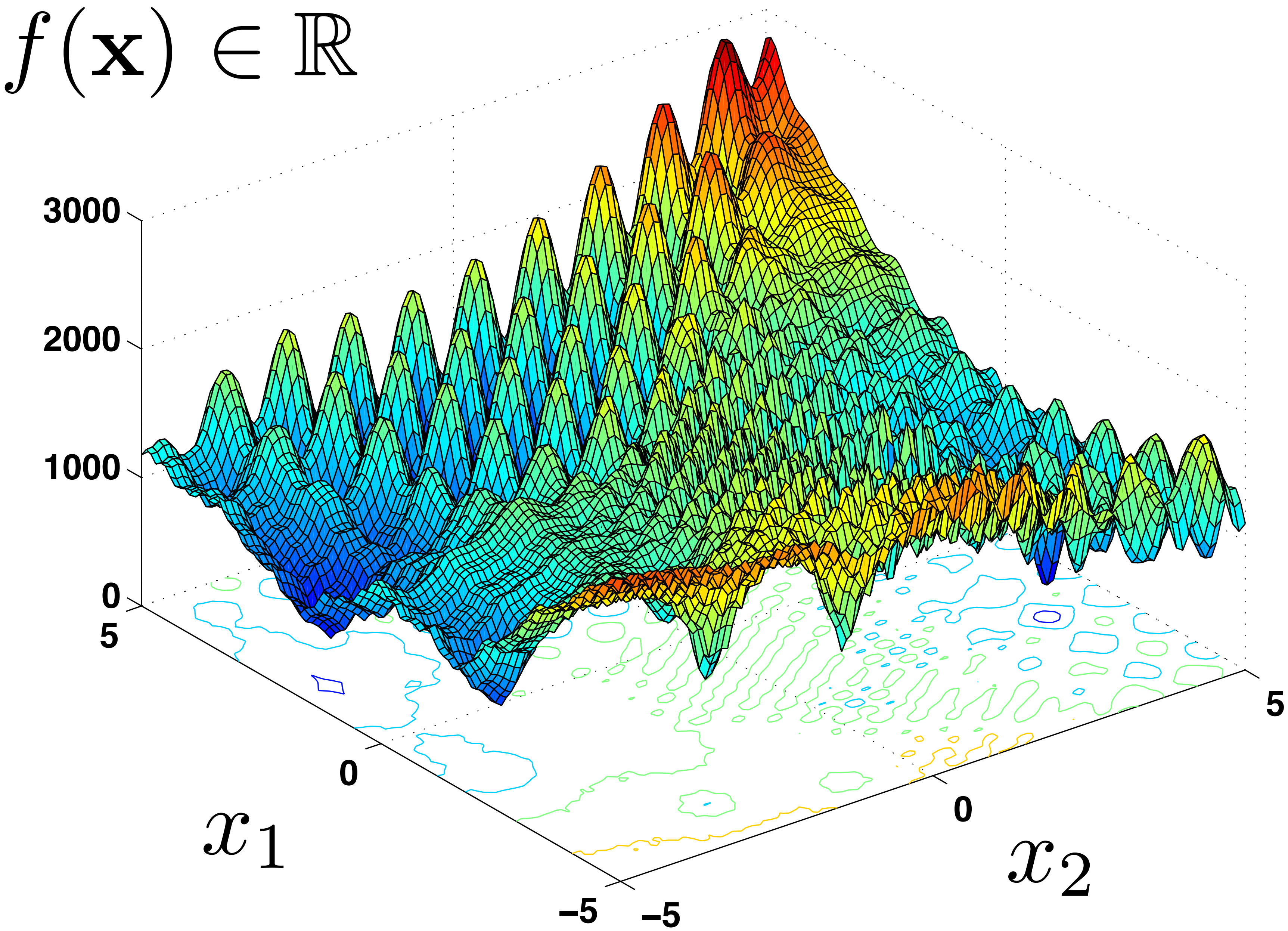
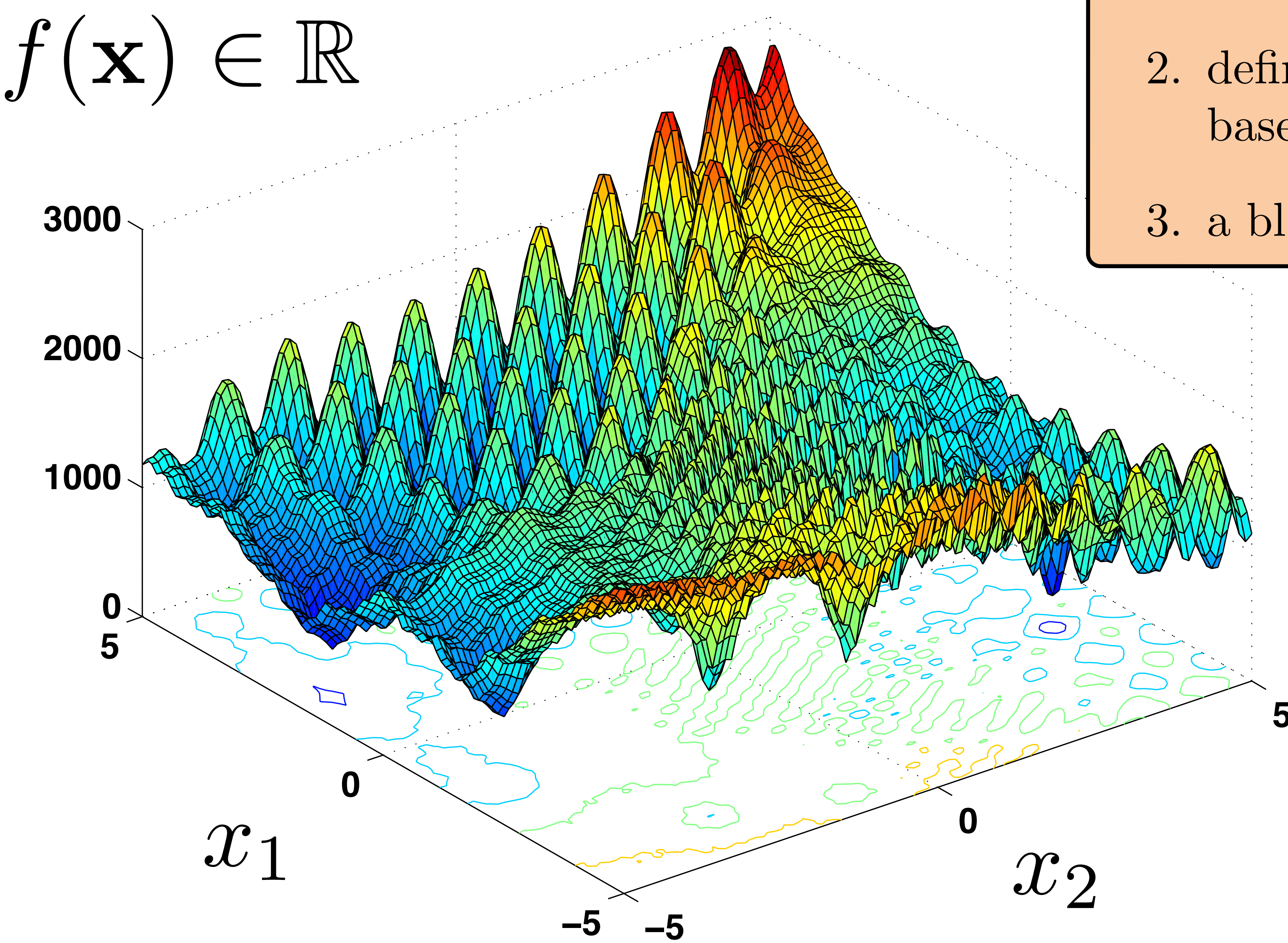


BLACK-BOX LANDSCAPES $\mathcal{L}_{\mathrm{B}}$

$\mathcal{L}_{\mathrm{B}}$ is the triple $(\mathcal{X}, d_{\mathrm{X}}, f)$ consisting of

1. $\mathcal{X} = [\mathbf{l}, \mathbf{u}] \subset \mathbb{R}^n$ with $\mathbf{l}, \mathbf{u} \in \mathbb{R}^n$.
2. definition of neighborhood/similarity based on a distance d_{X}.
3. a black-box function f.



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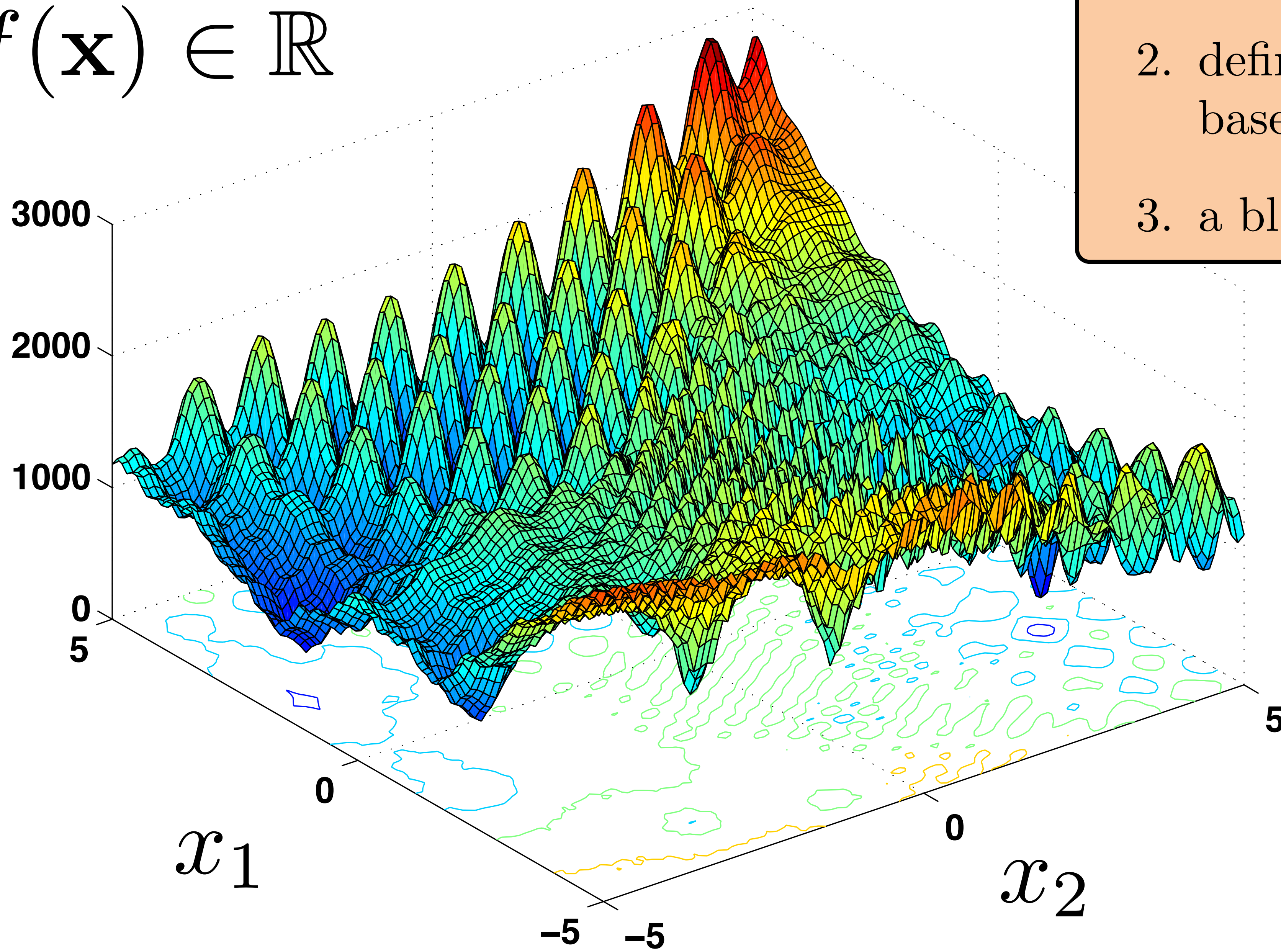
$f(\mathbf{x}) \in \mathbb{R}$



Topographic description:

- Peaks and valleys
- Plateaus and basins
- Ridges and funnels

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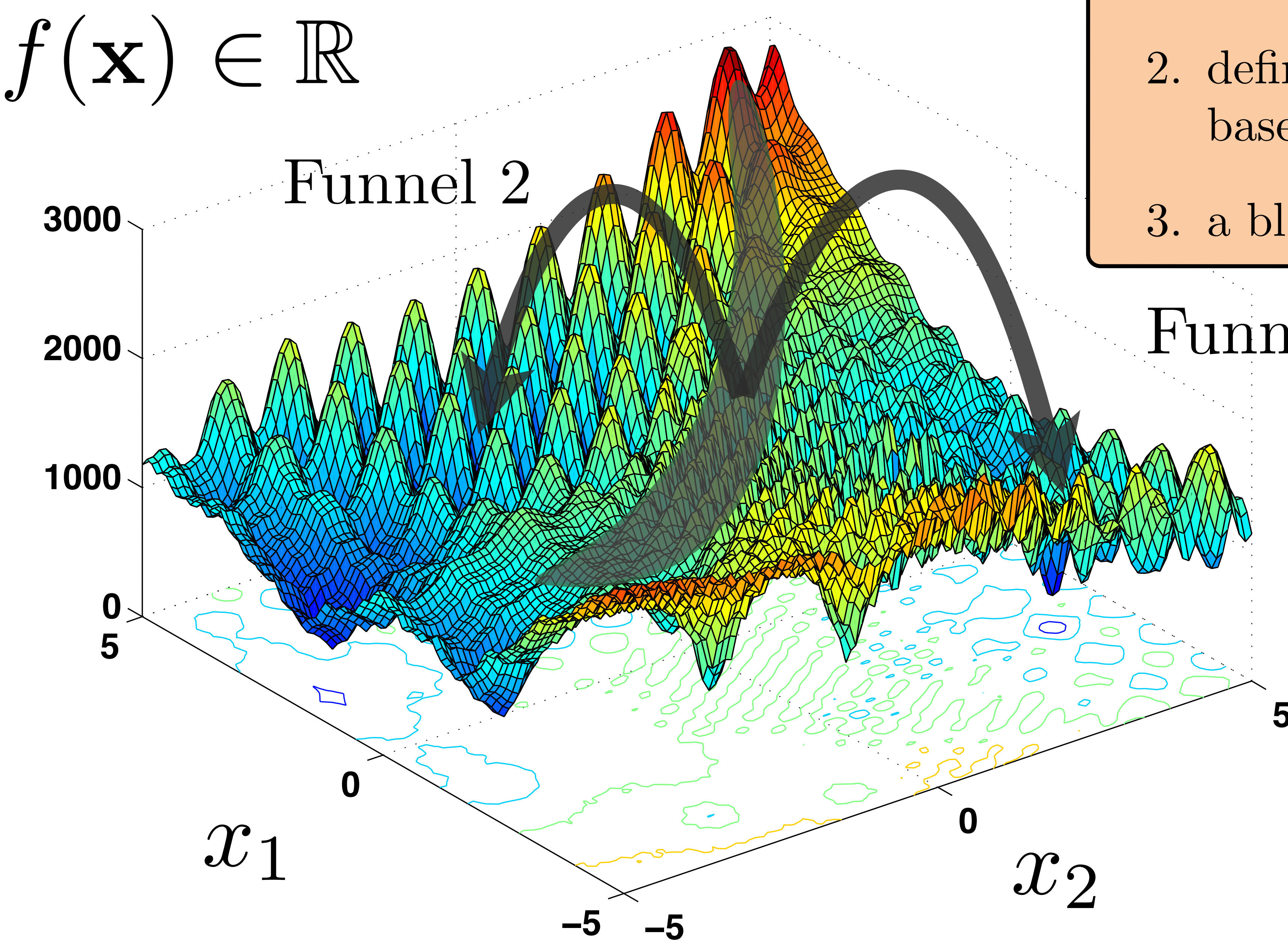

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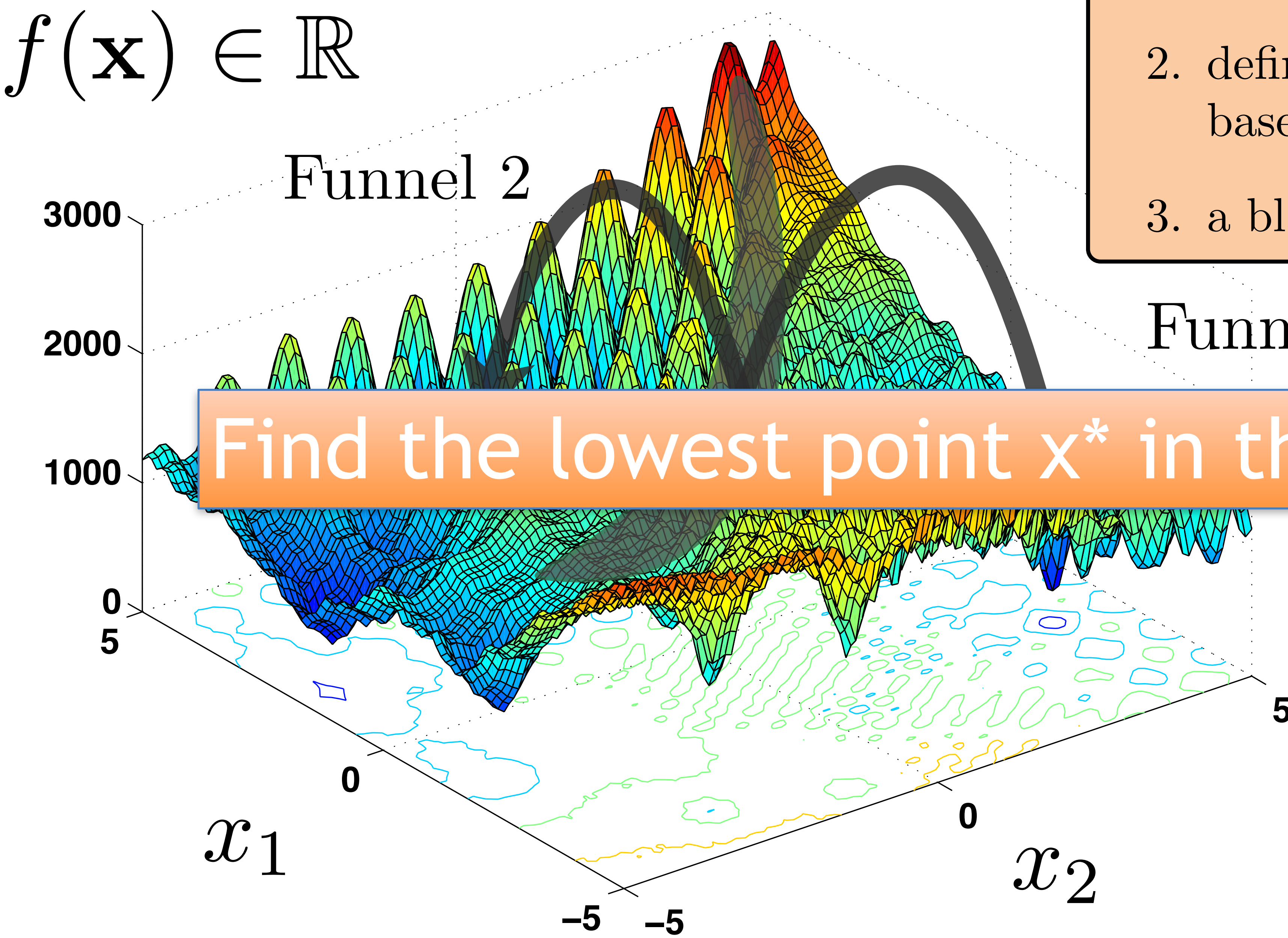
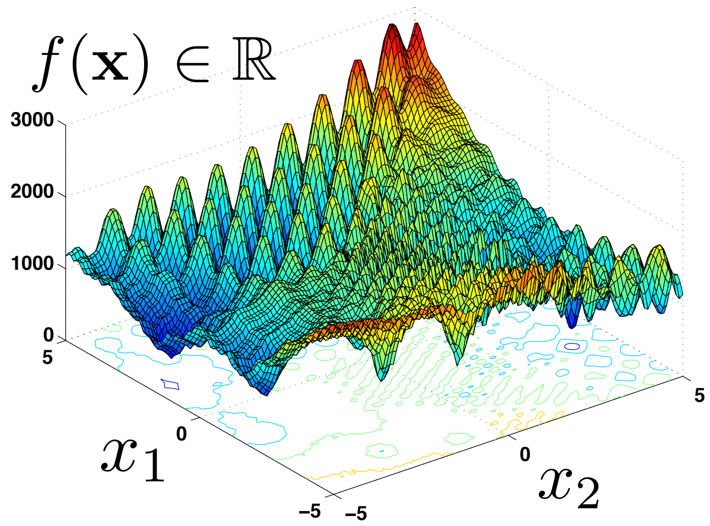


Find the lowest point x* in the landscape!

Topographic description:

- Peaks and valleys
- Plateaus and basins
- Ridges and funnels

LANDSCAPES IN SCIENCE



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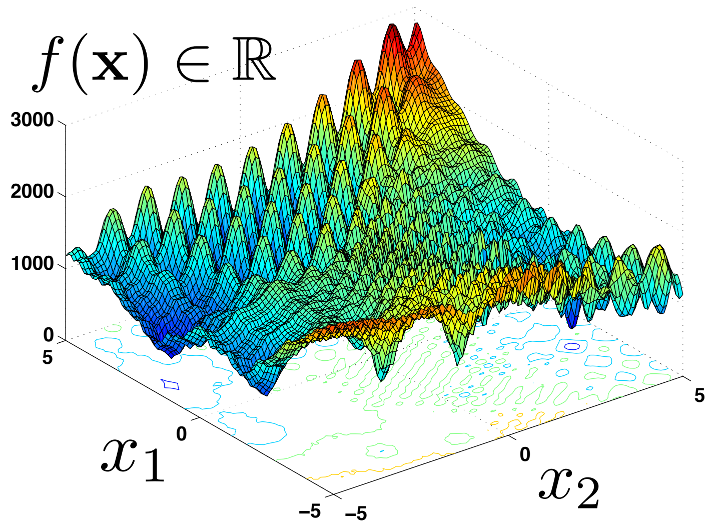
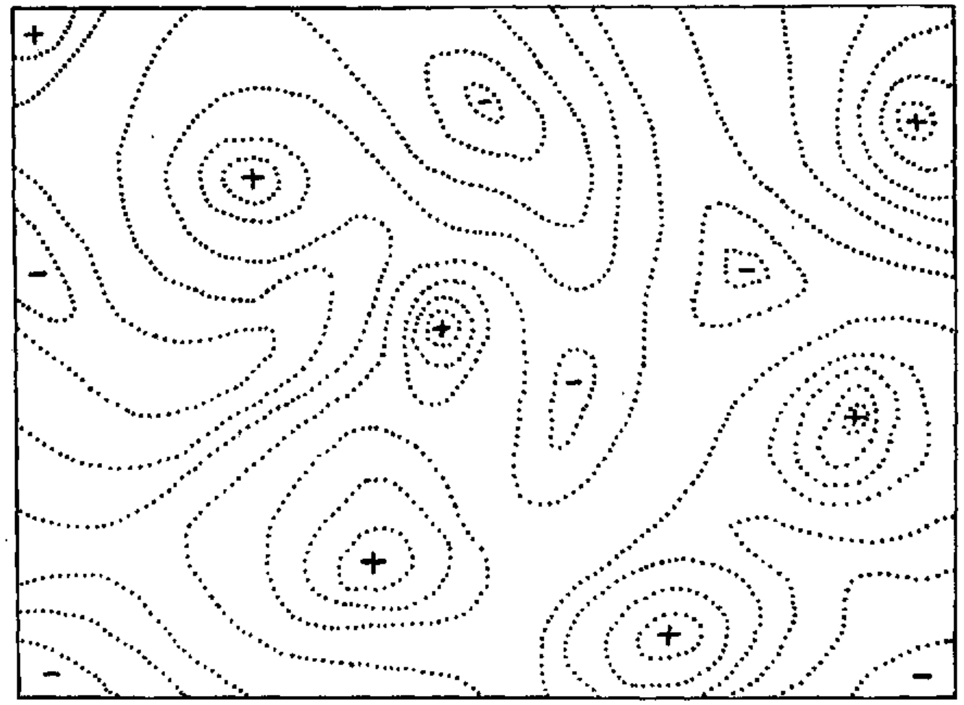
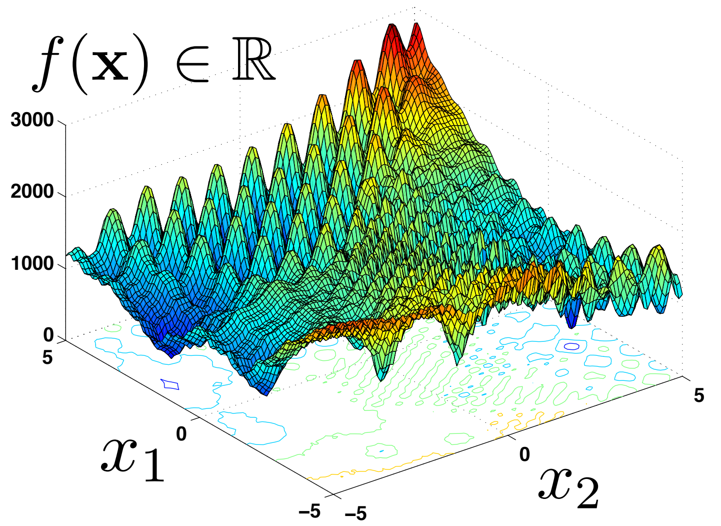
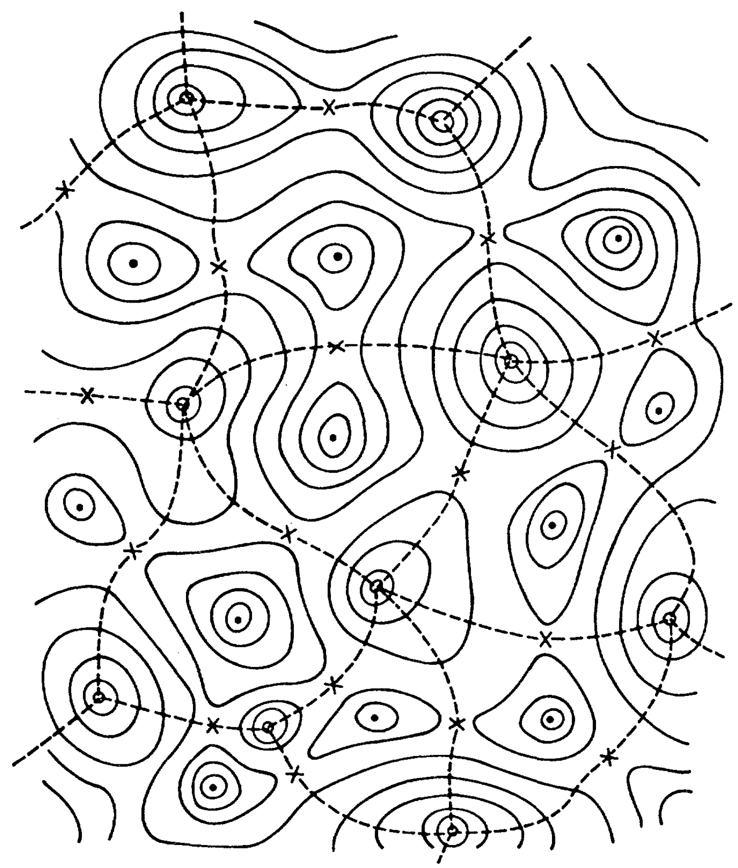




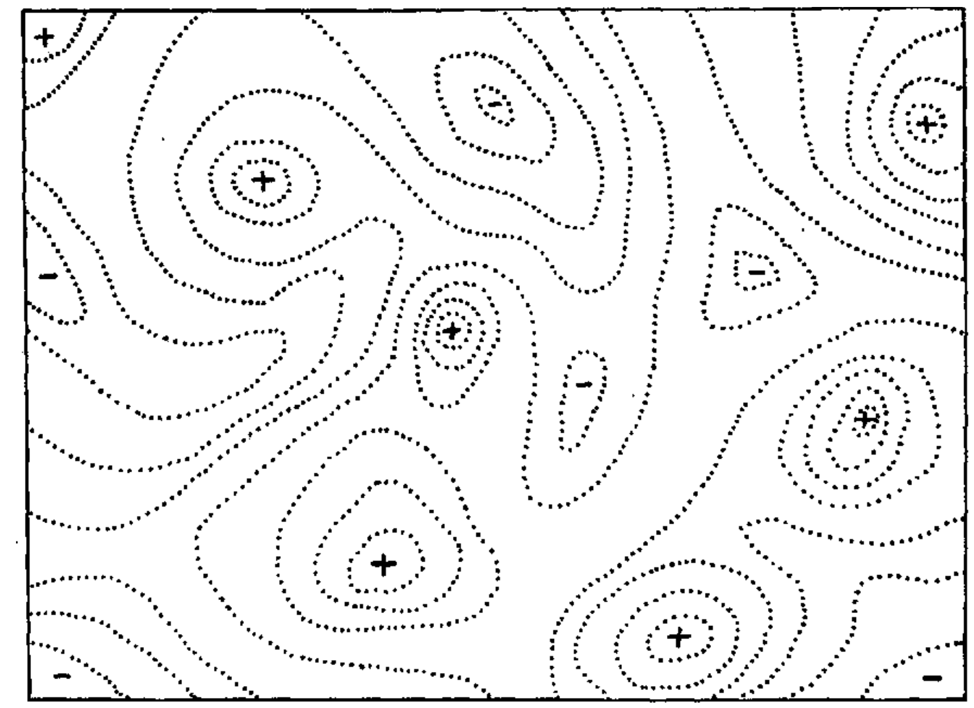
Fitness landscape

LANDSCAPES IN SCIENCE





Potential energy landscape



Fitness landscape

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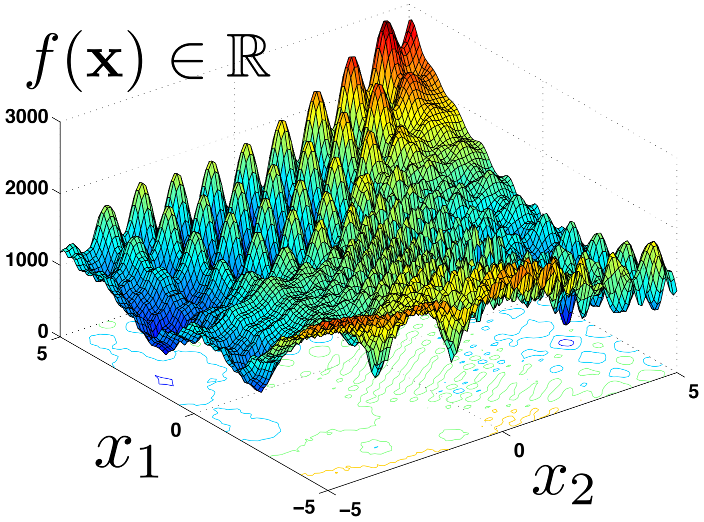
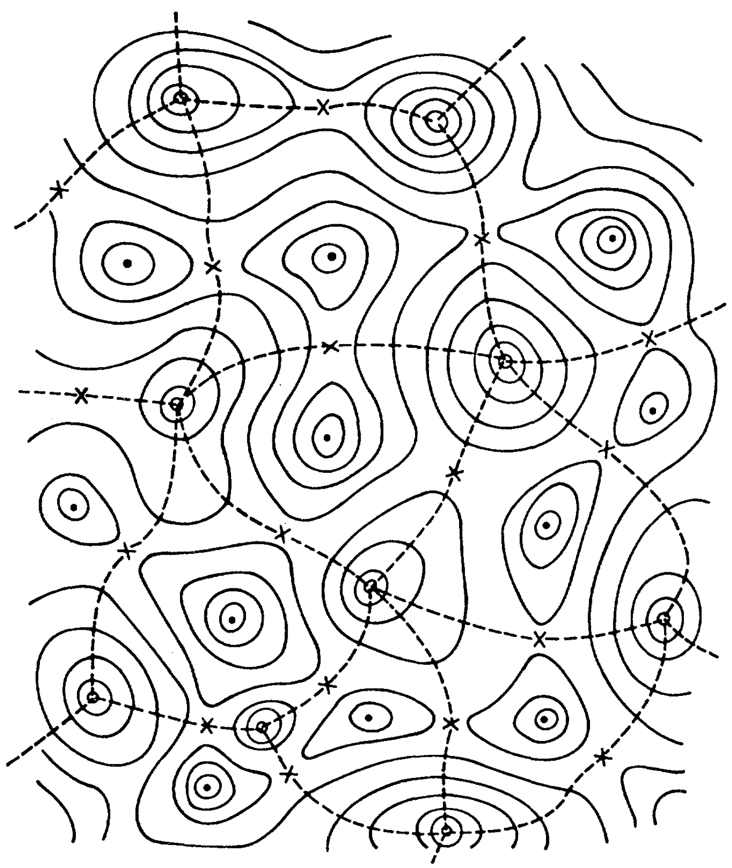
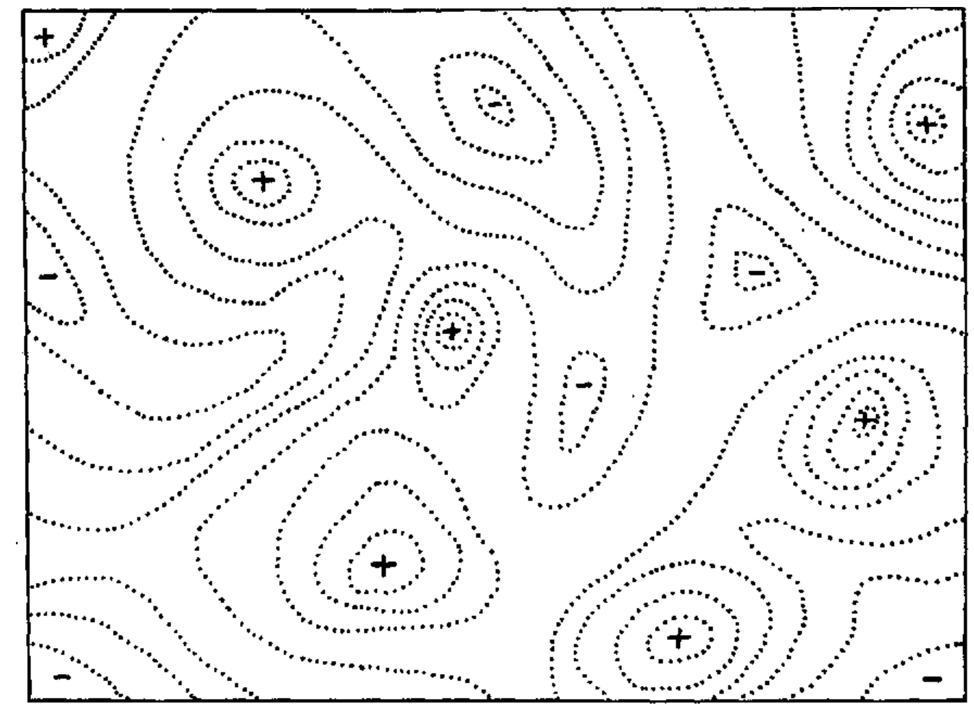




Potential energy landscape



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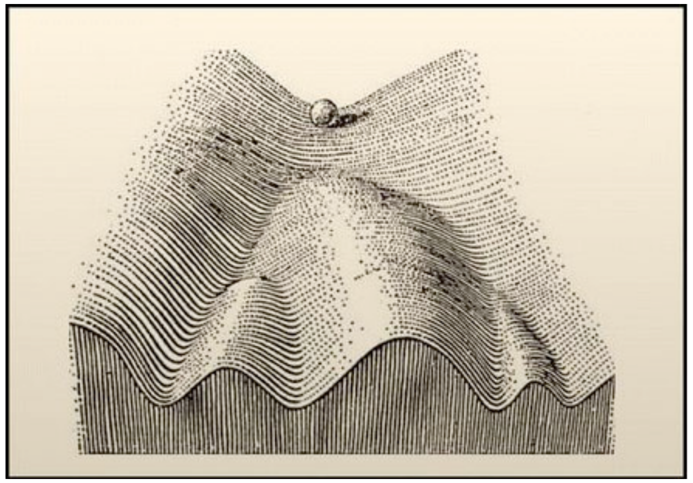
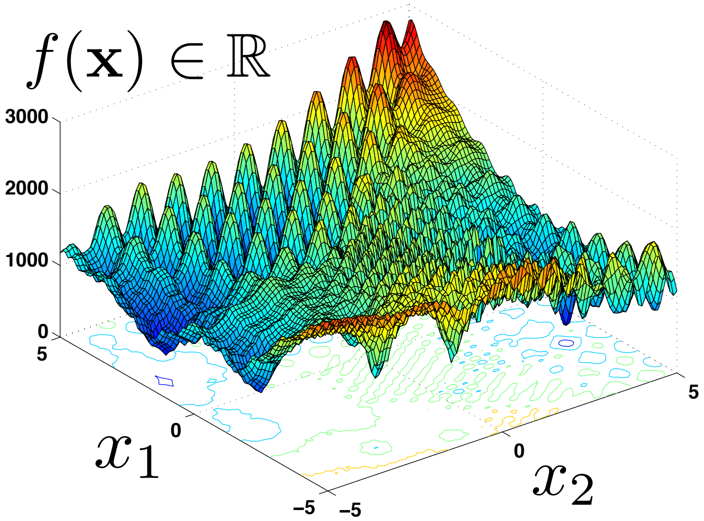
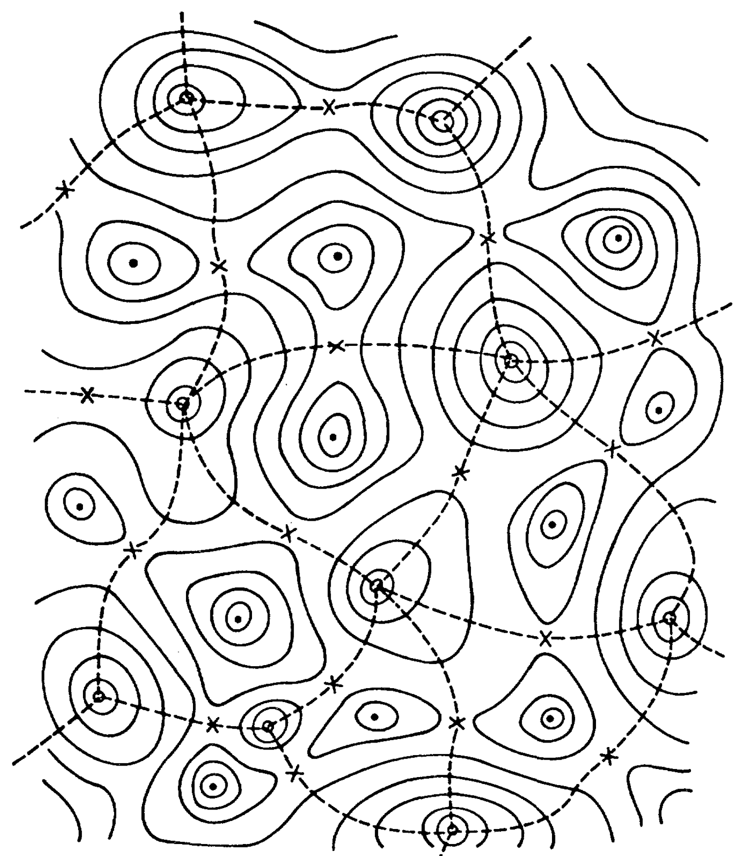


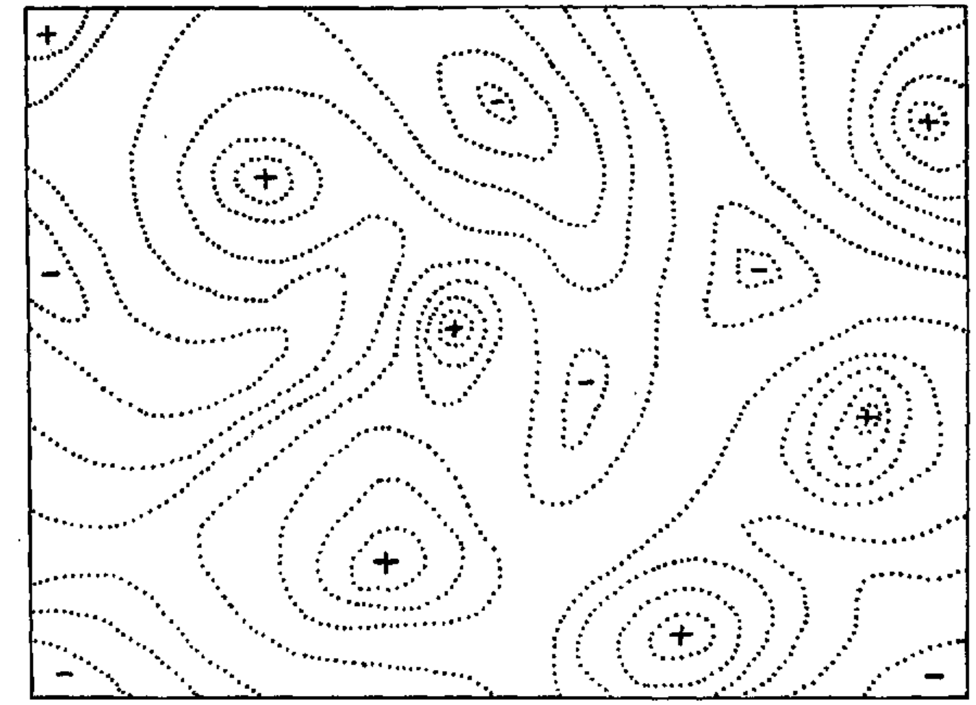
Epigenetic landscape

LANDSCAPES IN SCIENCE

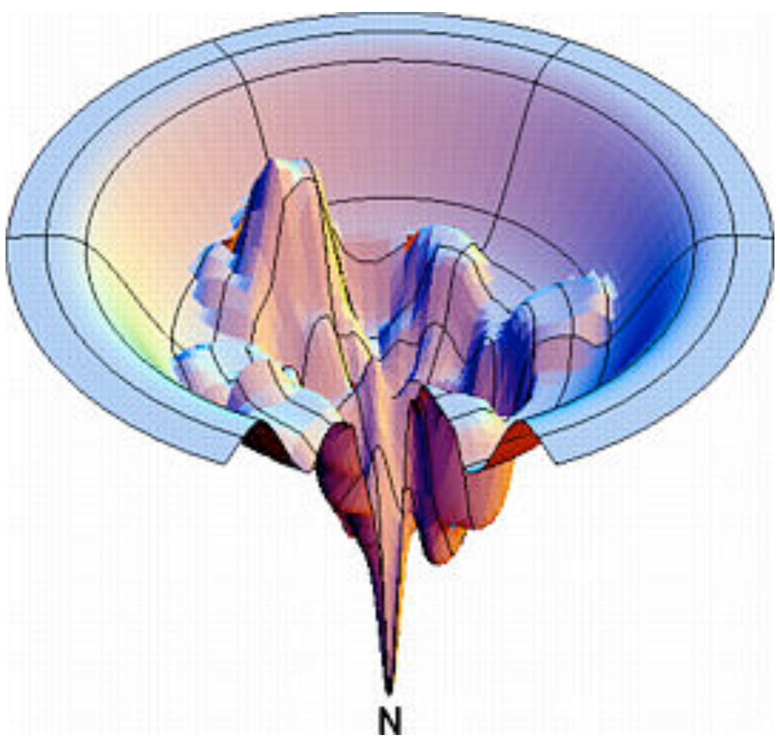




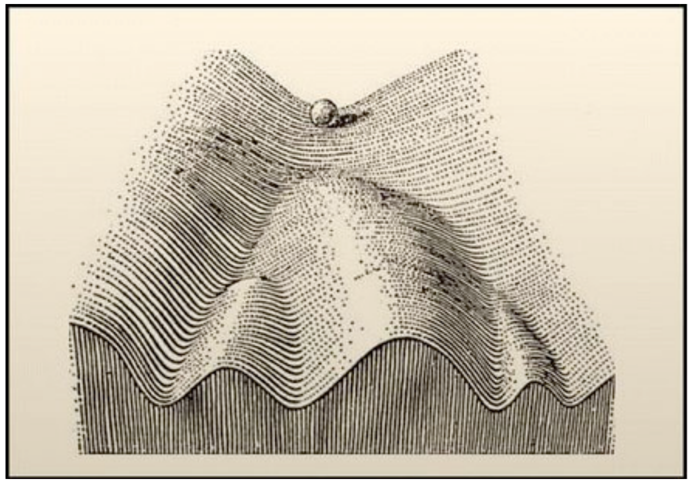
Potential energy landscape



Fitness landscape



Folding funnel



Epigenetic landscape

LANDSCAPES ARE METAPHORS

“The price of metaphor is eternal vigilance."

Norbert Wiener

La condition humaine, René Magritte

FITNESS LANDSCAPES

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Center for Computational Mathematics

Wright, S., “The Roles of Mutation, Inbreeding, Crossbreeding, and Selection in Evolution,”

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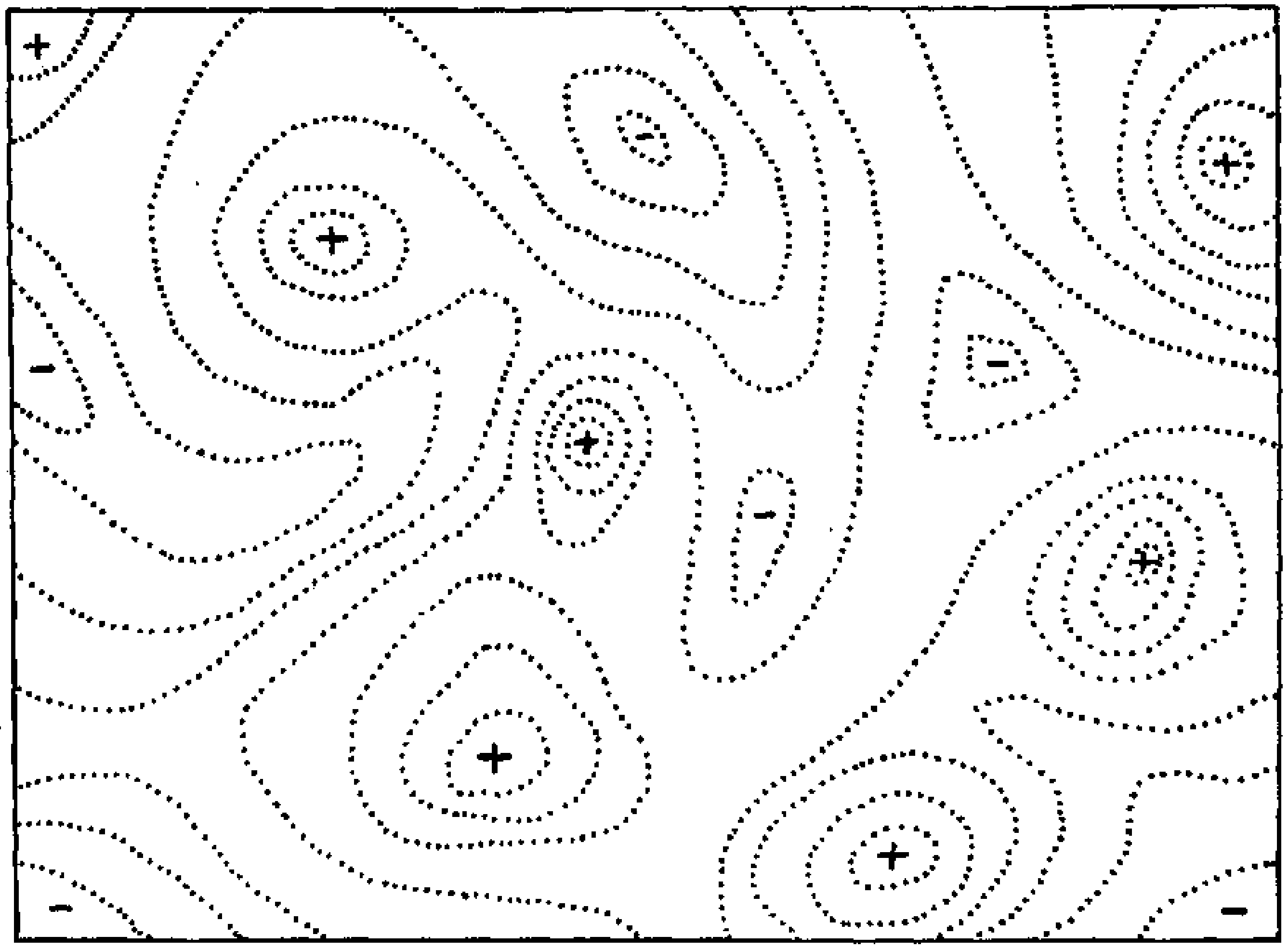

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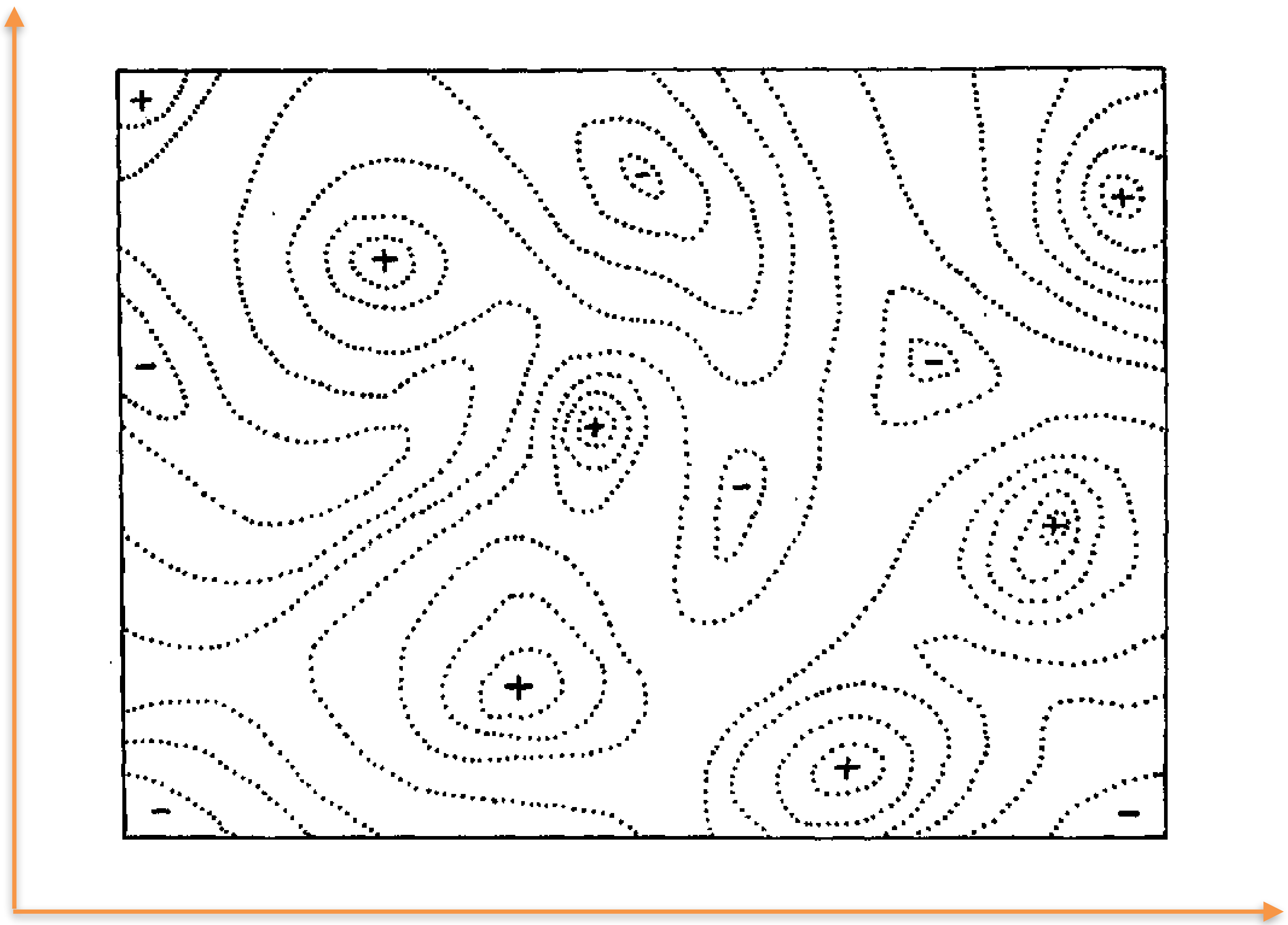
gene 1/
trait 1/…



gene 2/trait 2/…

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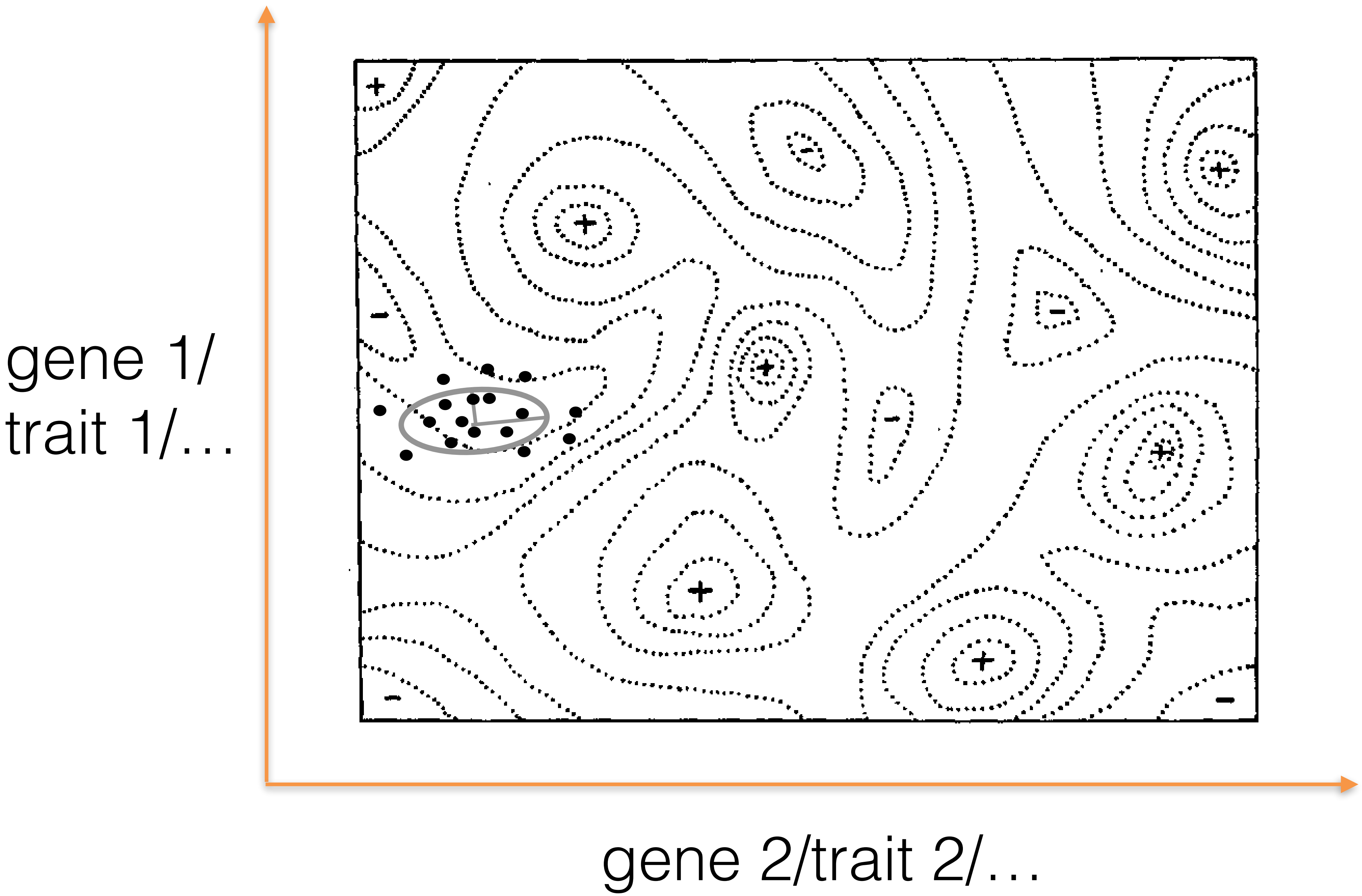

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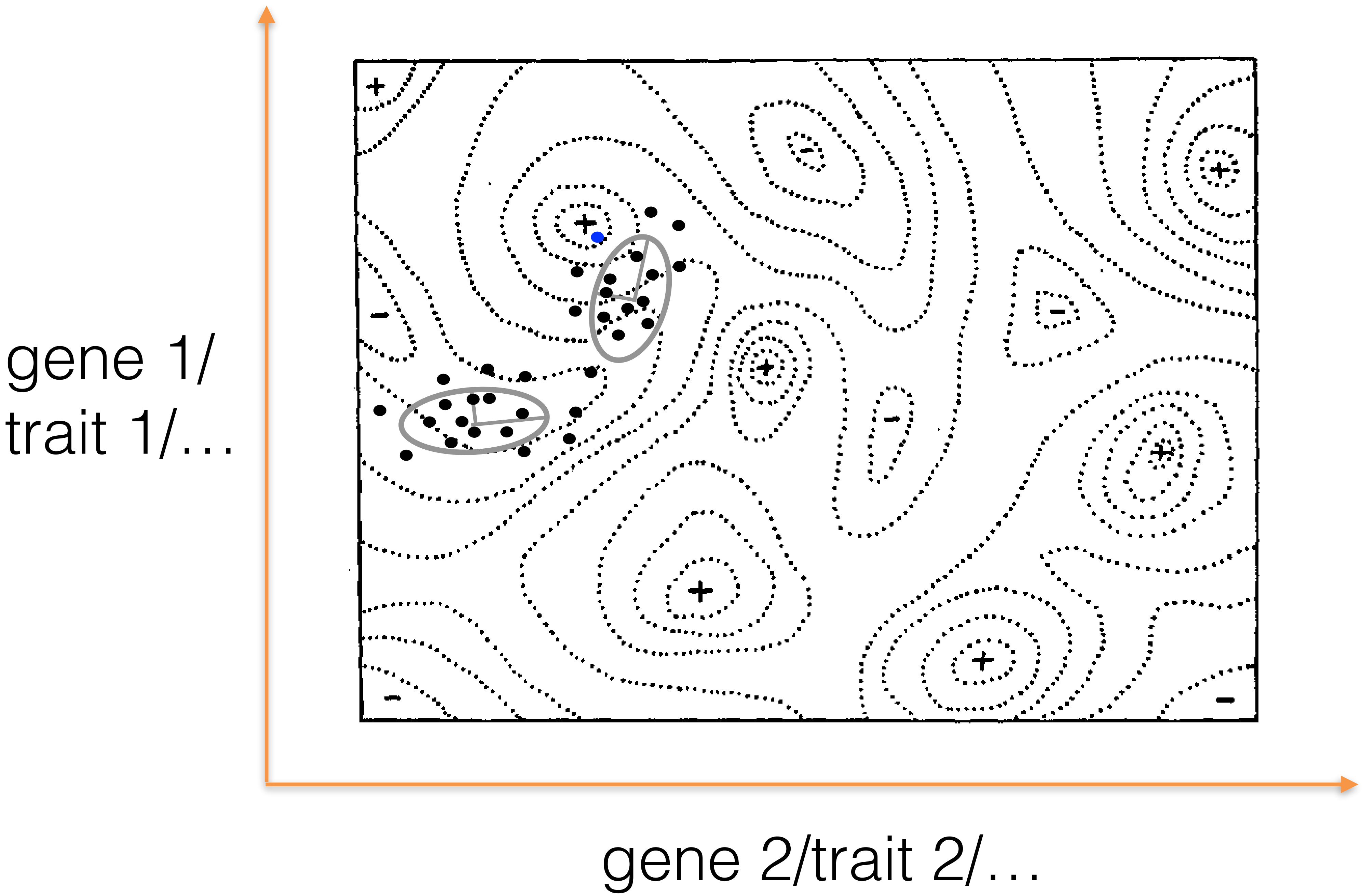
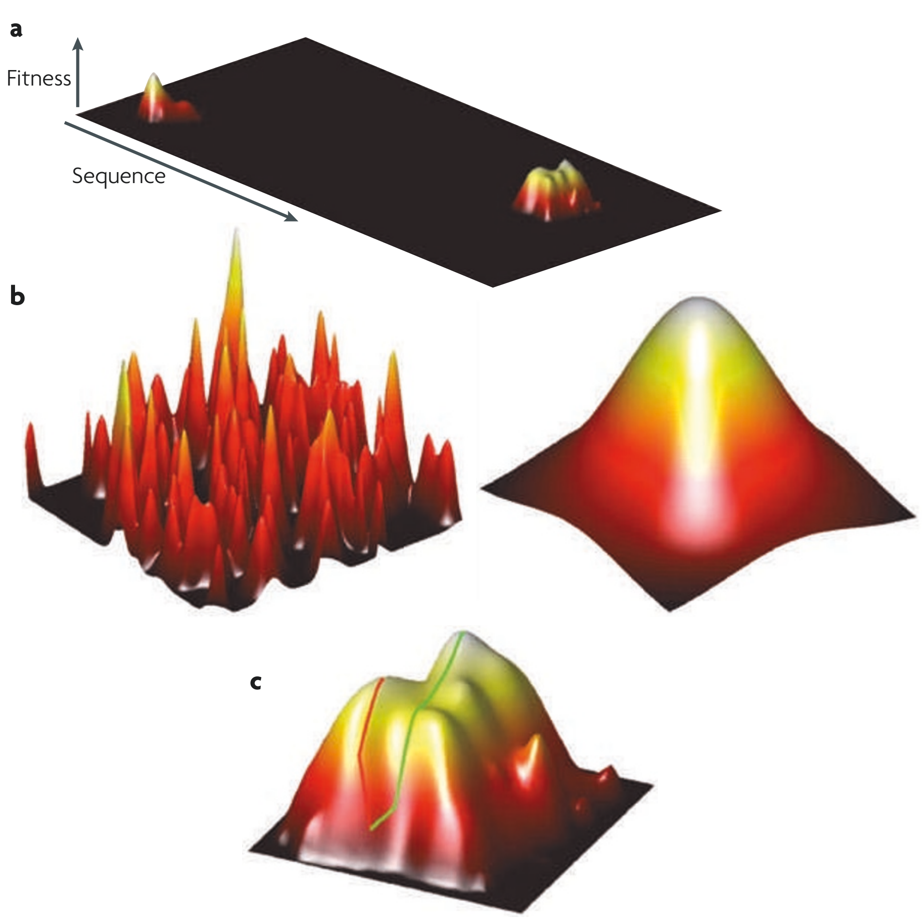


FITNESS LANDSCAPES

Exploring protein fitness landscapes by directed evolution

Philip A. Romero and Frances H. Arnold

Abstract | Directed evolution circumvents our profound ignorance of how a protein's sequence encodes its function by using iterative rounds of random mutation and artificial selection to discover new and useful proteins. Proteins can be tuned to adapt to new functions or environments by simple adaptive walks involving small numbers of mutations. Directed evolution studies have shown how rapidly some proteins can evolve under strong selection pressures and, because the entire 'fossil record' of evolutionary intermediates is available for detailed study, they have provided new insight into the relationship between sequence and function. Directed evolution has also shown how mutations that are functionally neutral can set the stage for further adaptation.



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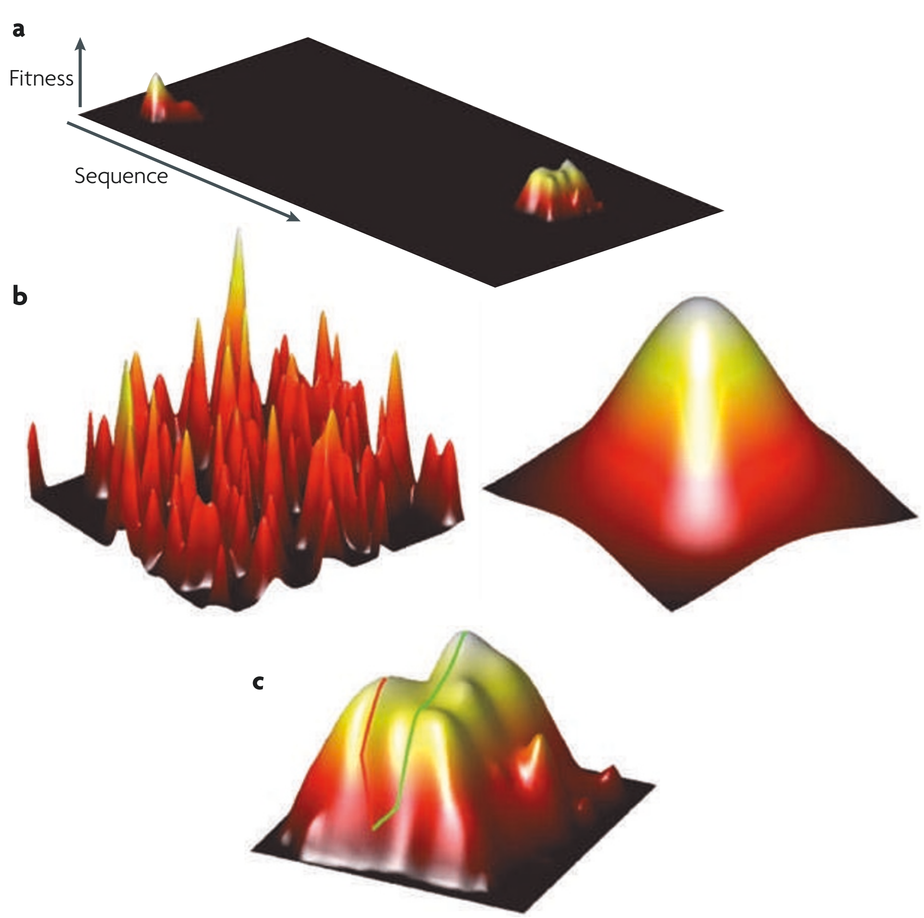
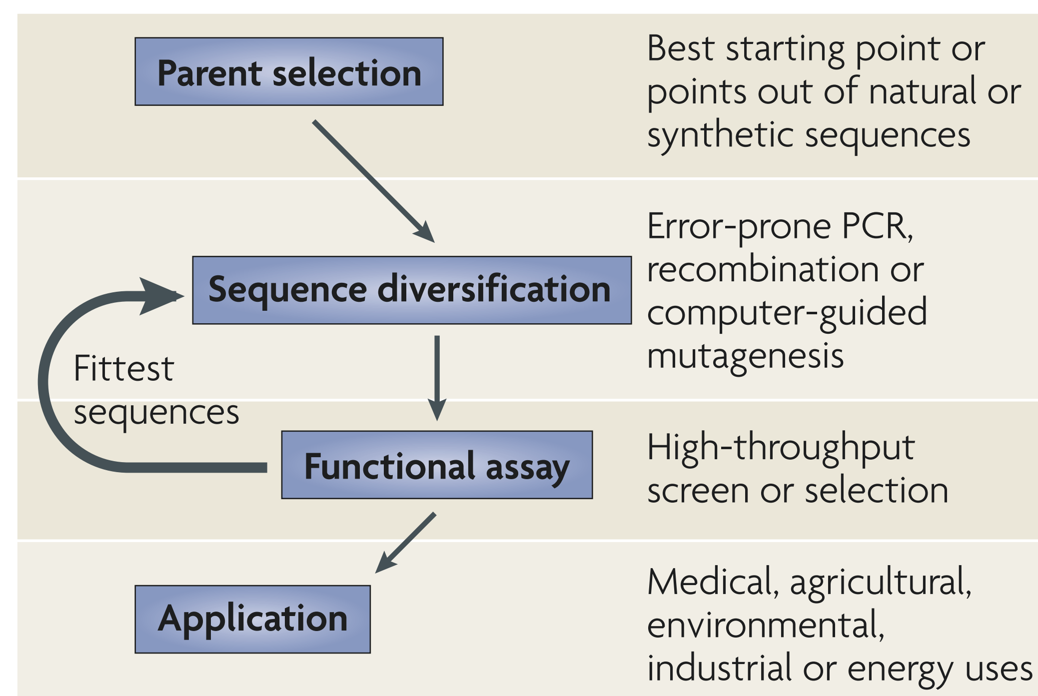




FITNESS LANDSCAPES

FLATIRON INSTITUTE
Center for Computational Mathematics

PNAS PLUS

Navigating the protein fitness landscape with Gaussian processes

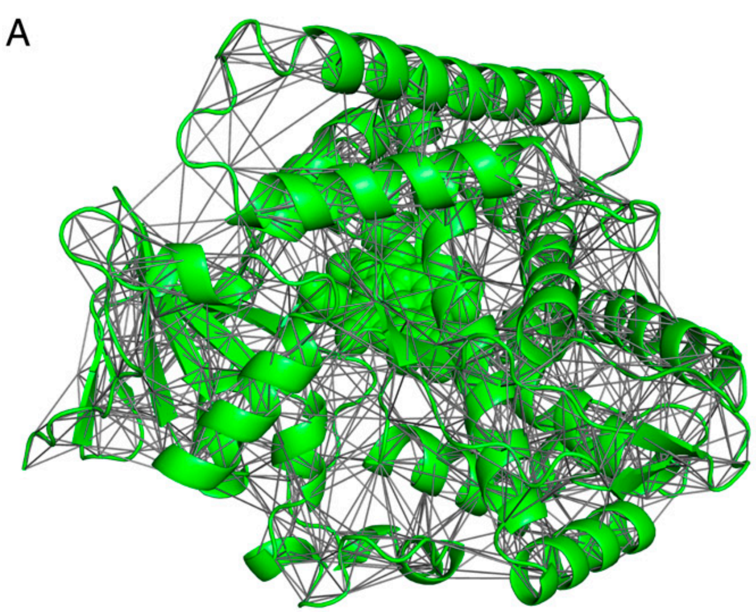
Philip A. Romero[a], Andreas Krause[b], and Frances H. Arnold[a,1]

[a]Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA 91125; and [b]Department of Computer Science, Swiss Federal Institute of Technology, 8092 Zurich, Switzerland

Edited by Michael Levitt, Stanford University School of Medicine, Stanford, CA, and approved November 28, 2012 (received for review September 9, 2012)

Enzyme to be optimized

A



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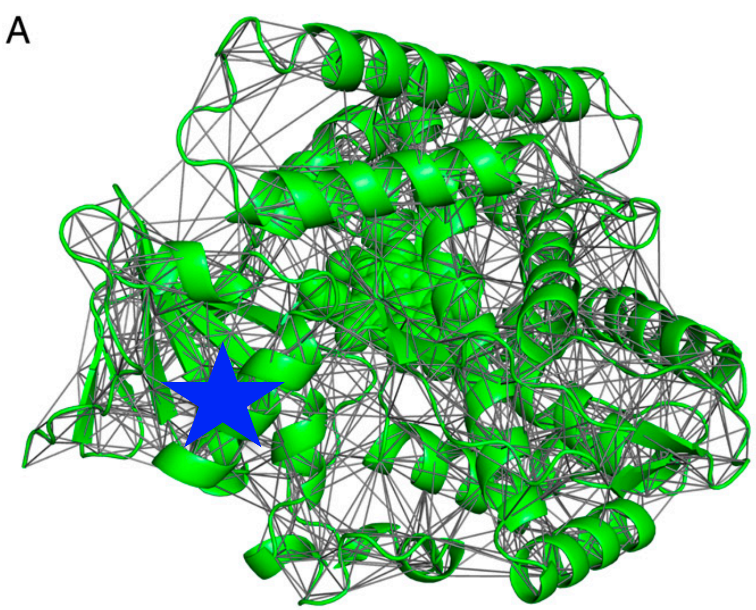

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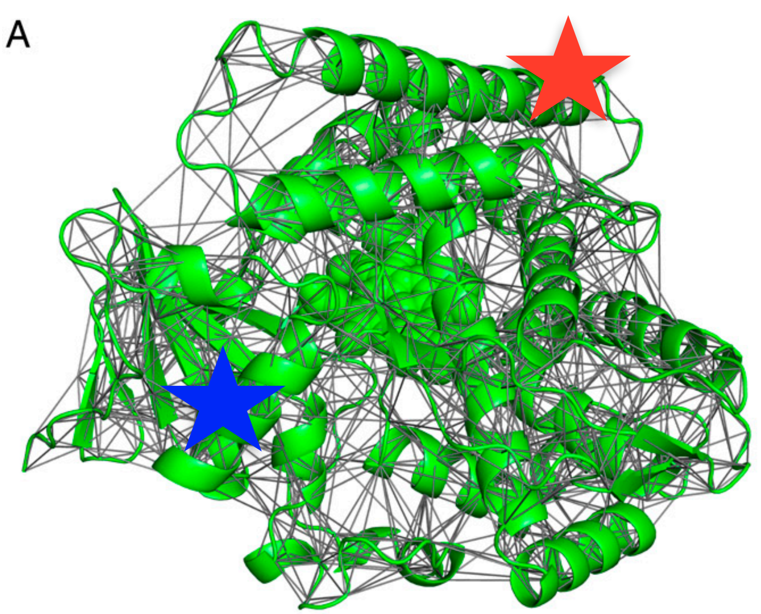

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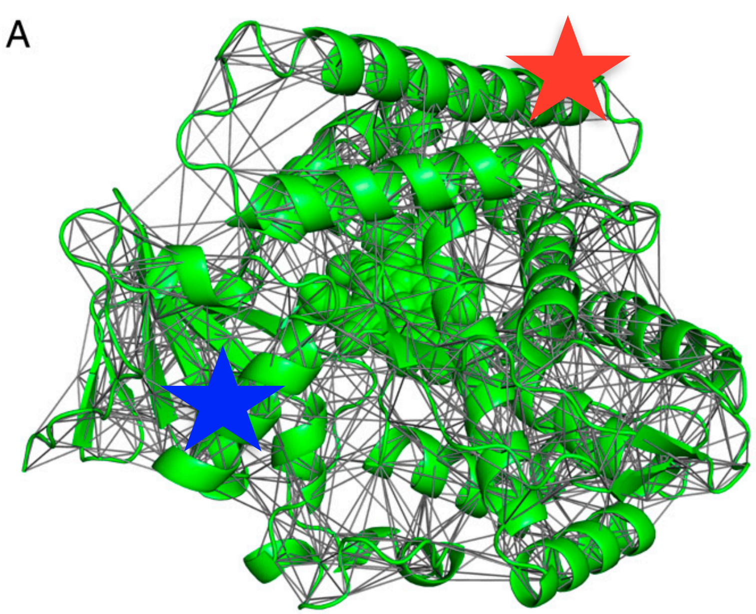
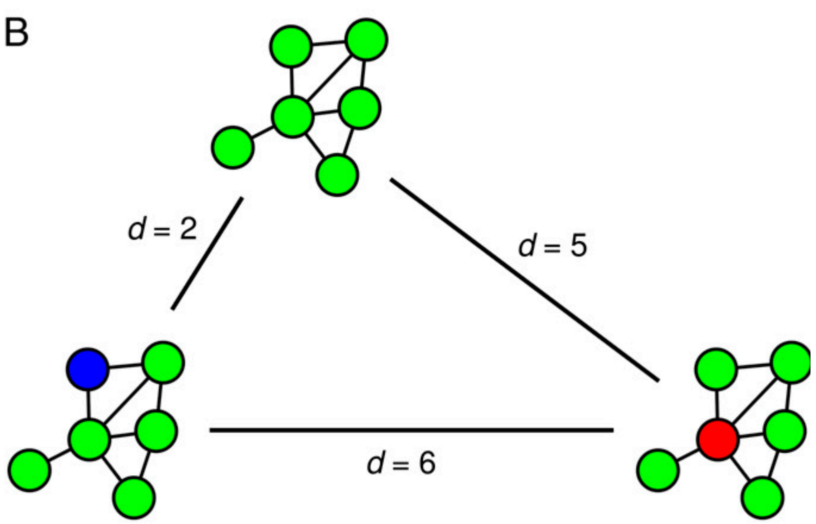


Network representation and distance definition

B



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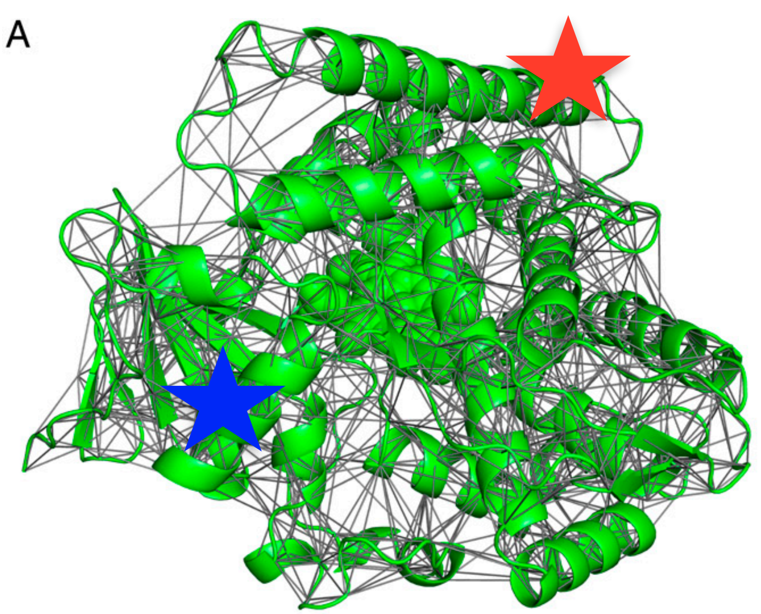

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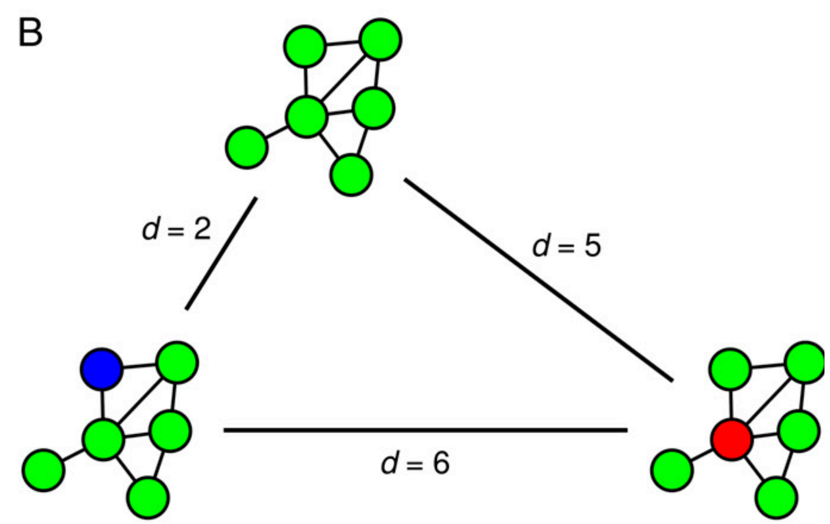
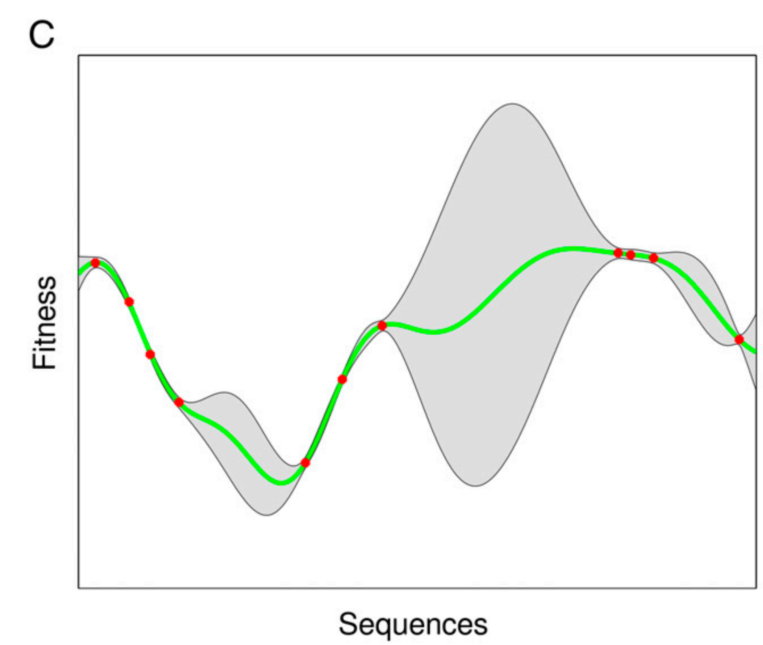


Modeling of measured fitness as GP



FITNESS LANDSCAPES

FLATIRON INSTITUTE
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PNAS PLUS

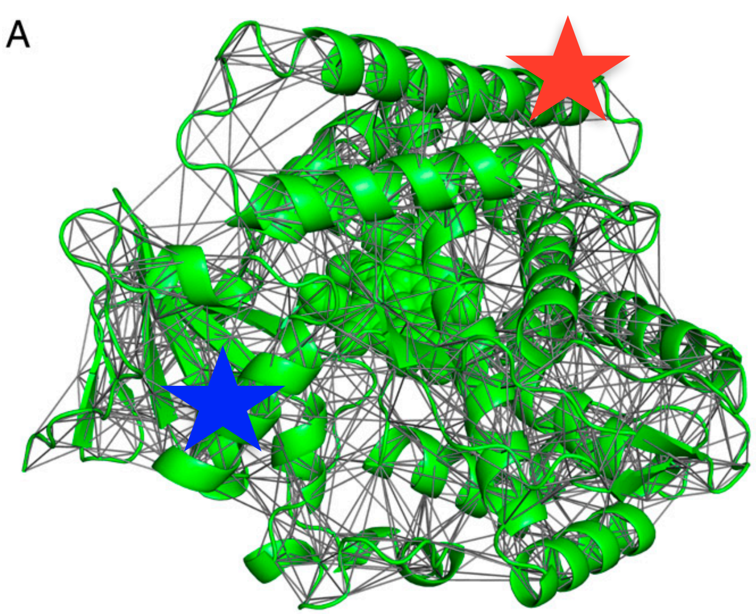
Navigating the protein fitness landscape with Gaussian processes

Philip A. Romero[a], Andreas Krause[b], and Frances H. Arnold[a,1]

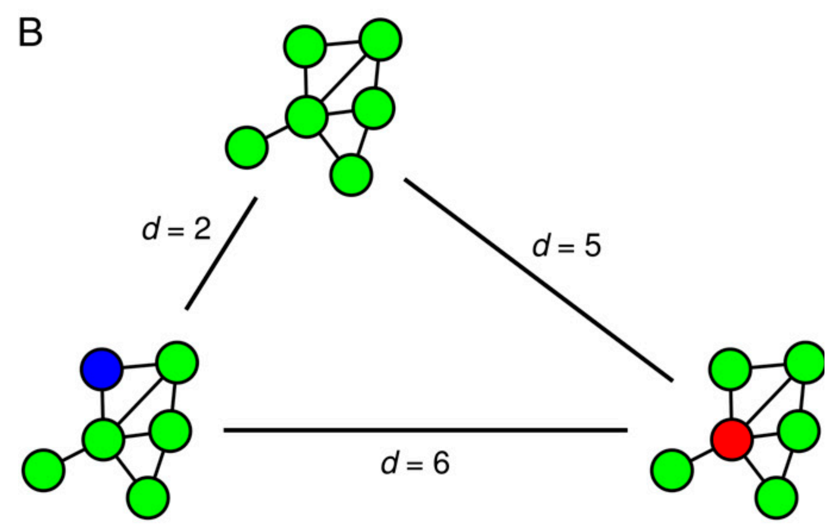
[a]Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA 91125; and [b]Department of Computer Science, Swiss Federal Institute of Technology, 8092 Zurich, Switzerland

Edited by Michael Levitt, Stanford University School of Medicine, Stanford, CA, and approved November 28, 2012 (received for review September 9, 2012)

Enzyme to be optimized



Network representation and distance definition



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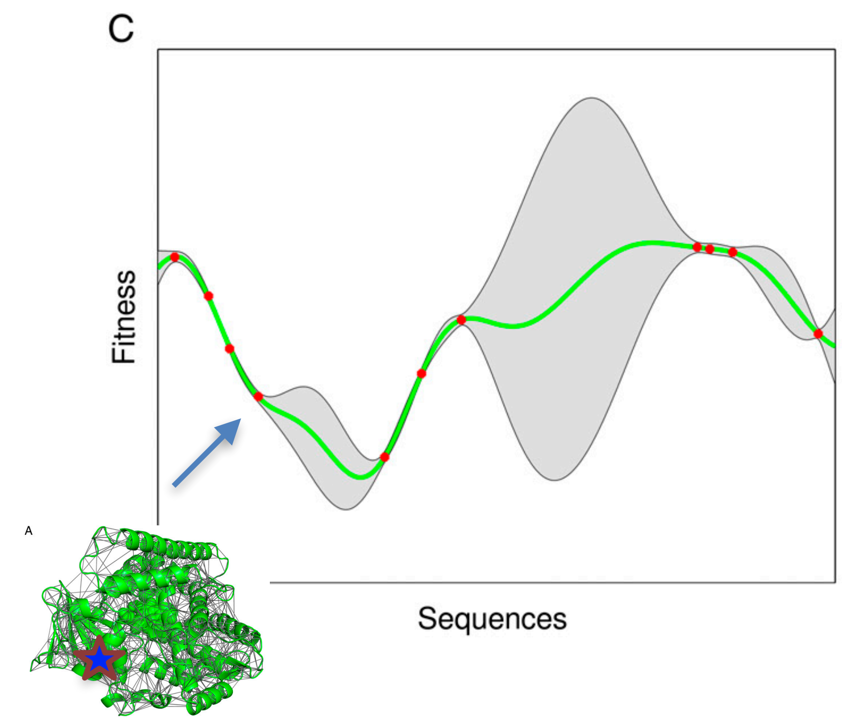

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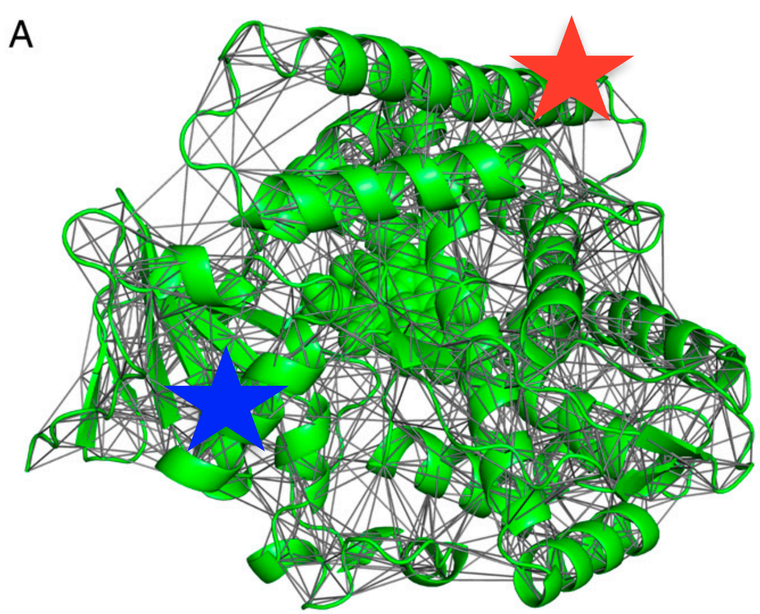

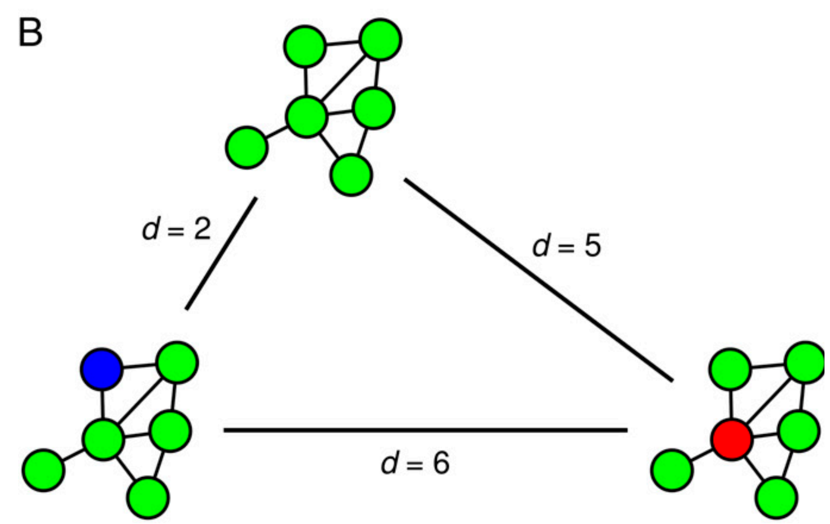

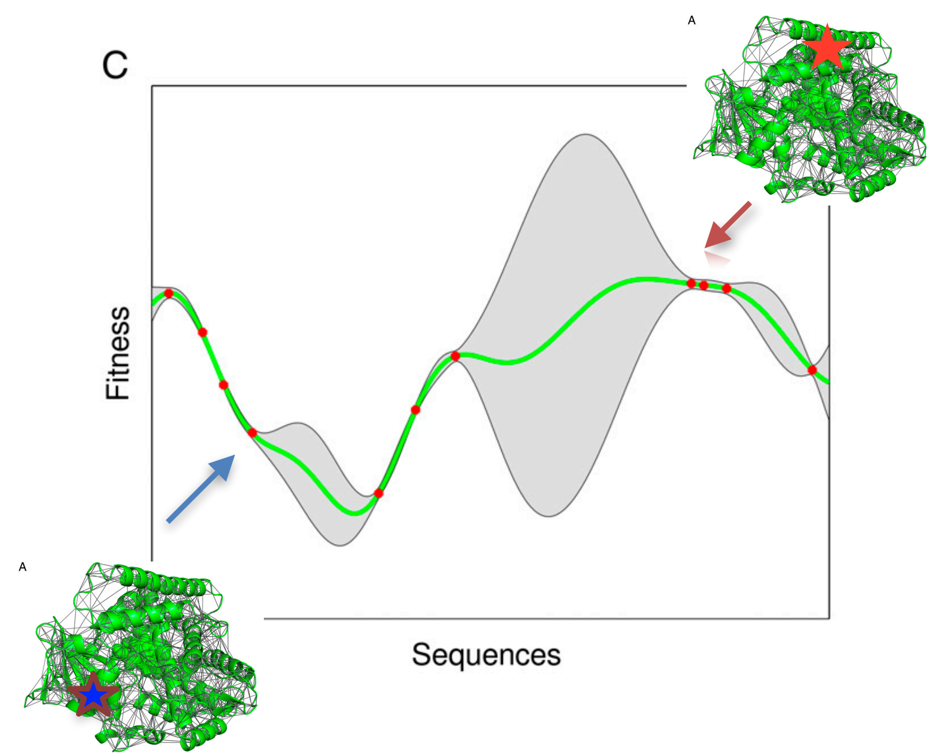

FITNESS LANDSCAPES AND OPTIMIZATION

- Evolution can be seen as optimization process over a fitness landscapes.
- The optimization process is based on a **population** of individuals.
- Key operations are **mutation** and **selection**.

FITNESS LANDSCAPES AND OPTIMIZATION

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Center for Computational Mathematics

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- The optimization process is based on a **population** of individuals.
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The entire field of *evolutionary computation*, a subfield of continuous optimization, is based on this idea (>100k publications).

Keywords: Genetic algorithms, genetic programs, Evolution Strategies

ENERGY LANDSCAPES -

LONDON-EYRING-POLANYI POTENTIAL ENERGY SURFACE

Eyring, H, Polanyi, M., “Über einfache Gasreaktionen,”

Zeitschrift für Physikalische Chemie B, Band 12, S. 279–311,1931

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$H + H_2 \Leftrightarrow H_2 + H$ reaction for a collinear collision geometry

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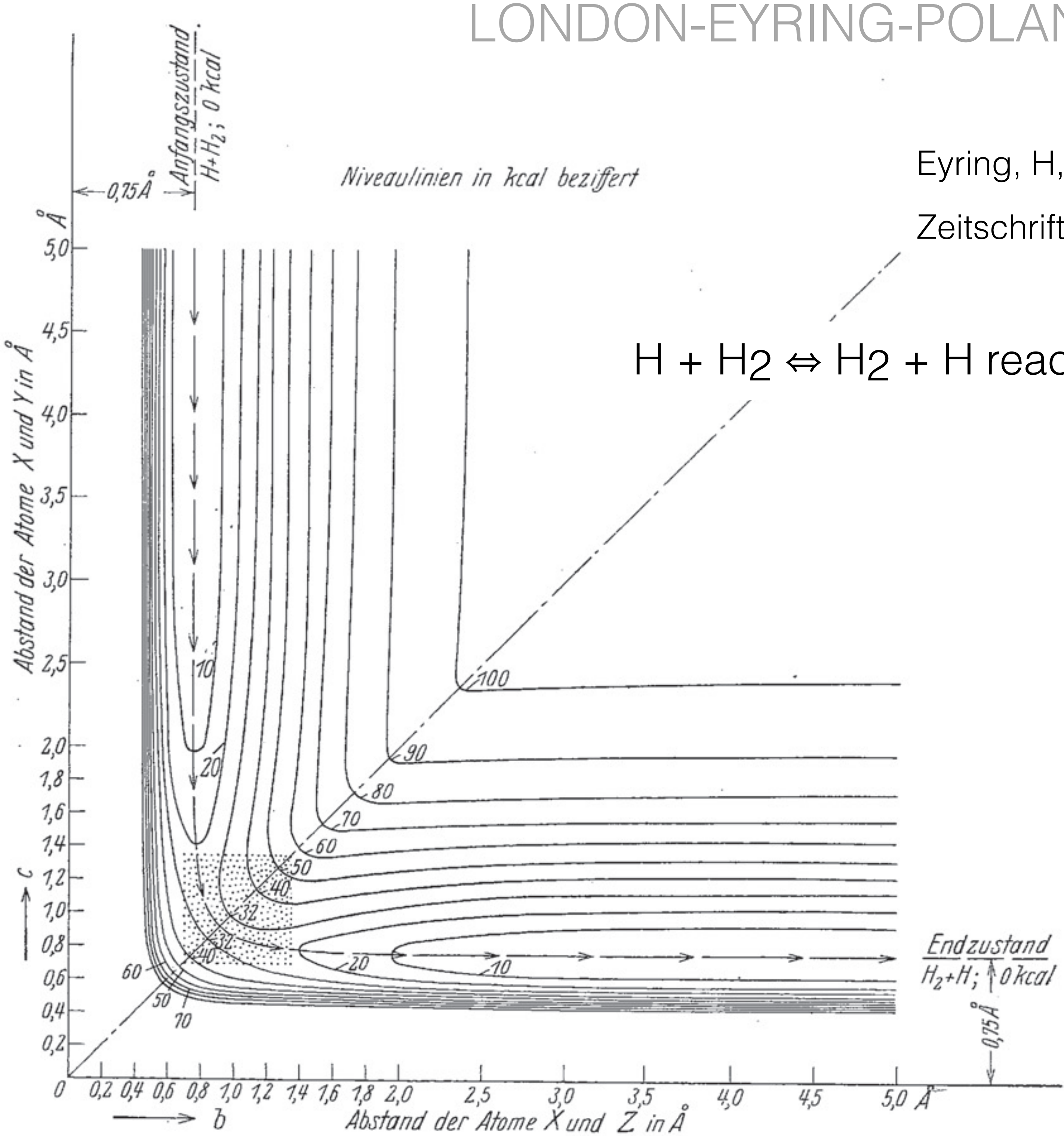

Fig. 5. Resonanzenergie von 3 geradlinig angeordneten H-Atomen als Funktion der Abstände („Resonanzgebirge“).
aus der optischen Energiekurve von H_2 (Fig. 4) unter Vernachlässigung des Coulombschen Anteils berechnet.

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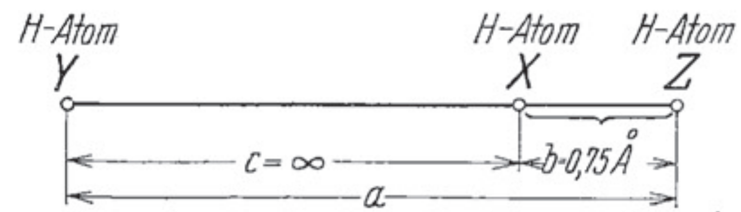

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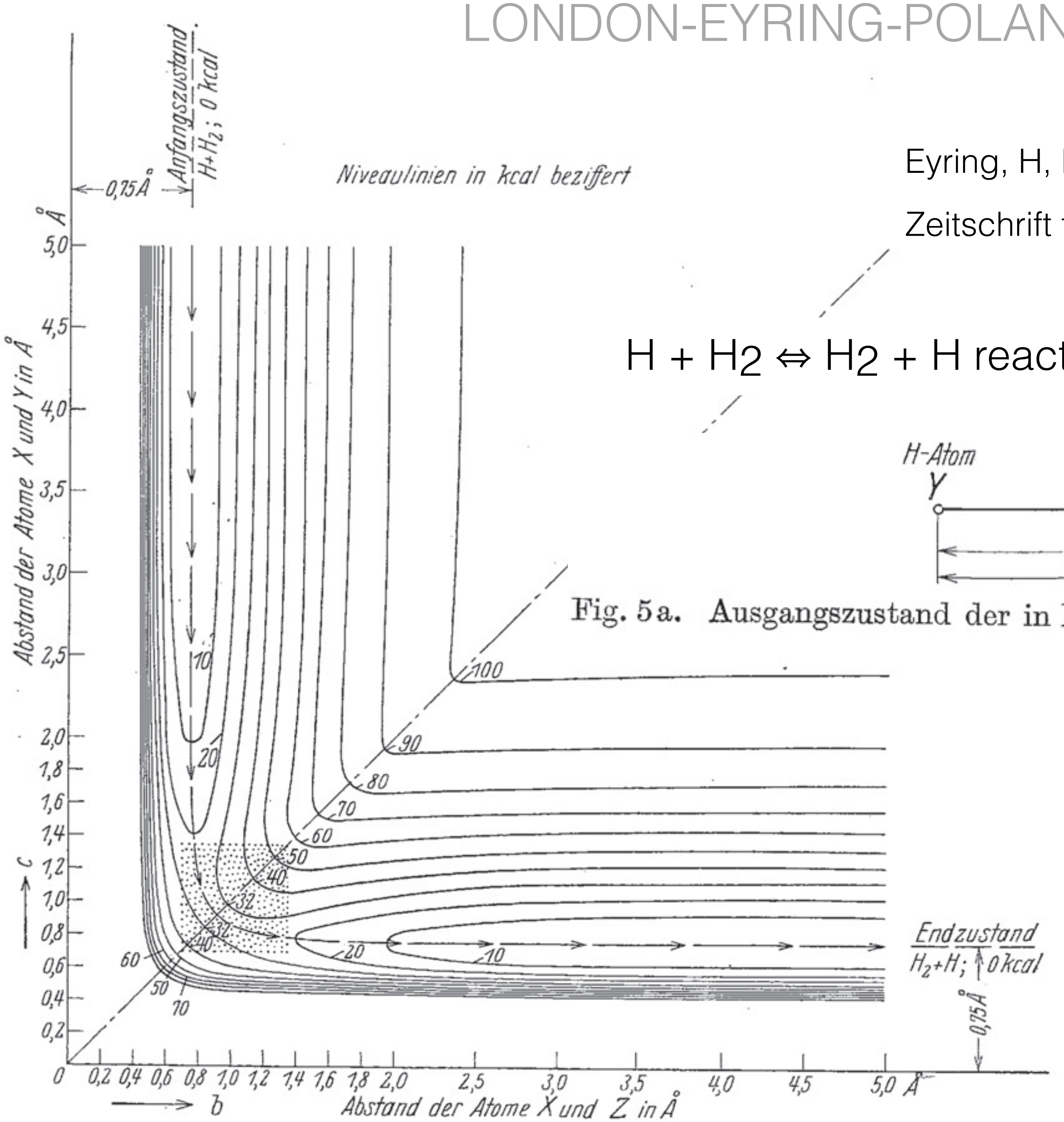

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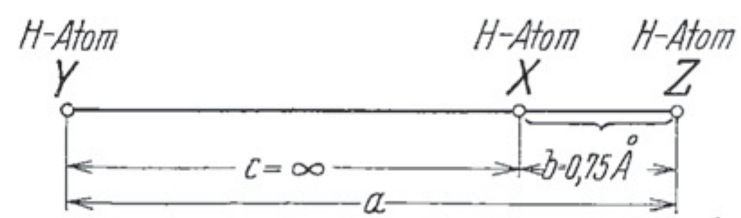

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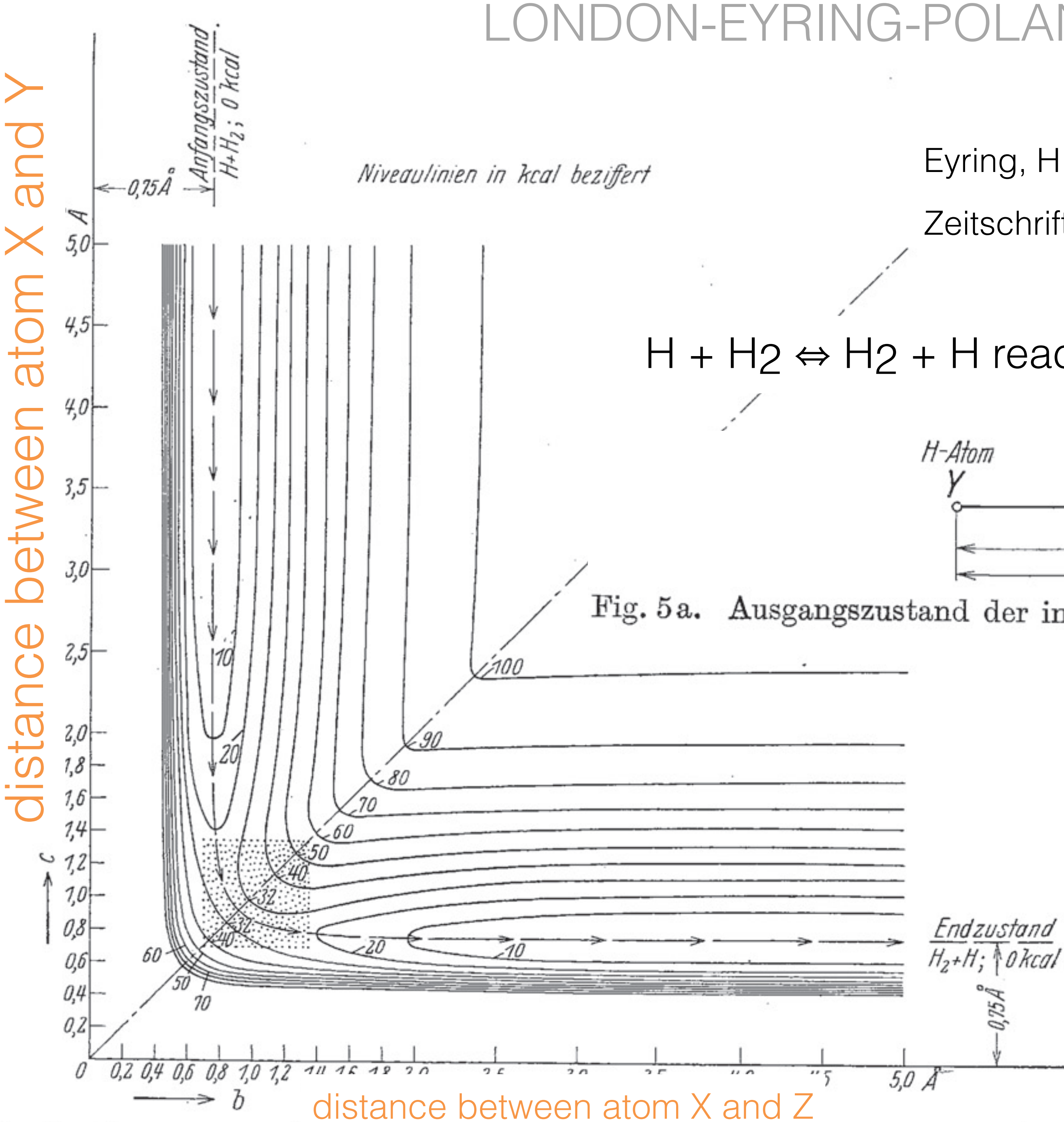

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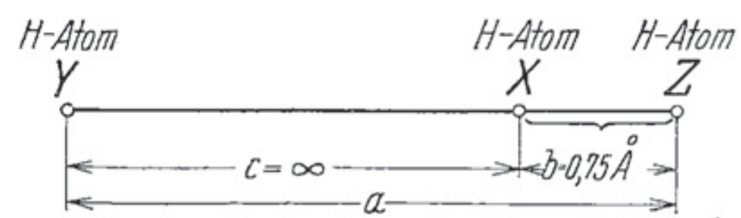

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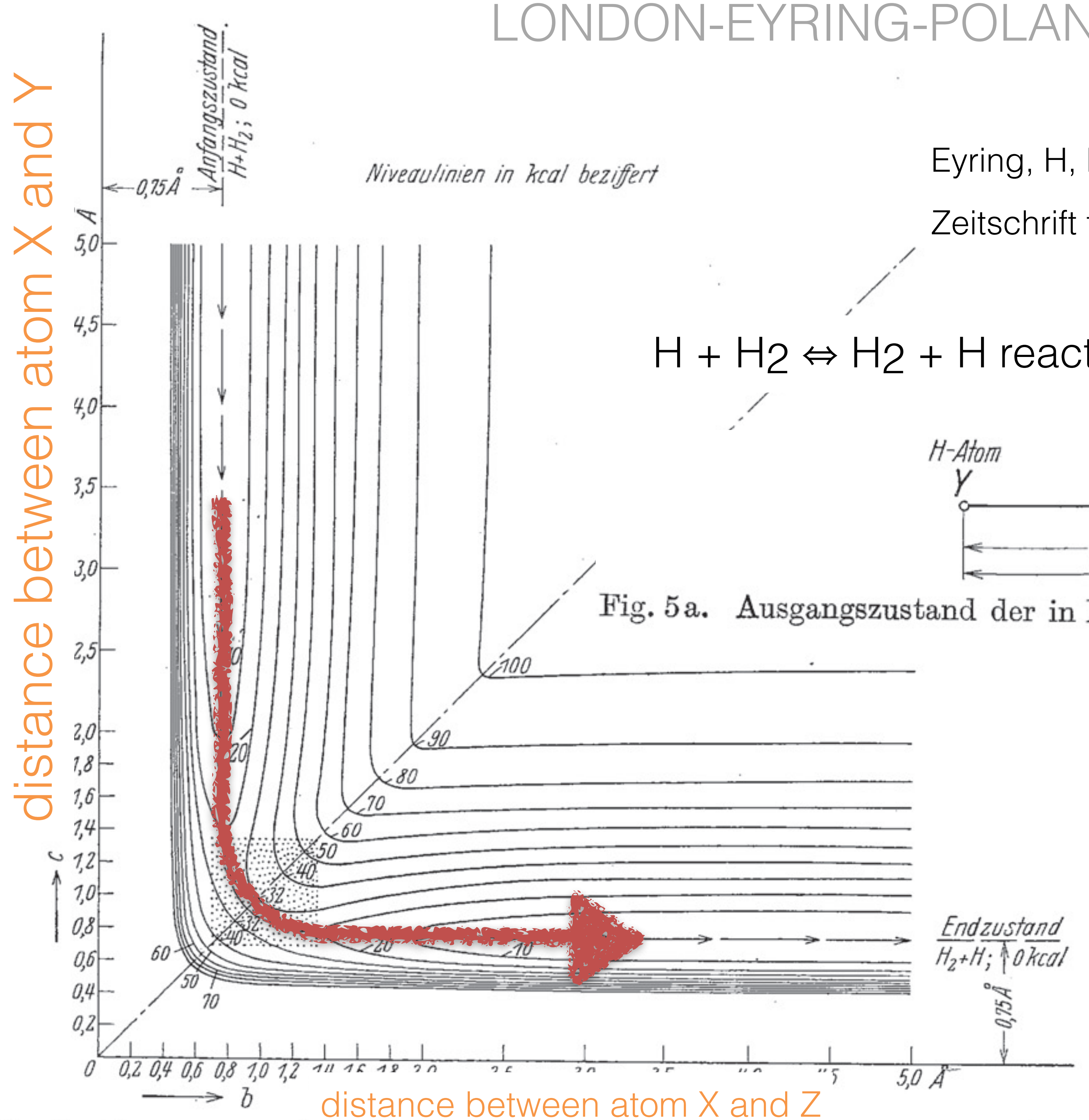

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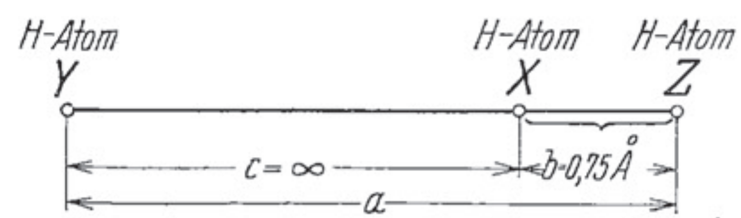

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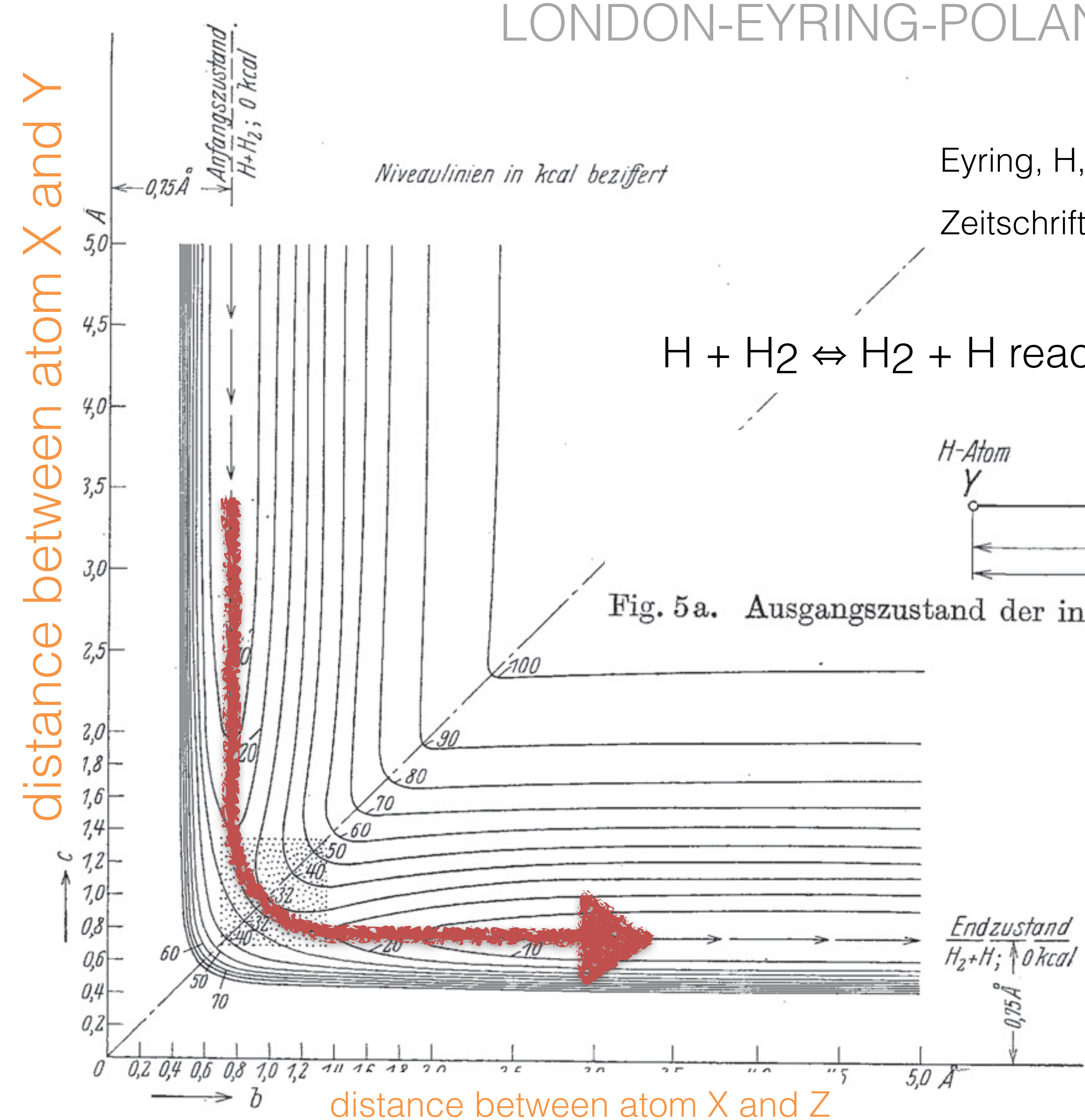

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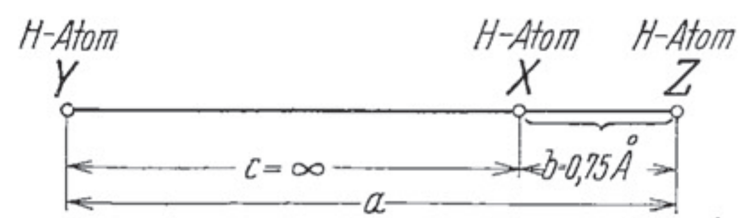

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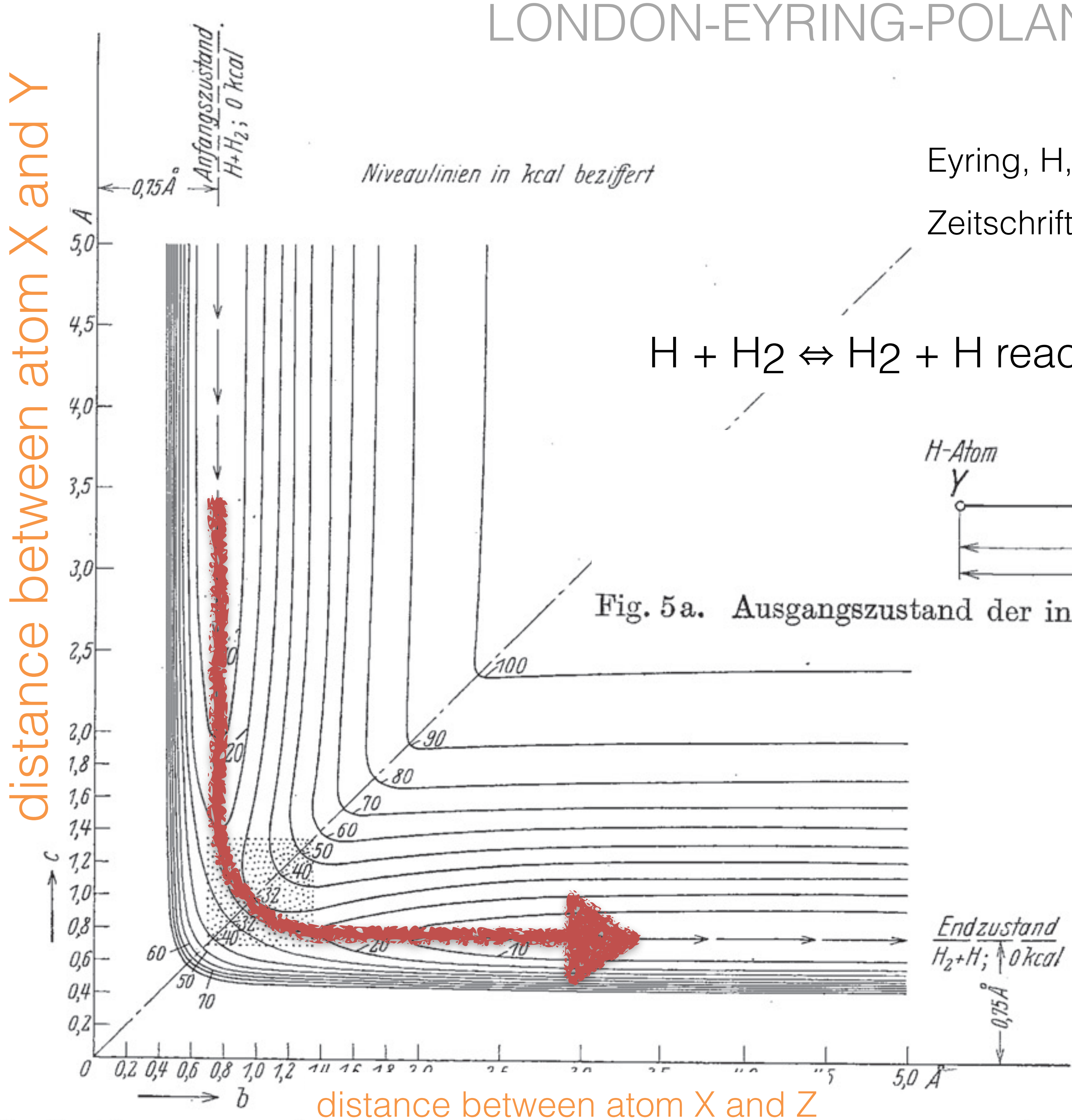

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Resonance energy as a function of distances (“resonance mountain”)

ENERGY LANDSCAPES

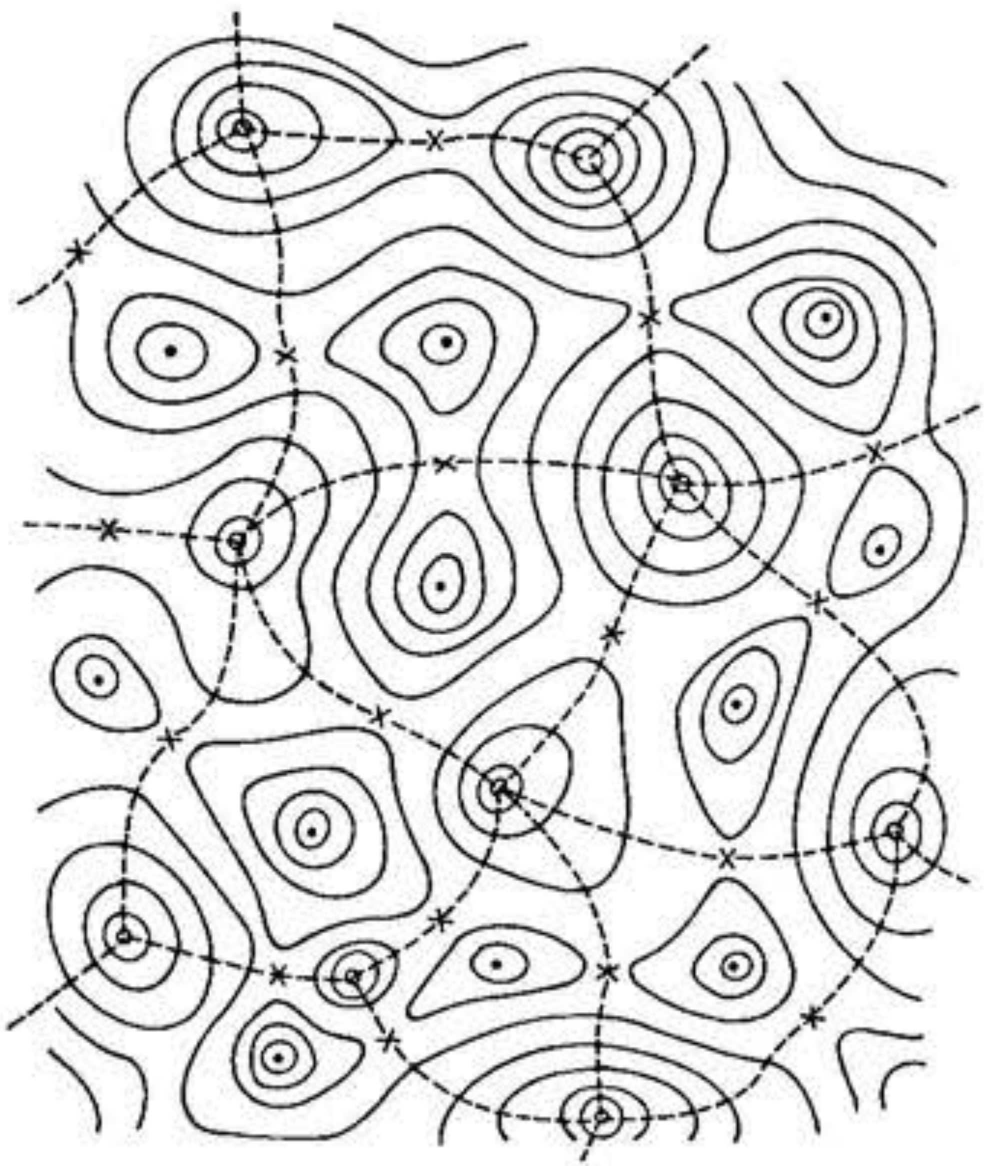

Fig. 1. Schematic representation of the potential energy surface for an *N*-atom system. Minima are shown as filled circles and saddle points as crosses. Potential energy is constant along the continuous curves. Regions belonging to different minima are indicated by dashed curves.

7 September 1984, Volume 225, Number 4666 **SCIENCE**

Packing Structures and Transitions in Liquids and Solids

Frank H. Stillinger and Thomas A. Weber

ENERGY LANDSCAPES

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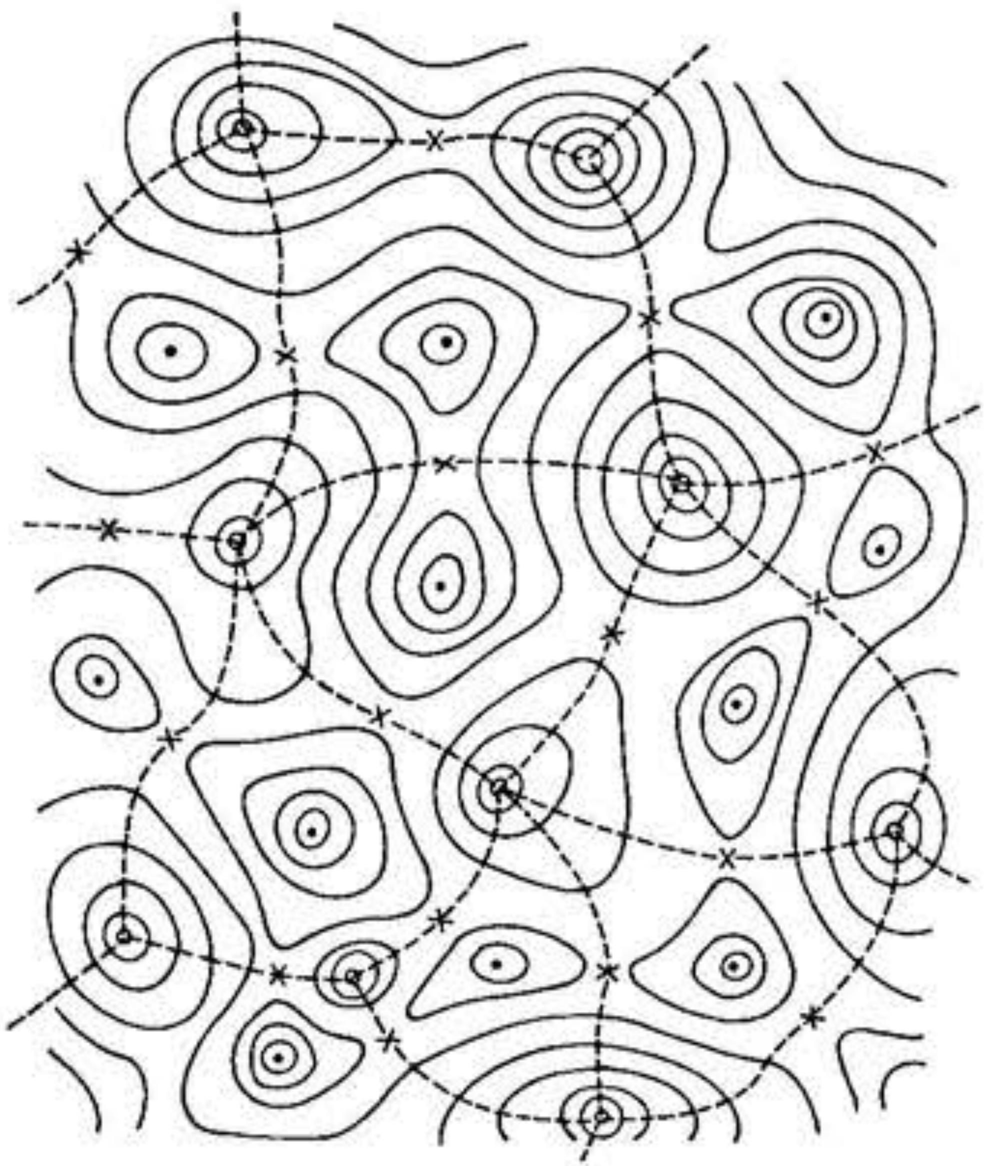

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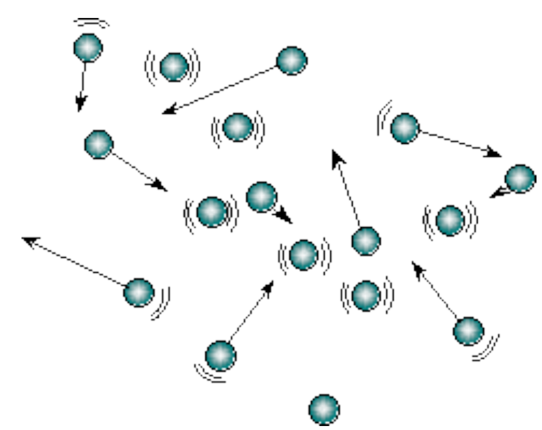
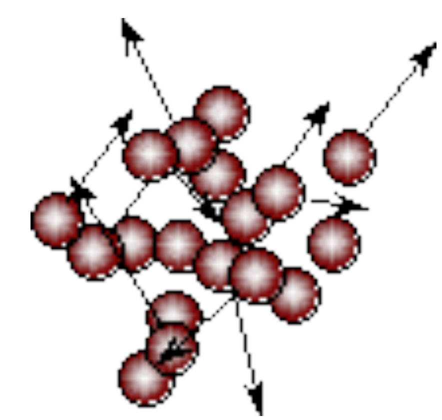
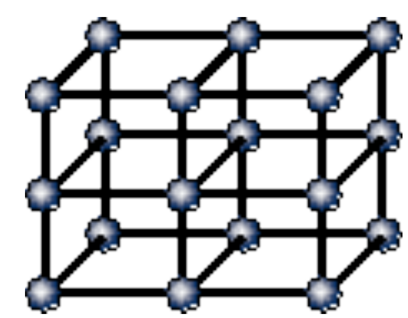


Liquid



Solid



https://www.learnthermo.com/T1-tutorial/ch03/lesson-A/pg01.php

ENERGY LANDSCAPES AND OPTIMIZATION

The transition process from gas to liquid to solid can be seen as optimization process

13 May 1983, Volume 220, Number 4598

SCIENCE

Optimization by Simulated Annealing

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ENERGY LANDSCAPES AND OPTIMIZATION

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Ingredients:

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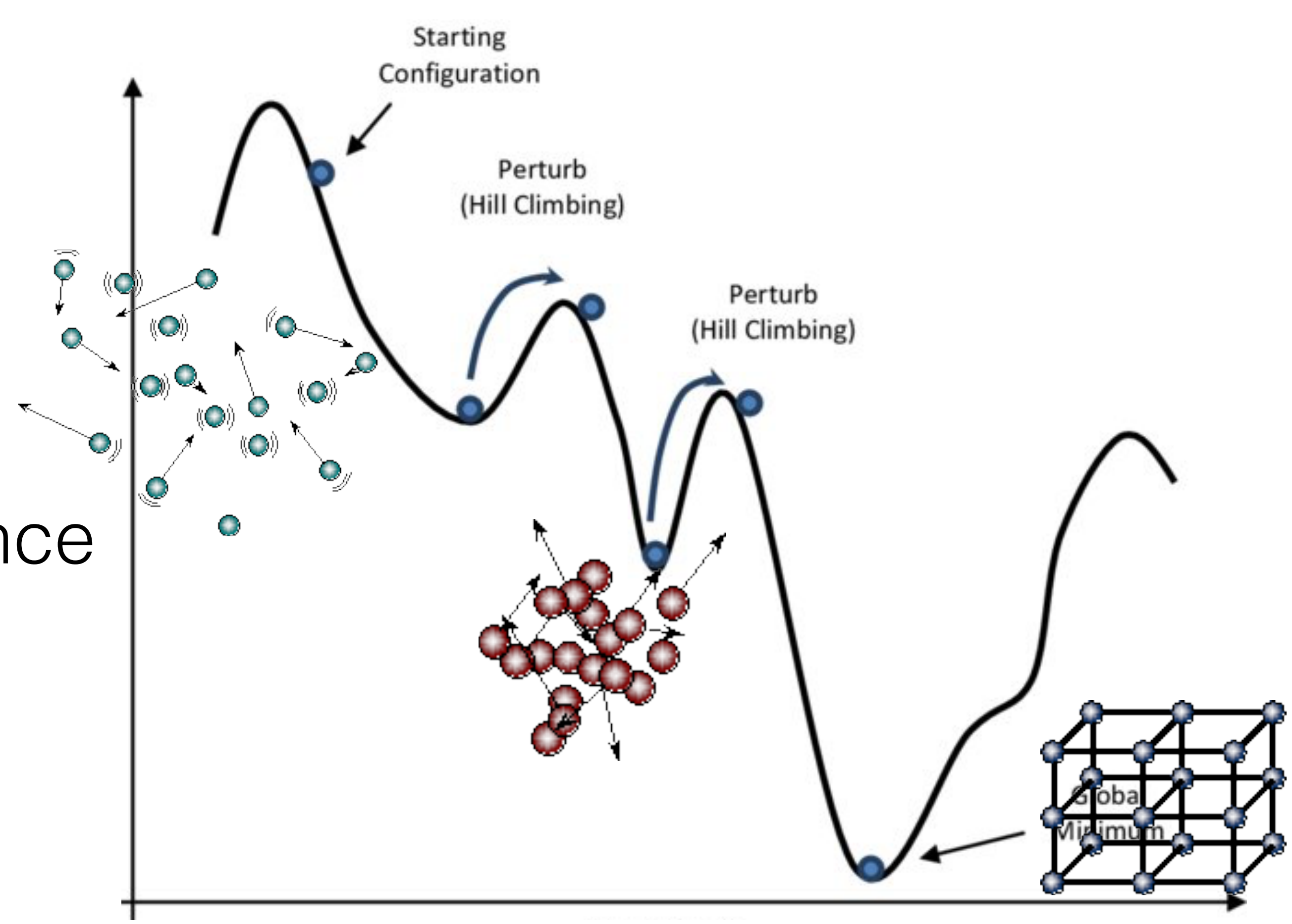
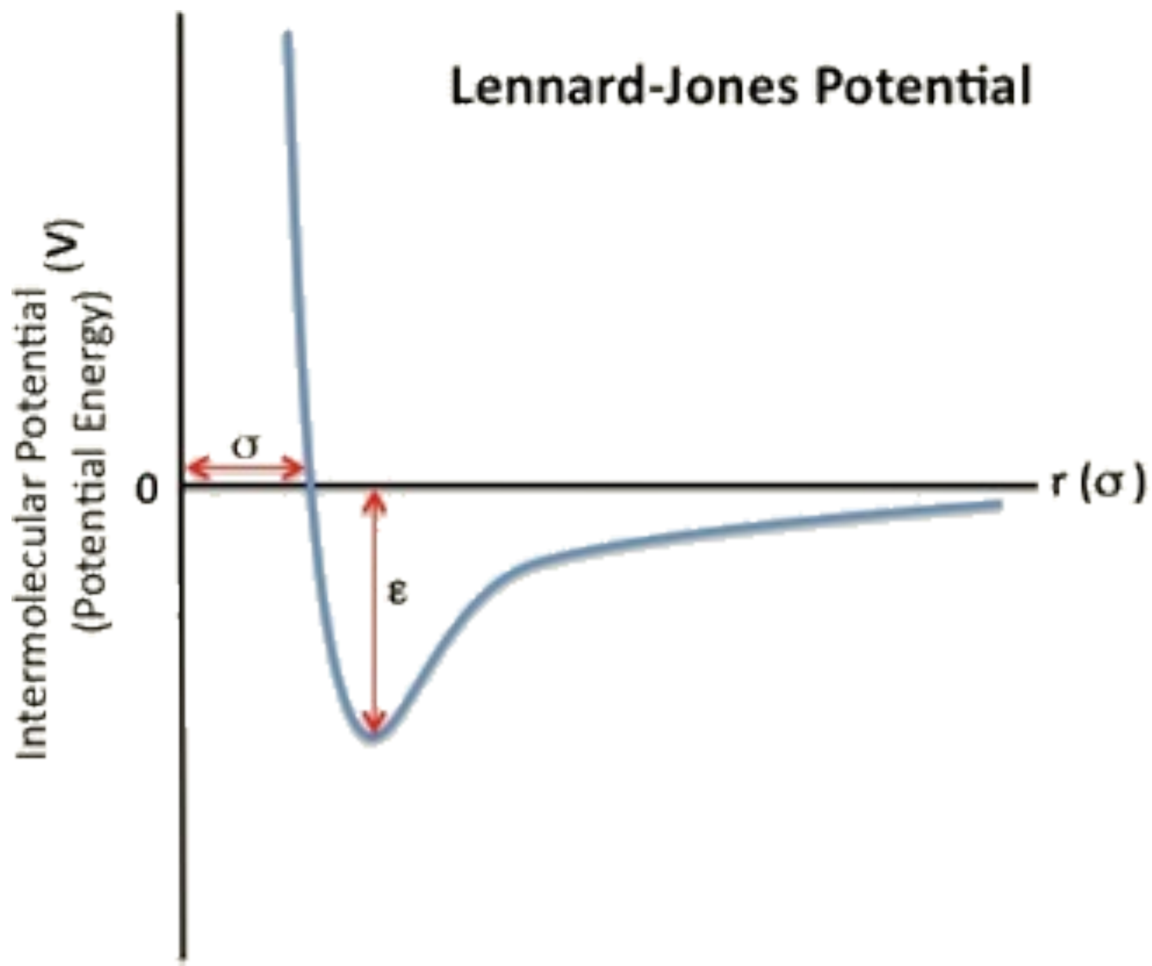
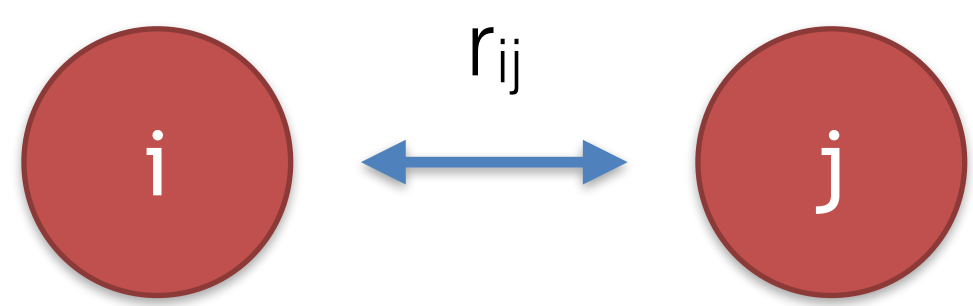


ENERGY LANDSCAPES - LENNARD-JONES CLUSTERS

- Lennard-Jones potential as pair potential between noble gas atoms
- What is the best (lowest potential energy) configuration at temperature T = 0?
- How does the energy landscape look like for N number of atoms?





$$E = 4\epsilon \sum_{i<j} \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right]$$

ENERGY LANDSCAPES - BASIN HOPPING

FLATIRON INSTITUTE
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J. Phys. Chem. A **1997,** *101,* 5111−5116 **5111**

Global Optimization by Basin-Hopping and the Lowest Energy Structures of Lennard-Jones Clusters Containing up to 110 Atoms

David J. Wales*
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Jonathan P. K. Doye
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Received: March 19, 1997; In Final Form: April 29, 1997⊗

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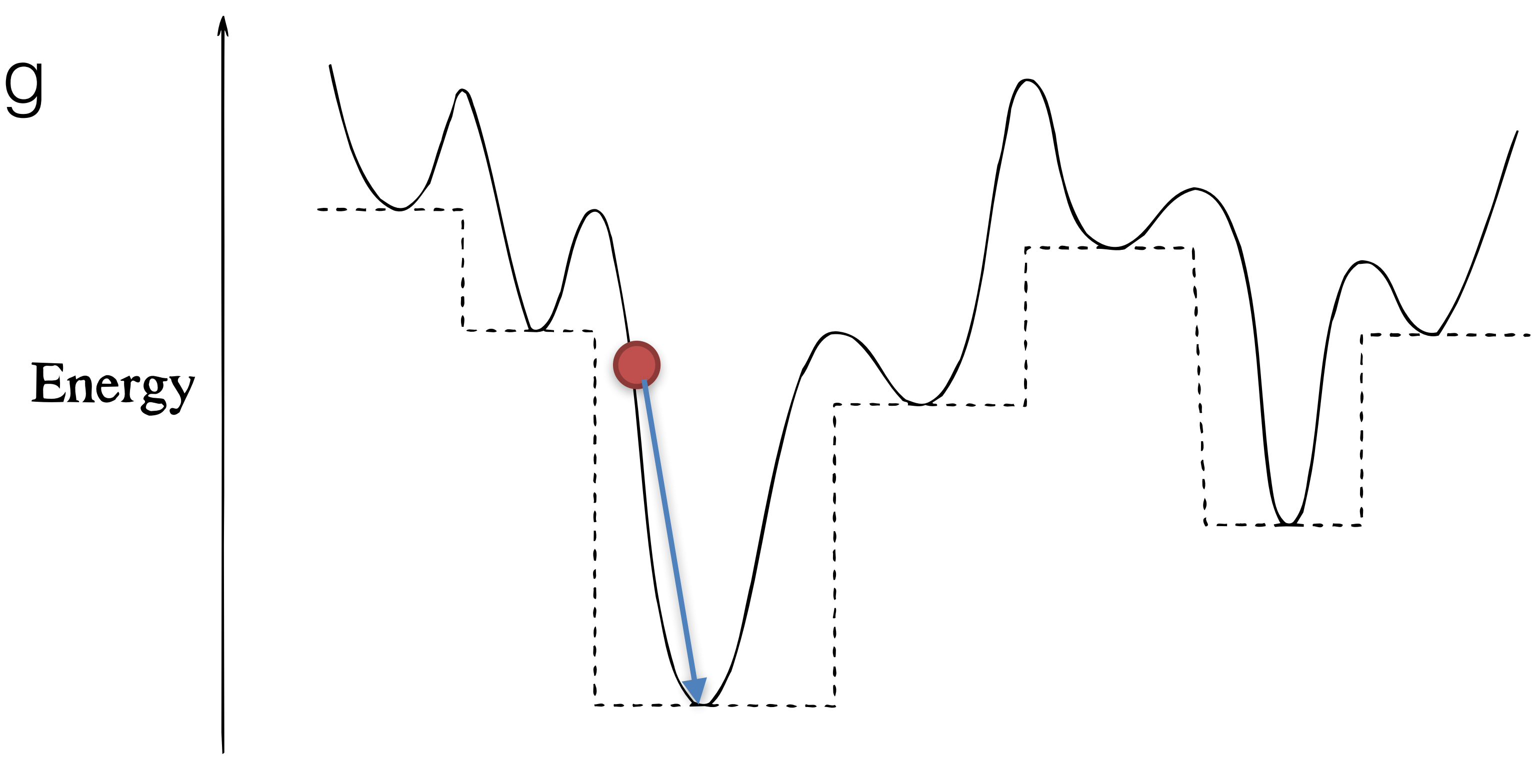

Figure 2. A schematic diagram illustrating the effects of our energy transformation for a one-dimensional example. The solid line is the energy of the original surface and the dashed line is the transformed energy $\tilde{E}$.

ENERGY LANDSCAPES - LJ CLUSTER MINIMA

FLATIRON INSTITUTE
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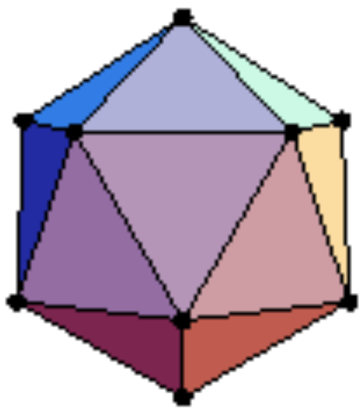
LJ 13



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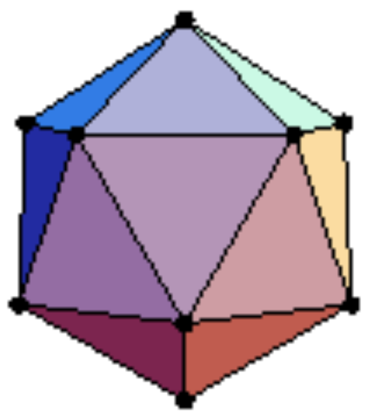

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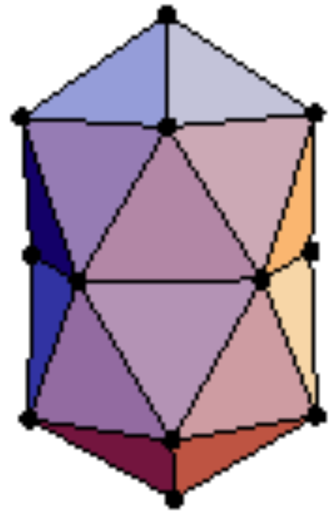
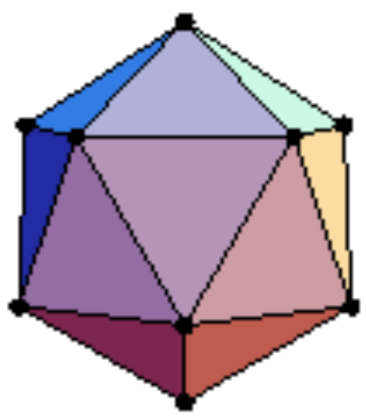


ENERGY LANDSCAPES - LJ CLUSTER MINIMA

LJ 13



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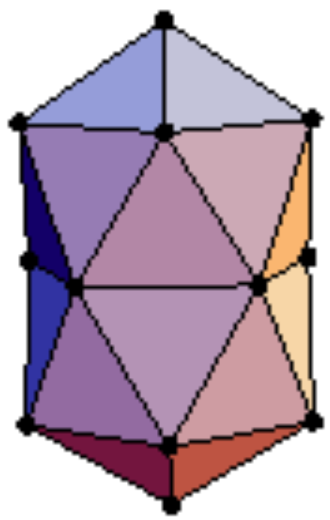
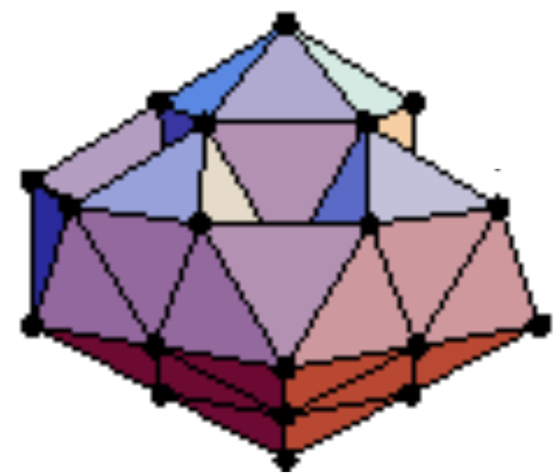
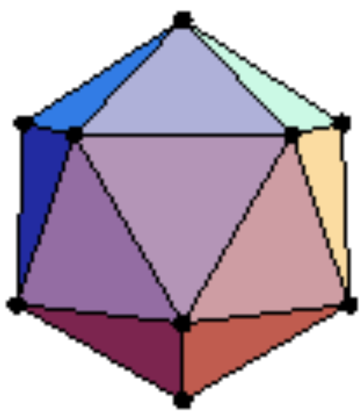


LJ 31



ENERGY LANDSCAPES - LJ CLUSTER MINIMA

LJ 13



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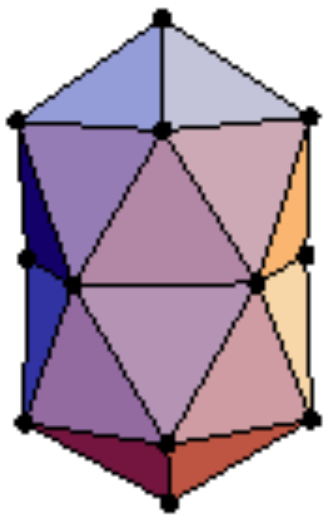

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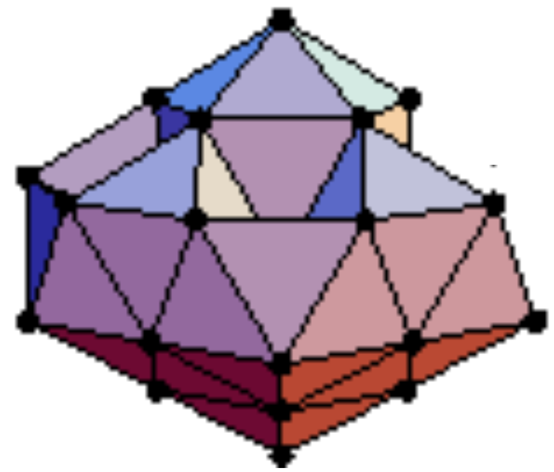
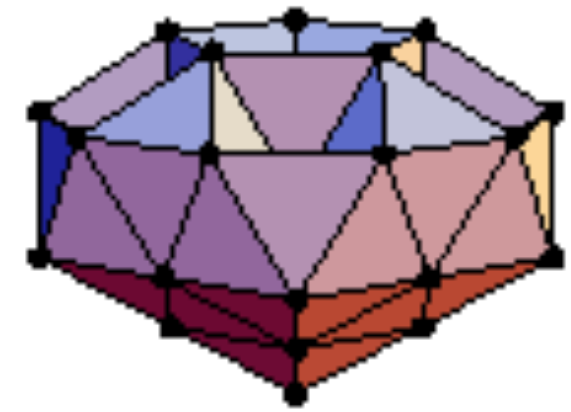
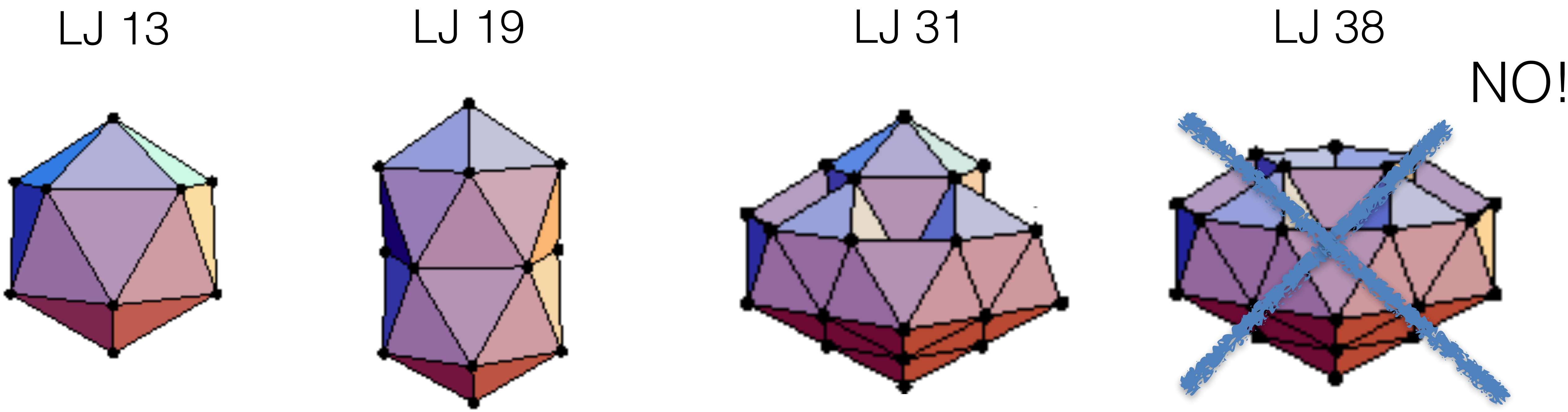


LJ 38

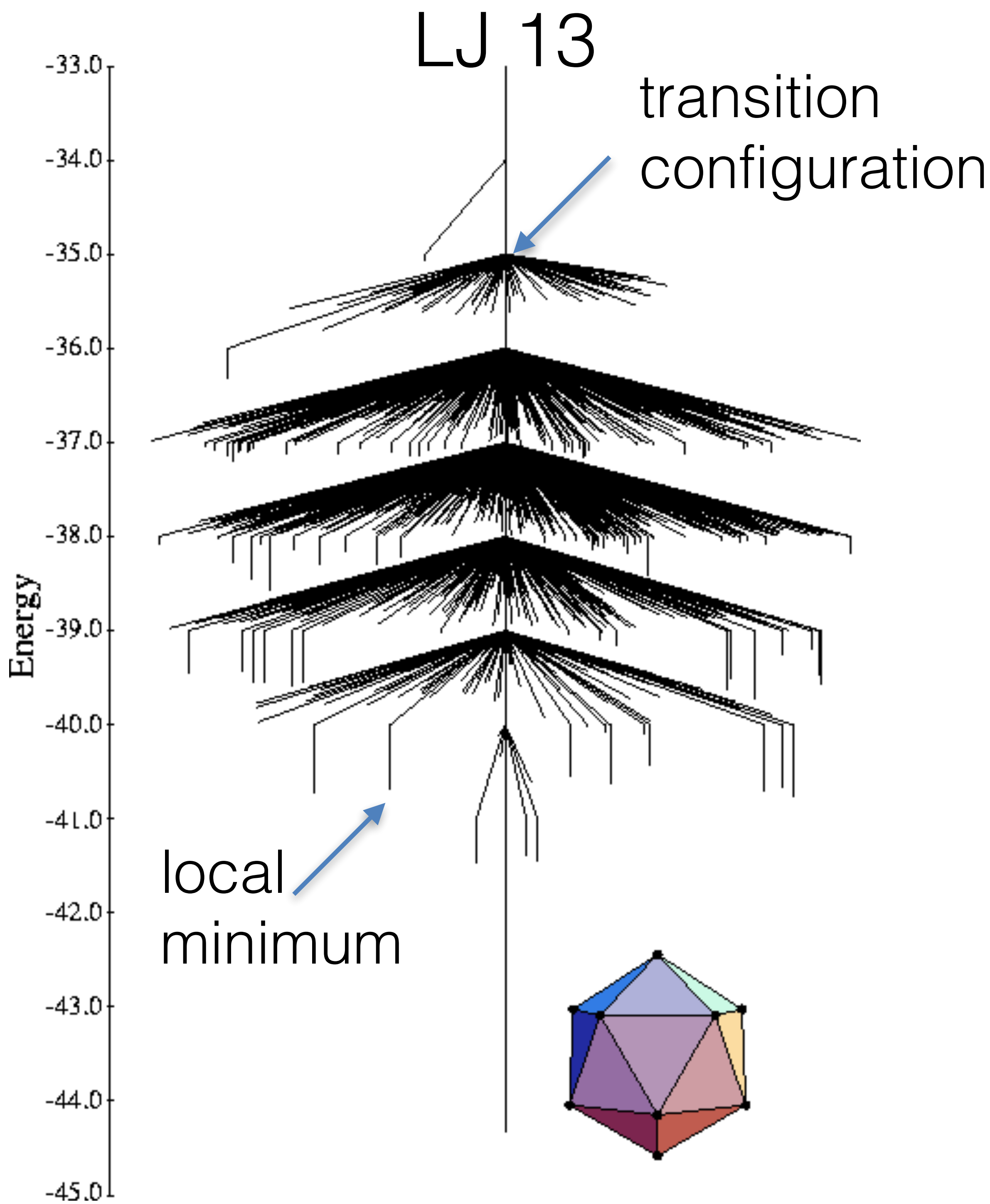


ENERGY LANDSCAPES - LJ CLUSTER MINIMA



This face-centered cubic octahedron (fcc) structure is the global minimum.

ENERGY LANDSCAPES AND DISCONNECTIVITY GRAPHS



ENERGY LANDSCAPES AND DISCONNECTIVITY GRAPHS

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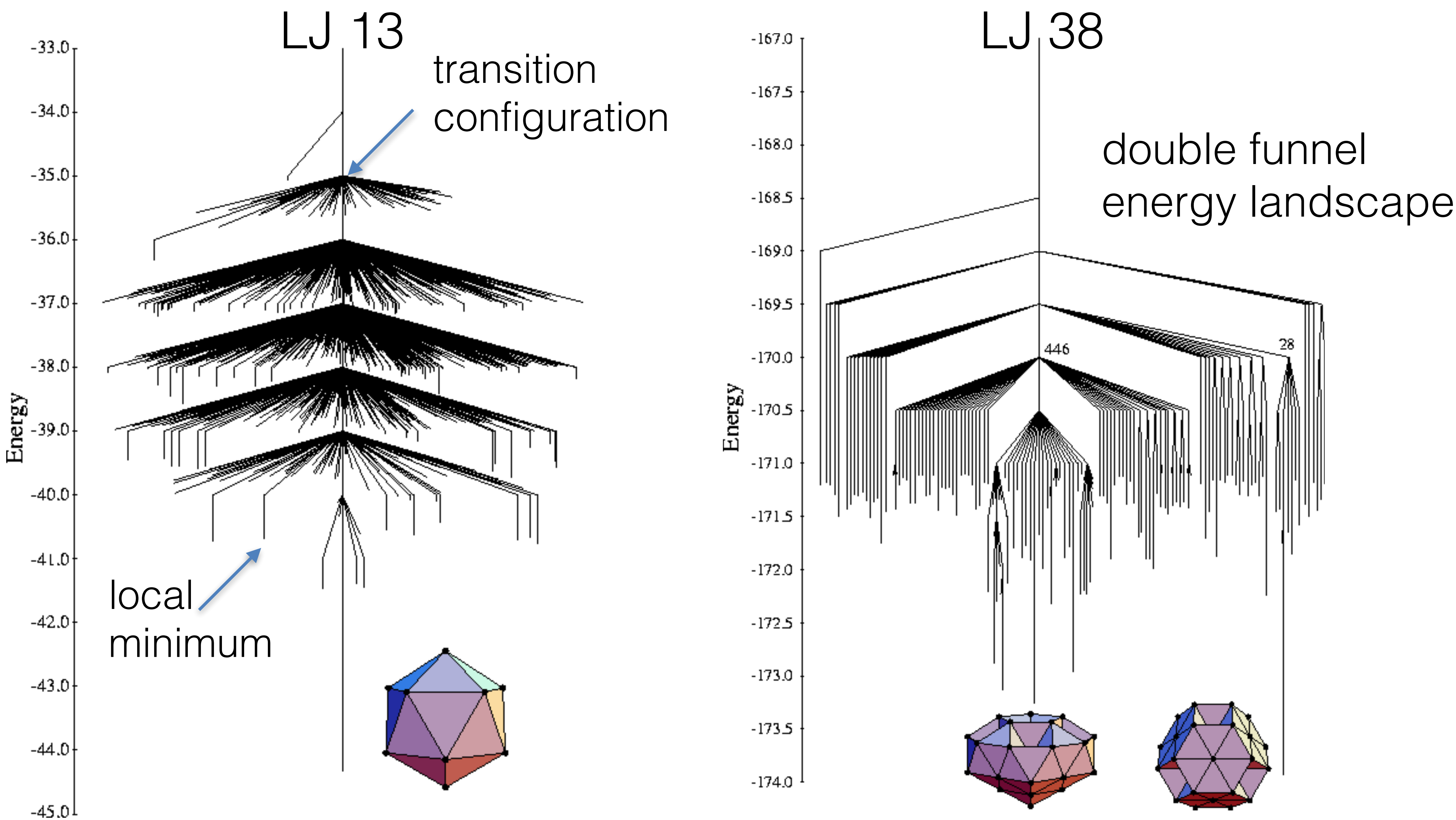

ENERGY LANDSCAPES AND THE SIMONS FOUNDATION

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SIMONS COLLABORATION ON CRACKING THE GLASS PROBLEM

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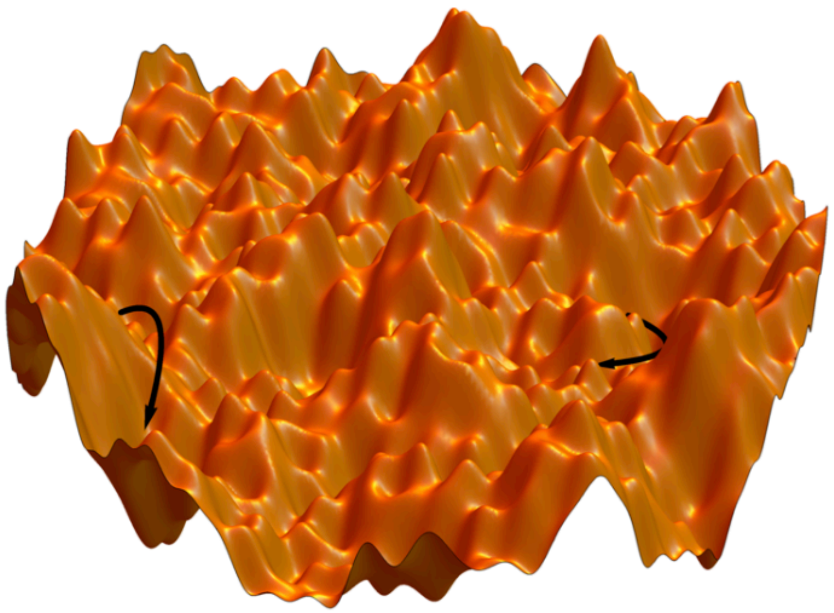
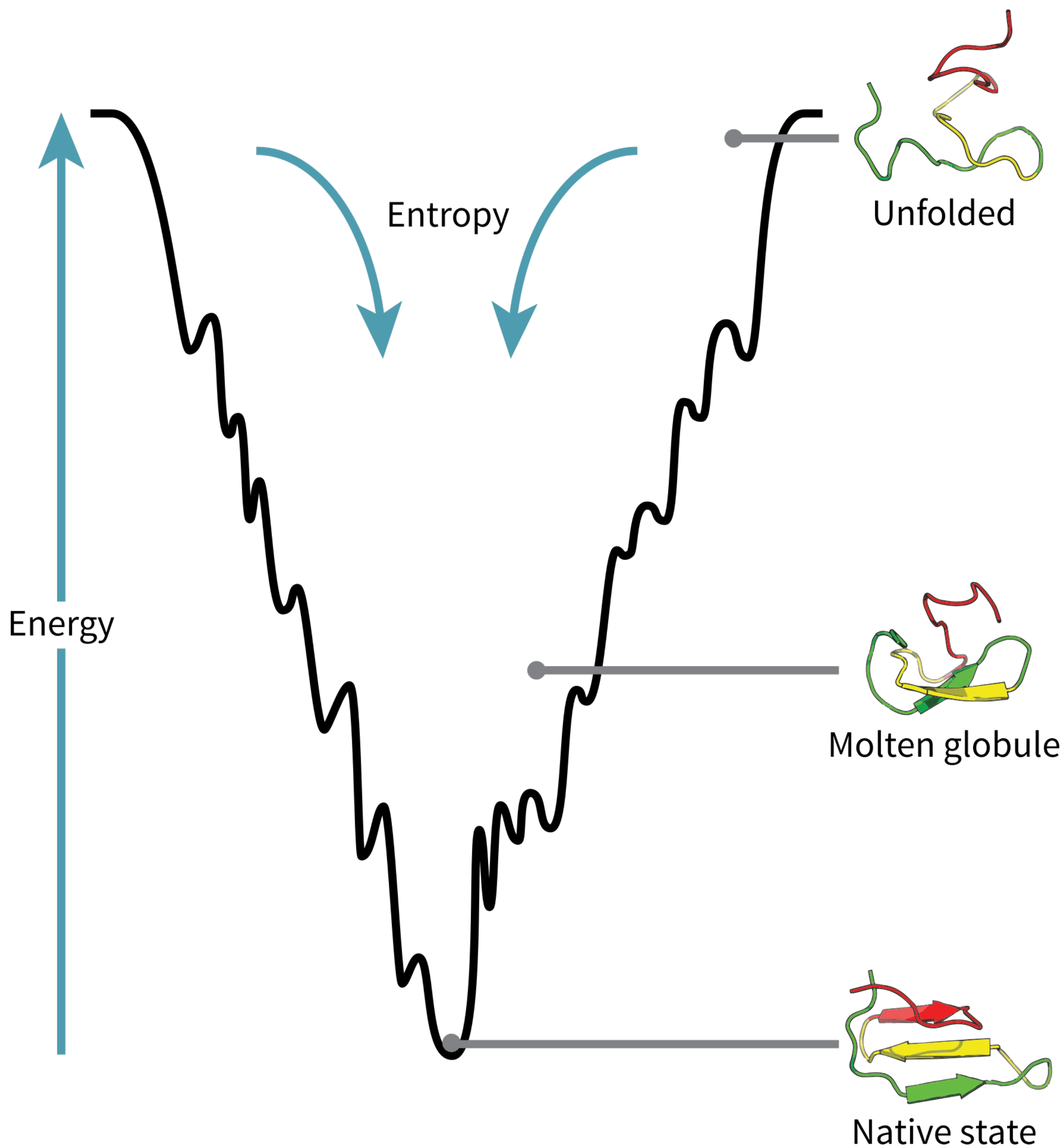


Figure (credit: Chiara Cammarota): A schematic rugged energy landscape with a multitude of energy minima, maxima, and saddles. Arrows denote some of the possible relaxation pathways.

ENERGY LANDSCAPES AND PROTEIN FOLDING



Science 13 Dec 1991:
Vol. 254, Issue 5038, pp. 1598-1603
DOI: 10.1126/science.1749933

Articles

The Energy Landscapes and Motions of Proteins

HANS FRAUENFELDER, STEPHEN G. SLIGAR, PETER G. WOLYNES

ENERGY LANDSCAPES AND DEEP MIND'S ALPHA-FOLD

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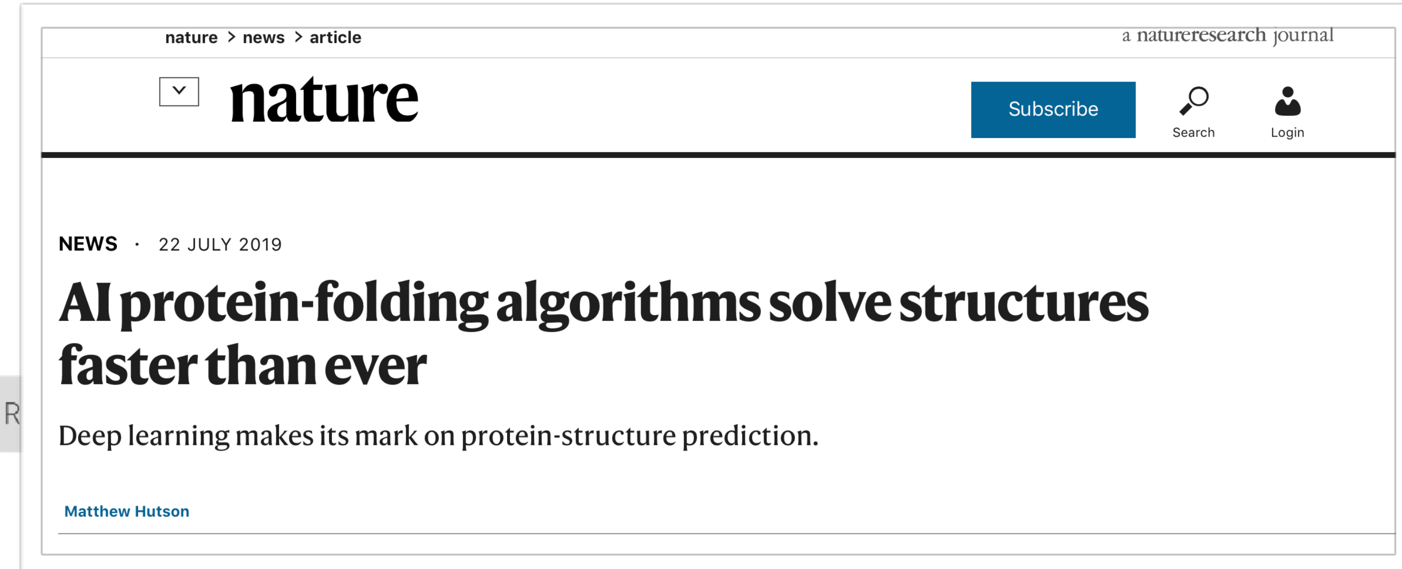
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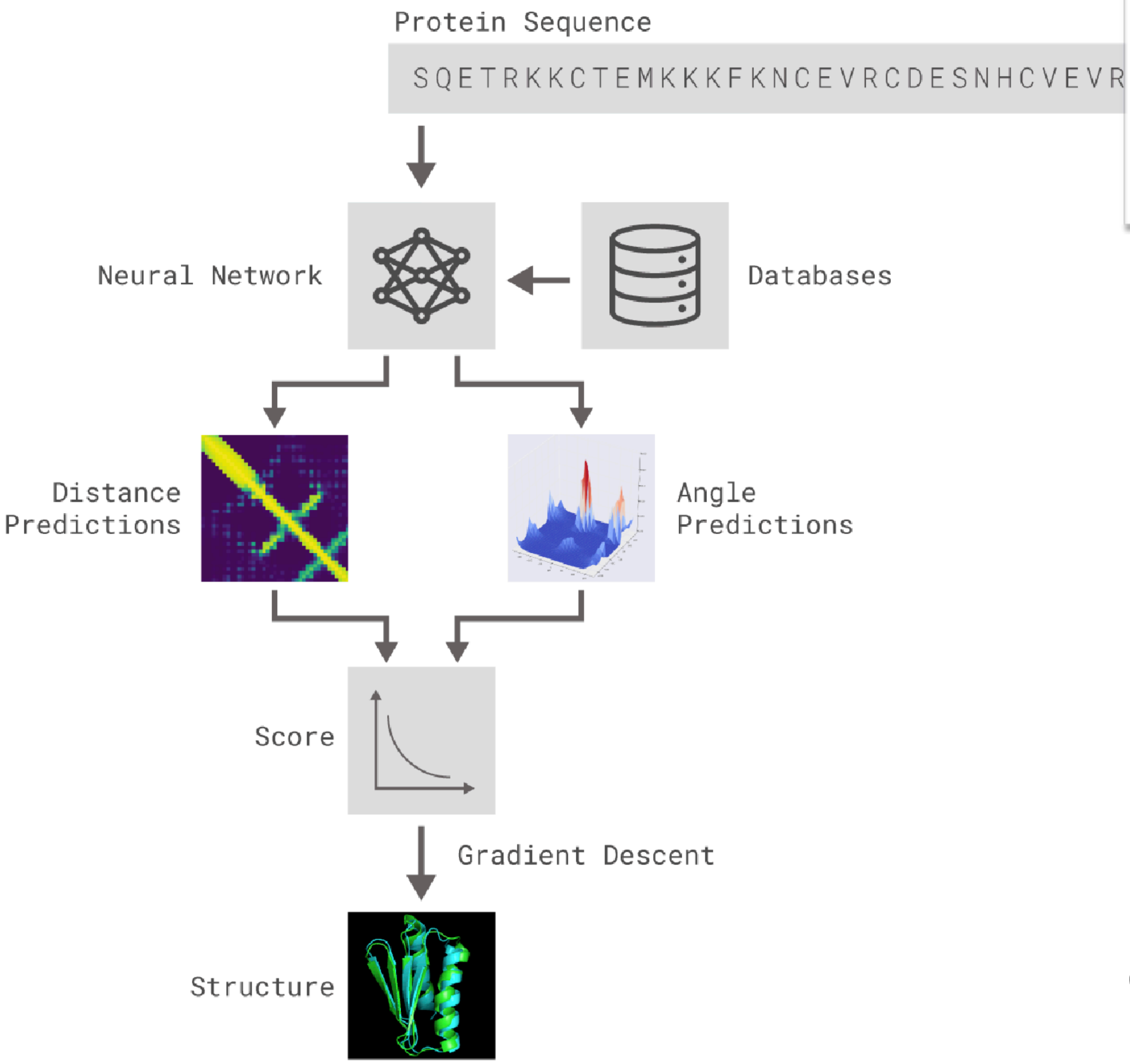
NEWS · 22 JULY 2019

AI protein-folding algorithms solve structures faster than ever

Deep learning makes its mark on protein-structure prediction.

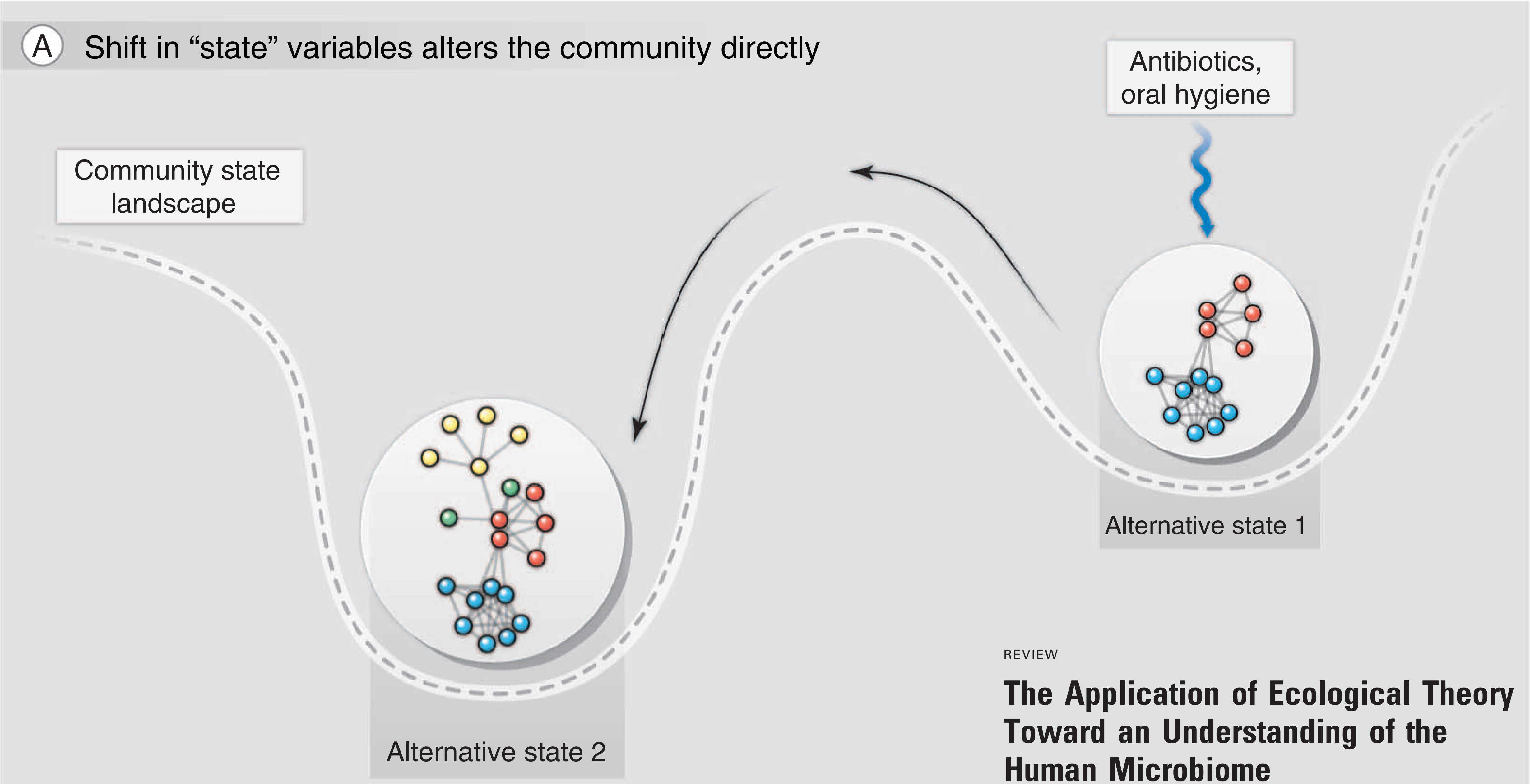
Matthew Hutson



Build a single-funnel energy landscape approximation

Gradient descent on landscape

COMMUNITY STATE LANDSCAPES AND ECOSYSTEMS



REVIEW

The Application of Ecological Theory Toward an Understanding of the Human Microbiome

Elizabeth K. Costello,[1] Keaton Stagaman,[2] Les Dethlefsen,[1,3] Brendan J. M. Bohannan,[2] David A. Relman[1,3,4]*

COMMUNITY STATE LANDSCAPES AND ECOSYSTEMS

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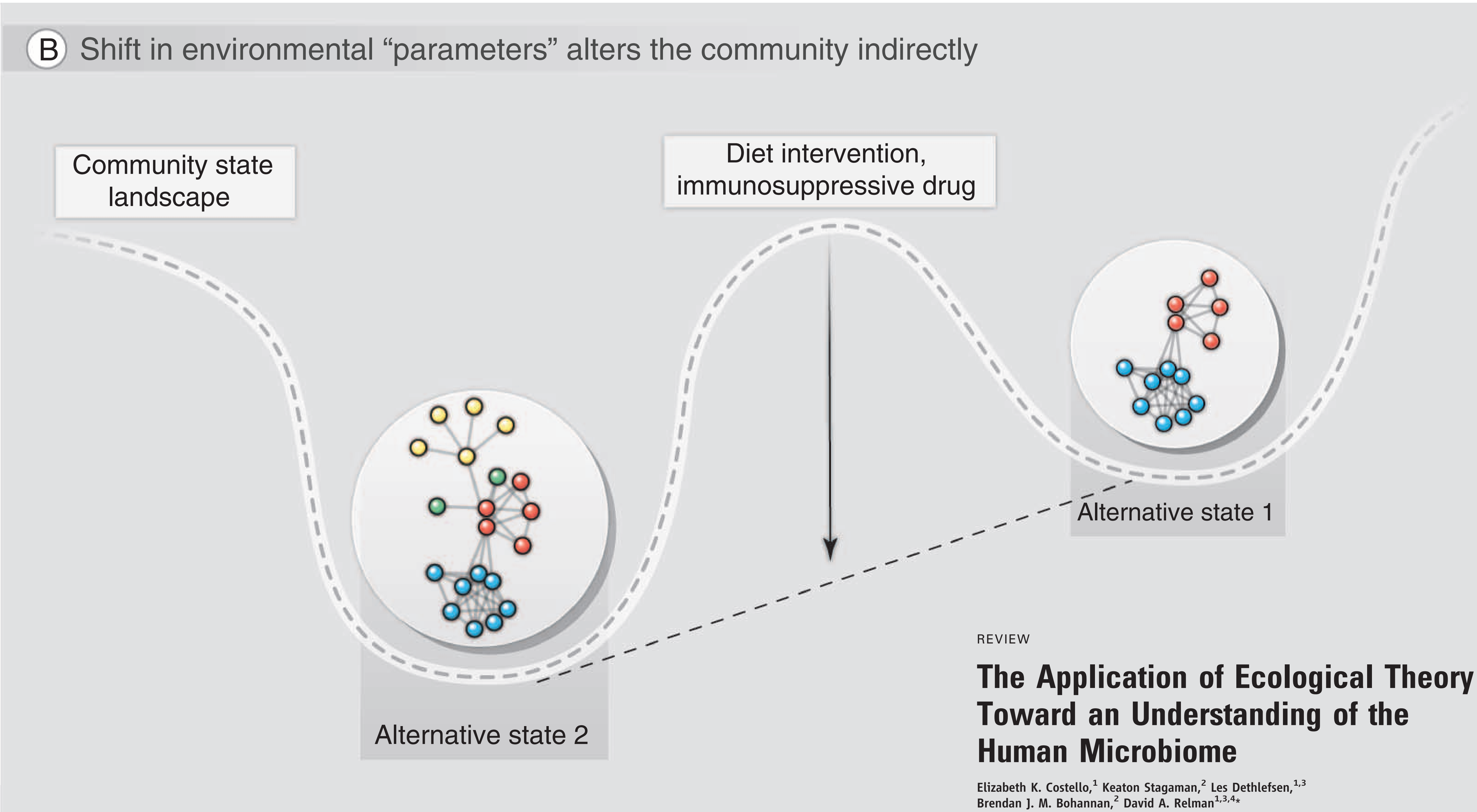

WANT TO KNOW MORE?

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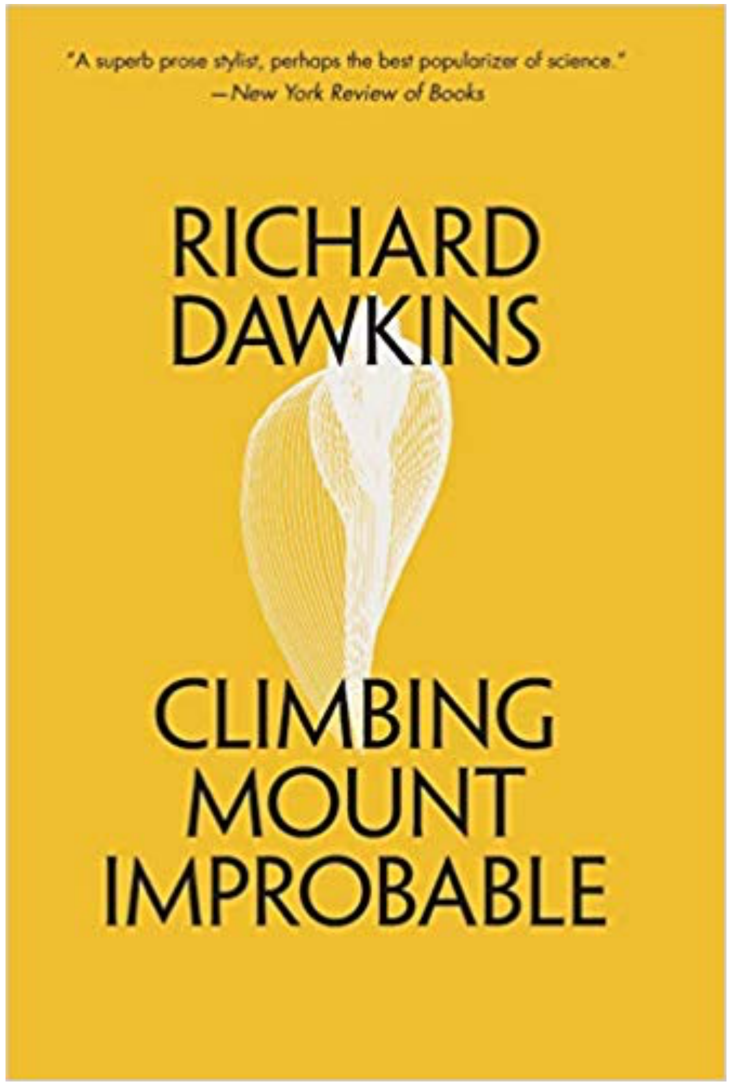

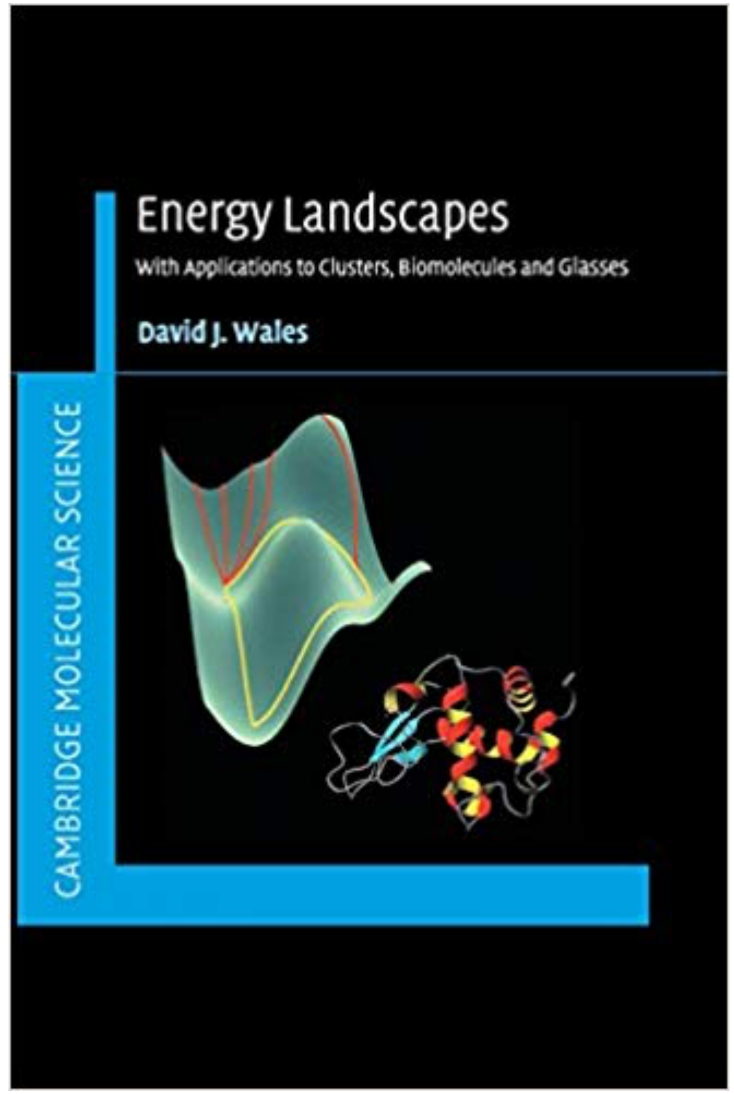

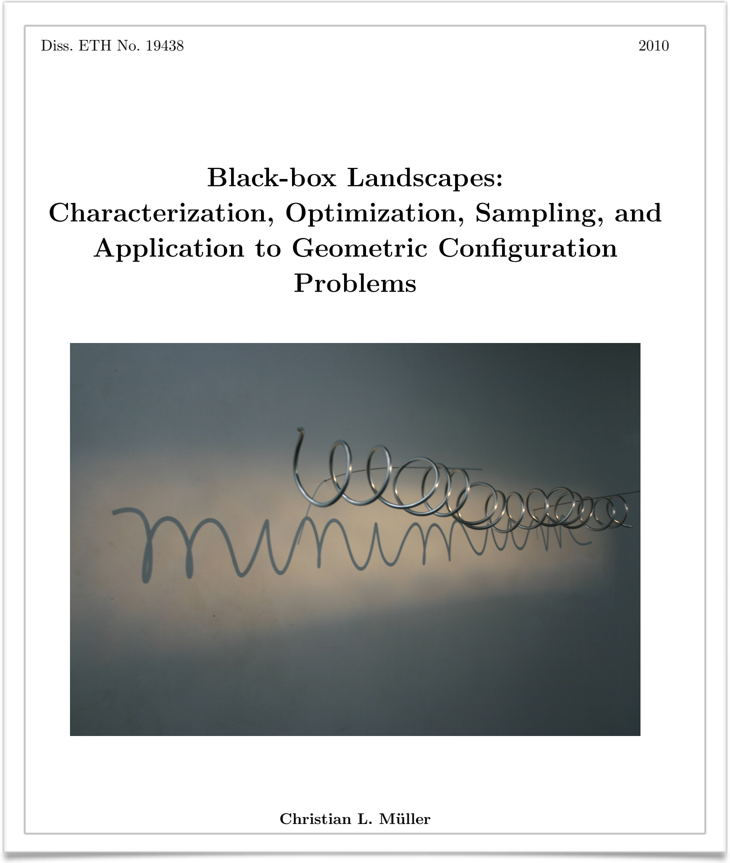

FROM LANDSCAPES TO MATHEMATICAL OPTIMIZATION

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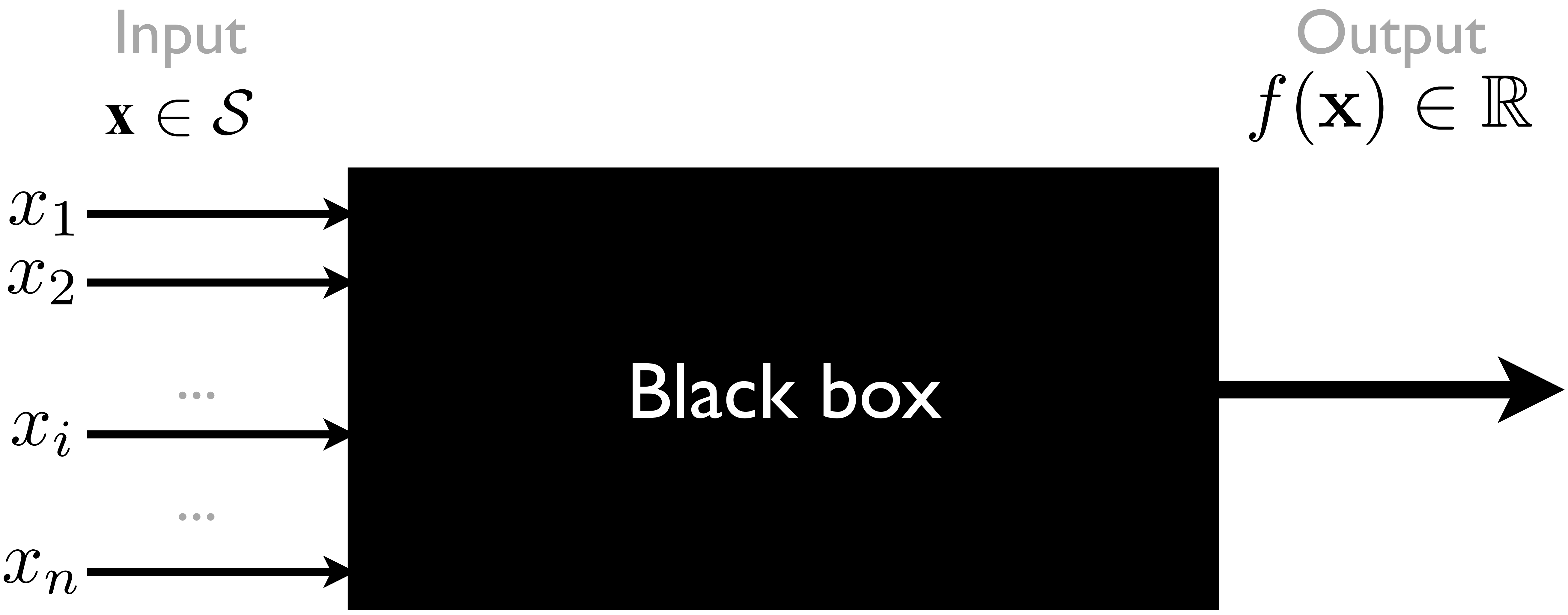

FROM LANDSCAPES TO MATHEMATICAL OPTIMIZATION

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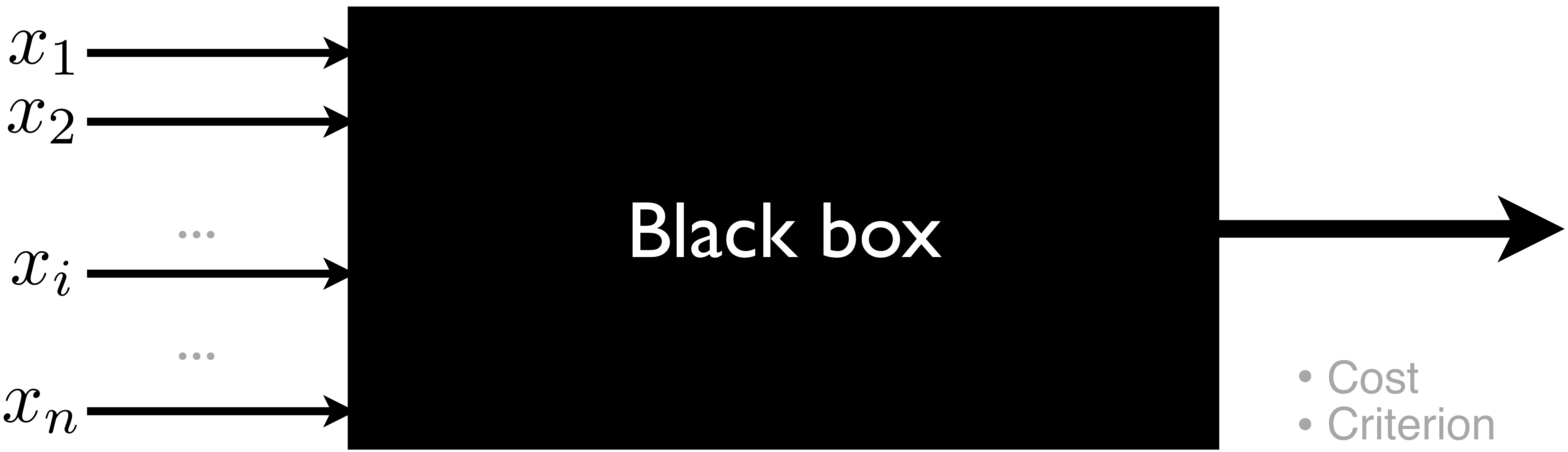
Input

$\mathbf{x} \in \mathcal{S}$

Output

$f(\mathbf{x}) \in \mathbb{R}$



- Variables
- Parameters
- Configuration
- Factors

- Cost
- Criterion
- Objective
- Energy
- Fitness

OPENING UP THE BLACK-BOX: CONTINUOUS OPTIMIZATION PROBLEM

The *standard form* of a continuous optimization problem is[1]

$$\begin{aligned} &\underset{x}{\operatorname{minimize}} && f(x) \\ &\operatorname{subject\ to} && g_i(x) \leq 0, \quad i = 1, \dots, m \\ &&& h_j(x) = 0, \quad j = 1, \dots, p \end{aligned}$$

where

- $f : \mathbb{R}^n \to \mathbb{R}$ is the **objective function** to be minimized over the n-variable vector x,
- $g_i(x) \leq 0$ are called **inequality constraints**
- $h_j(x) = 0$ are called **equality constraints**, and
- $m \geq 0$ and $p \geq 0$.

If $m = p = 0$, the problem is an unconstrained optimization problem. By convention, the standard form defines a **minimization problem**. A **maximization problem** can be treated by negating the objective function.

wikipedia

OPENING UP THE BLACK BOX

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- What do you know about $\mathbf{x} \in \mathcal{S}$?
- What is the dimensionality of the problem?
- Does the function $f(\mathbf{x})$ have special properties? What are good properties?
- Can you evaluate gradients or higher-order information of the function?

OPENING UP THE BLACK BOX

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- What is the dimensionality of the problem?
- Does the function $f(\mathbf{x})$ have special properties? What are good properties?
- Can you evaluate gradients or higher-order information of the function?
- How much does it cost (in computation time/experimental time) to evaluate the function? How often can you evaluate it?
- Is the function value deterministic? Is it stochastic?
- How accurate does the solution need to be?
- …

PURE RANDOM SEARCH

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Rastrigin, L.A. (1963). "The convergence of the random search method in the extremal control of a many parameter system". *Automation and Remote Control*. **24** (10): 1337–1342.

PURE RANDOM SEARCH

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- Useful when your input domain is simple, e.g., a hyper-cube
- Only requires function evaluations, no other information needed
- Better coverage than grid search

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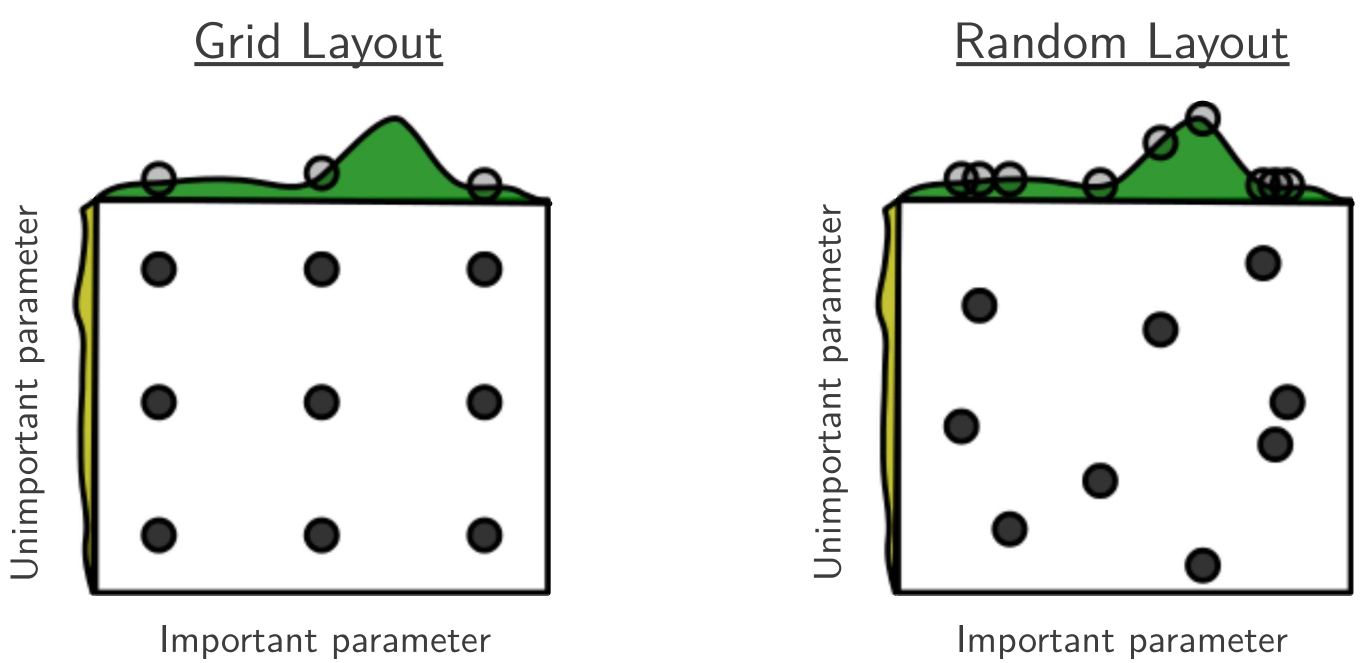

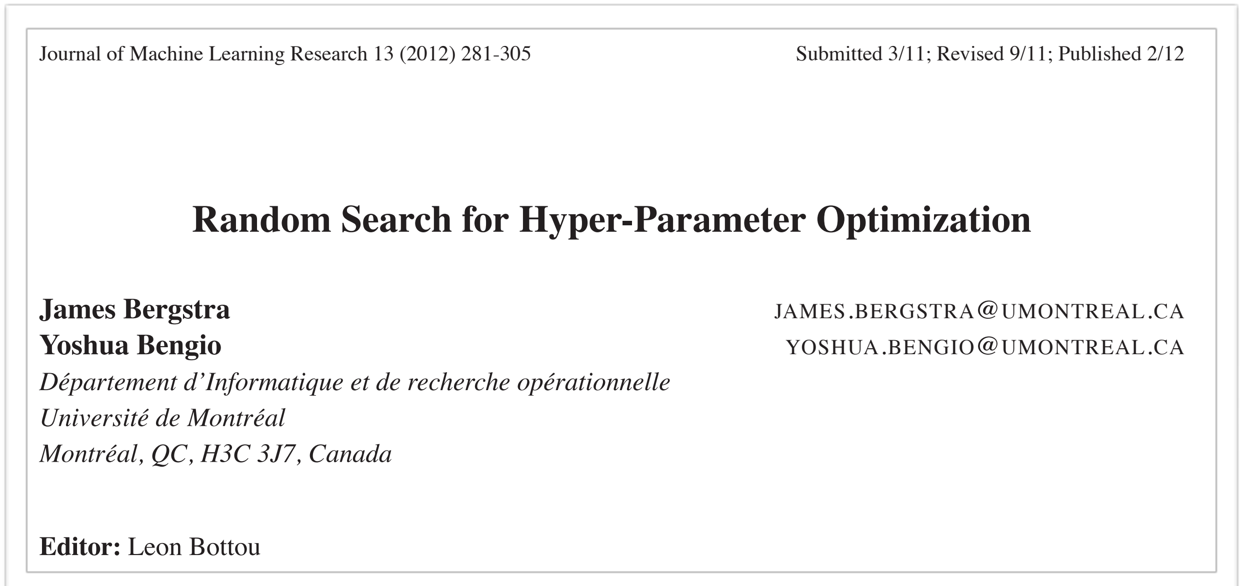
Journal of Machine Learning Research 13 (2012) 281-305 Submitted 3/11; Revised 9/11; Published 2/12

Random Search for Hyper-Parameter Optimization

James Bergstra JAMES.BERGSTRA@UMONTREAL.CA
Yoshua Bengio YOSHUA.BENGIO@UMONTREAL.CA
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Editor: Leon Bottou

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QUASI-RANDOM SEARCH

Sobol,I.M. (1967), "Distribution of points in a cube and approximate evaluation of integrals". *Zh. Vych. Mat. Mat. Fiz.* **7**: 784–802 (in Russian); *U.S.S.R Comput. Maths. Math. Phys.* **7**: 86–112 (in English).

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- Use quasi-random points rather than random ones to cover the space
- Better space-filling properties
- Works well for up to n=50 dimensions
- (Scrambled) Sobol sequences are good

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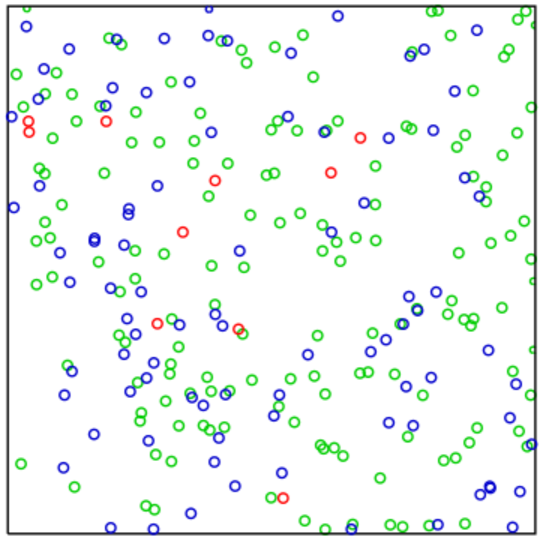
Pseudo-random points



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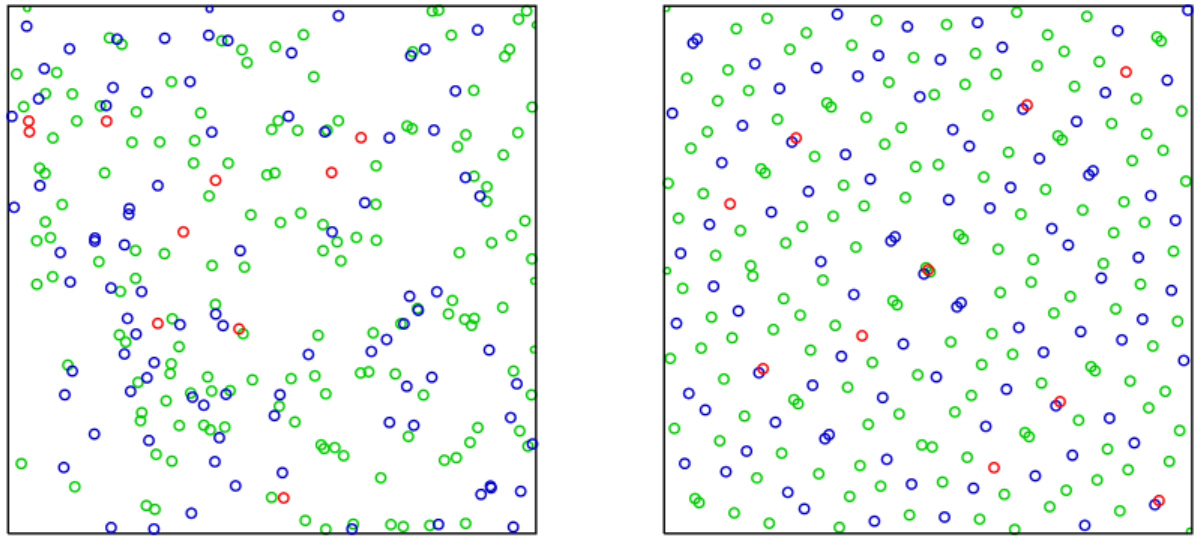

QUASI-RANDOM SEARCH

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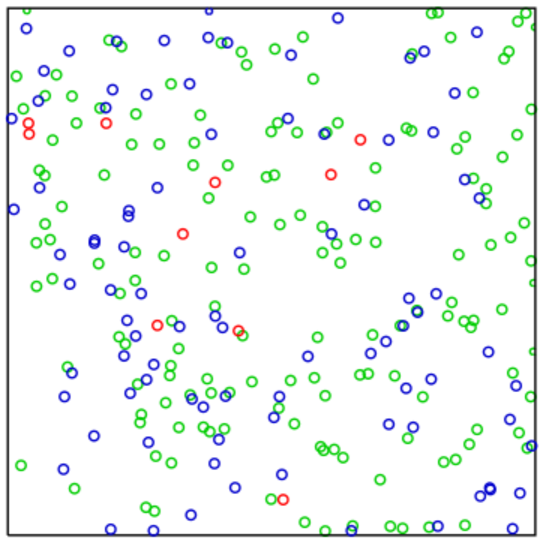

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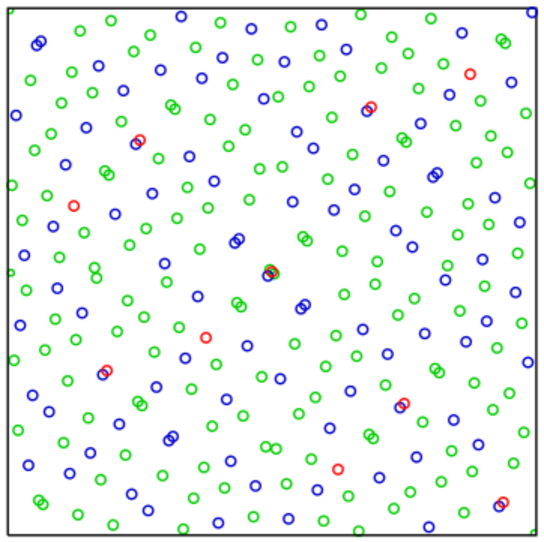

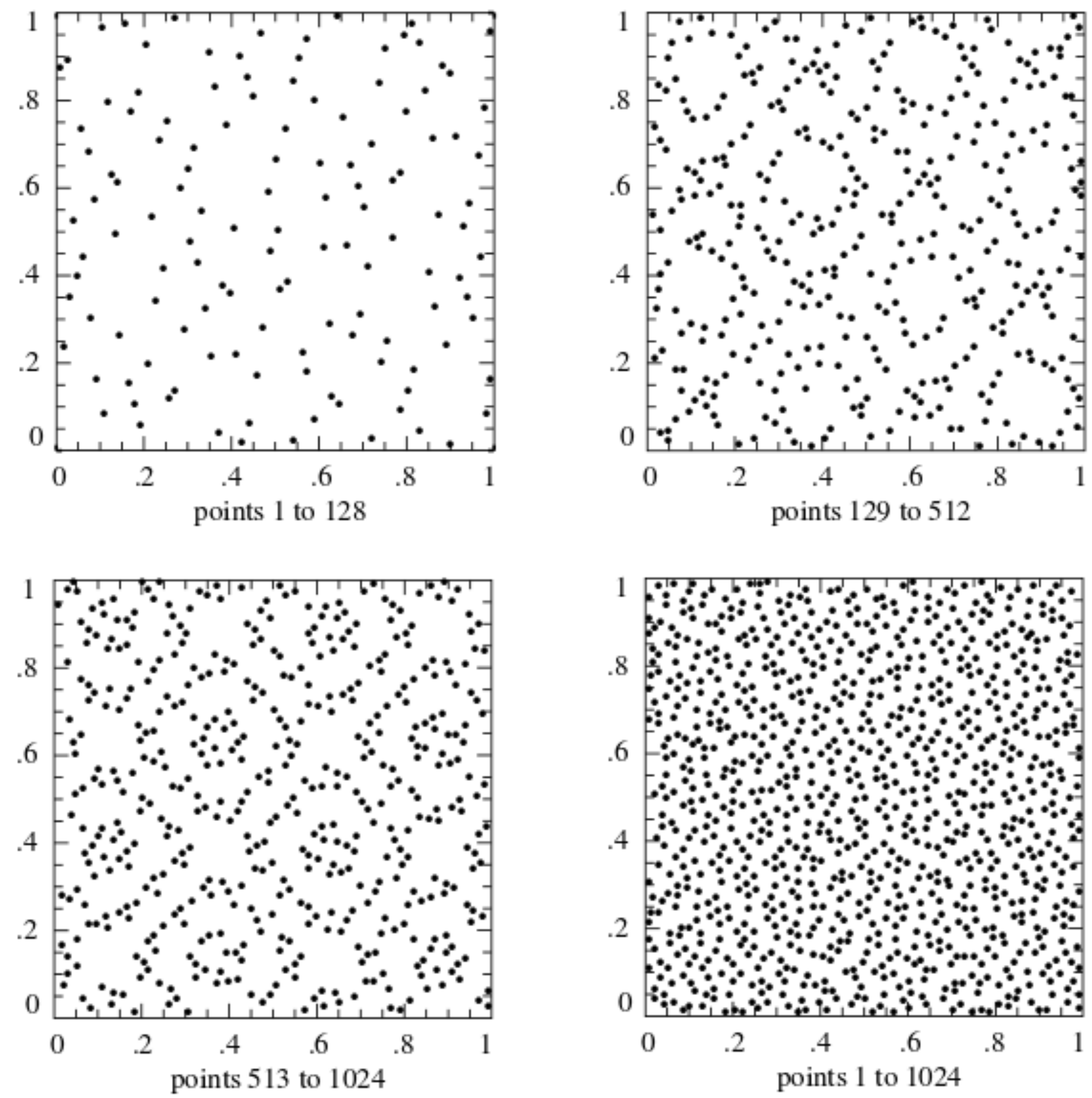

DERIVATIVE-FREE OPTIMIZATION AND EVOLUTION STRATEGIES

- Use it when you know very little about the function and the function is **not costly**, i.e., you can evaluate $O(n^2)$ points
- Input domain is simple, e.g. a hyper-cube, not too high-dimensional
- Typically used in **simulation-based optimization** where only function evaluations are available
- Popular method: Nelder-Mead Simplex method (not recommended), Pattern search, Covariance Matrix Adaptation ES

CMA-ES resources

http://www.cmap.polytechnique.fr/~nikolaus.hansen/

GRADIENT-FREE OPTIMIZATION WITH CMA-ES

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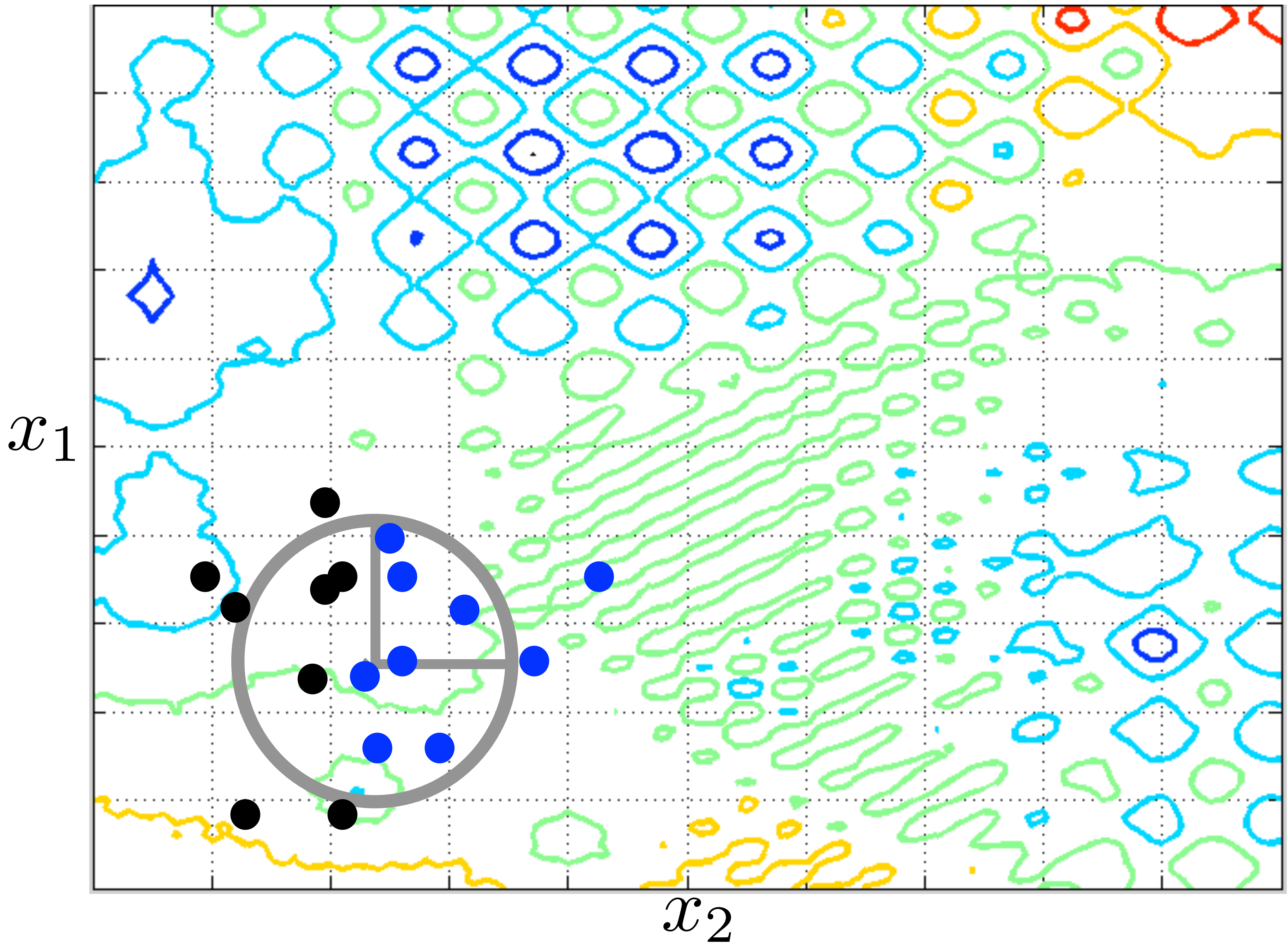

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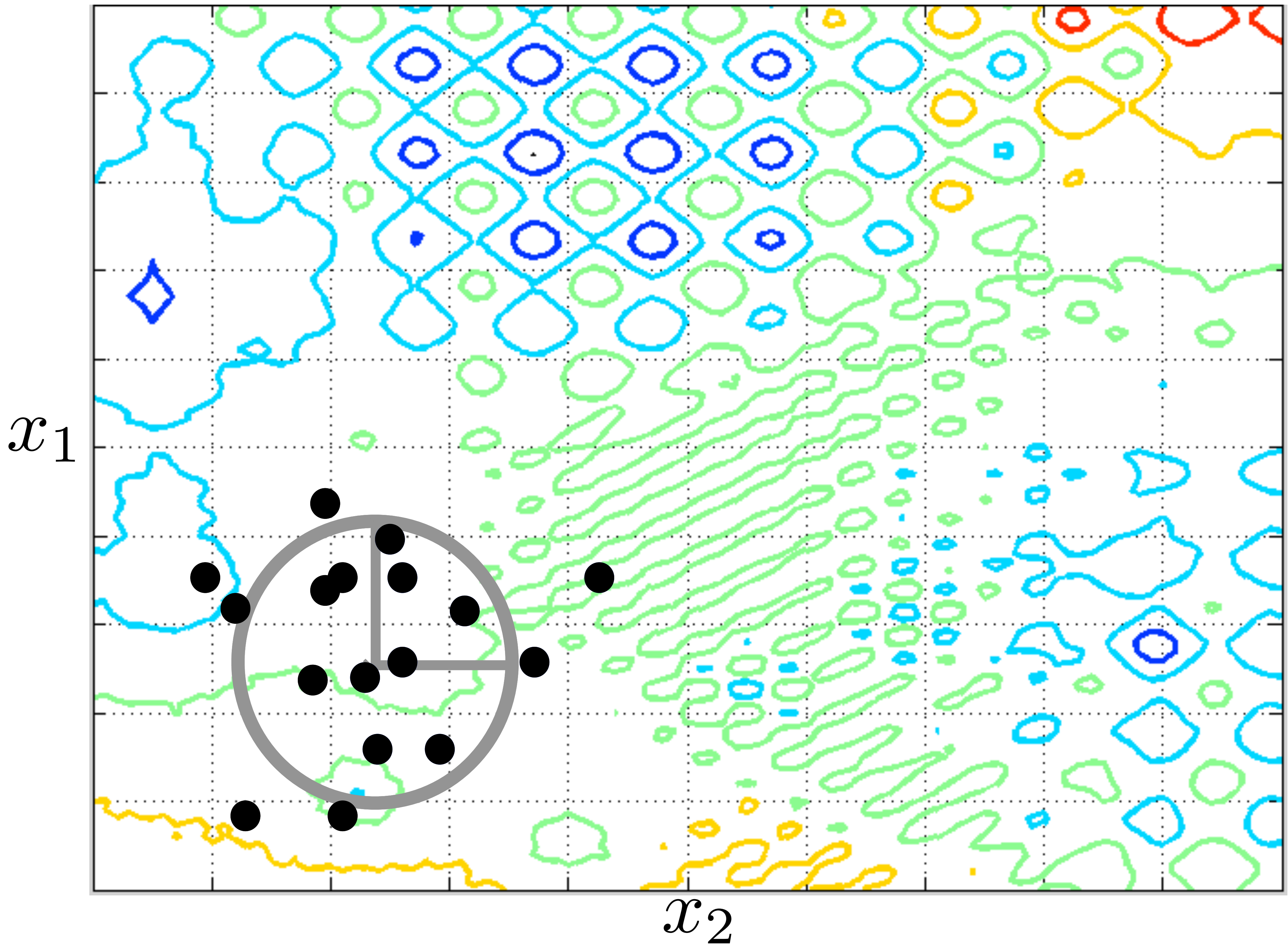

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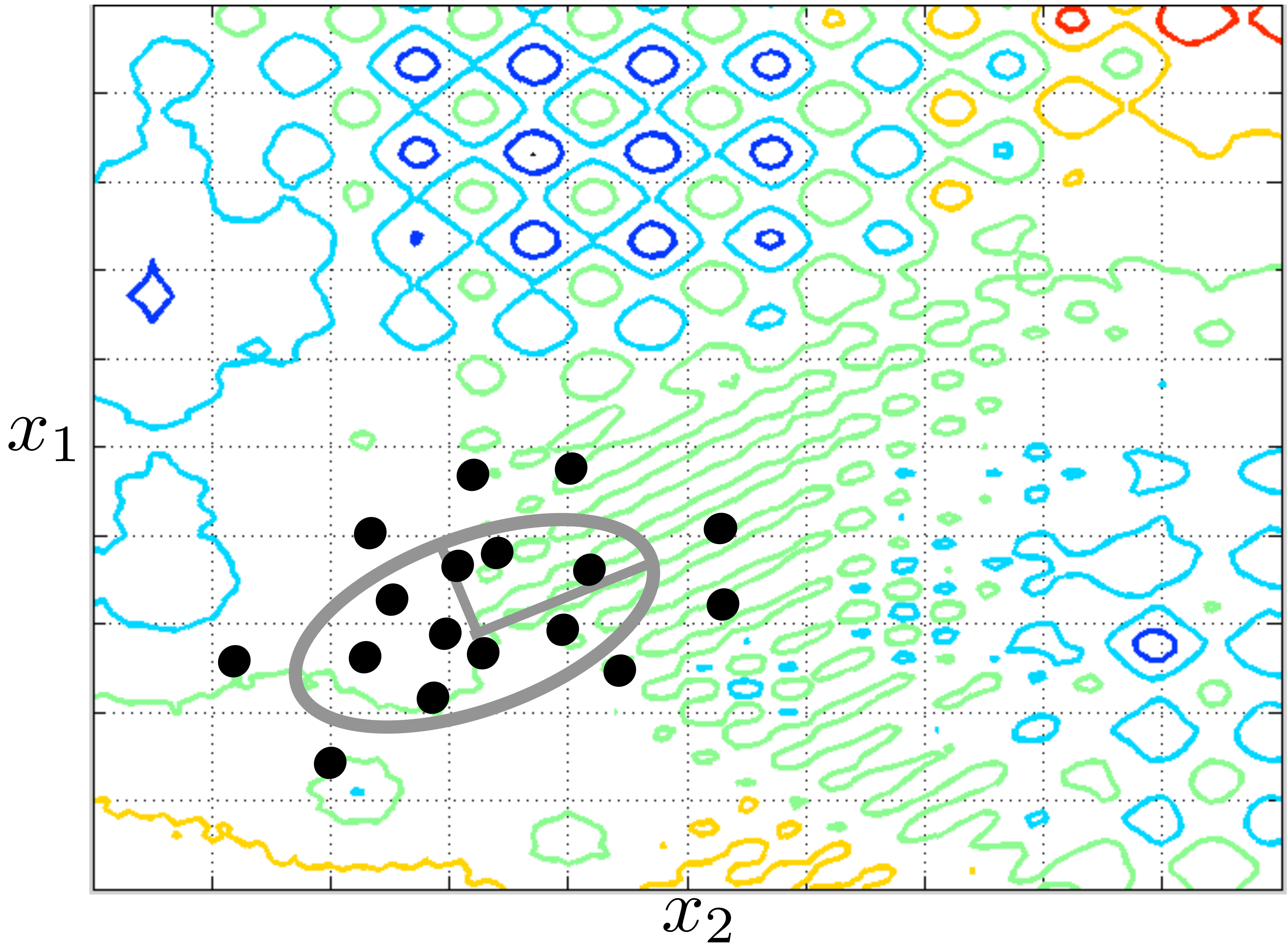

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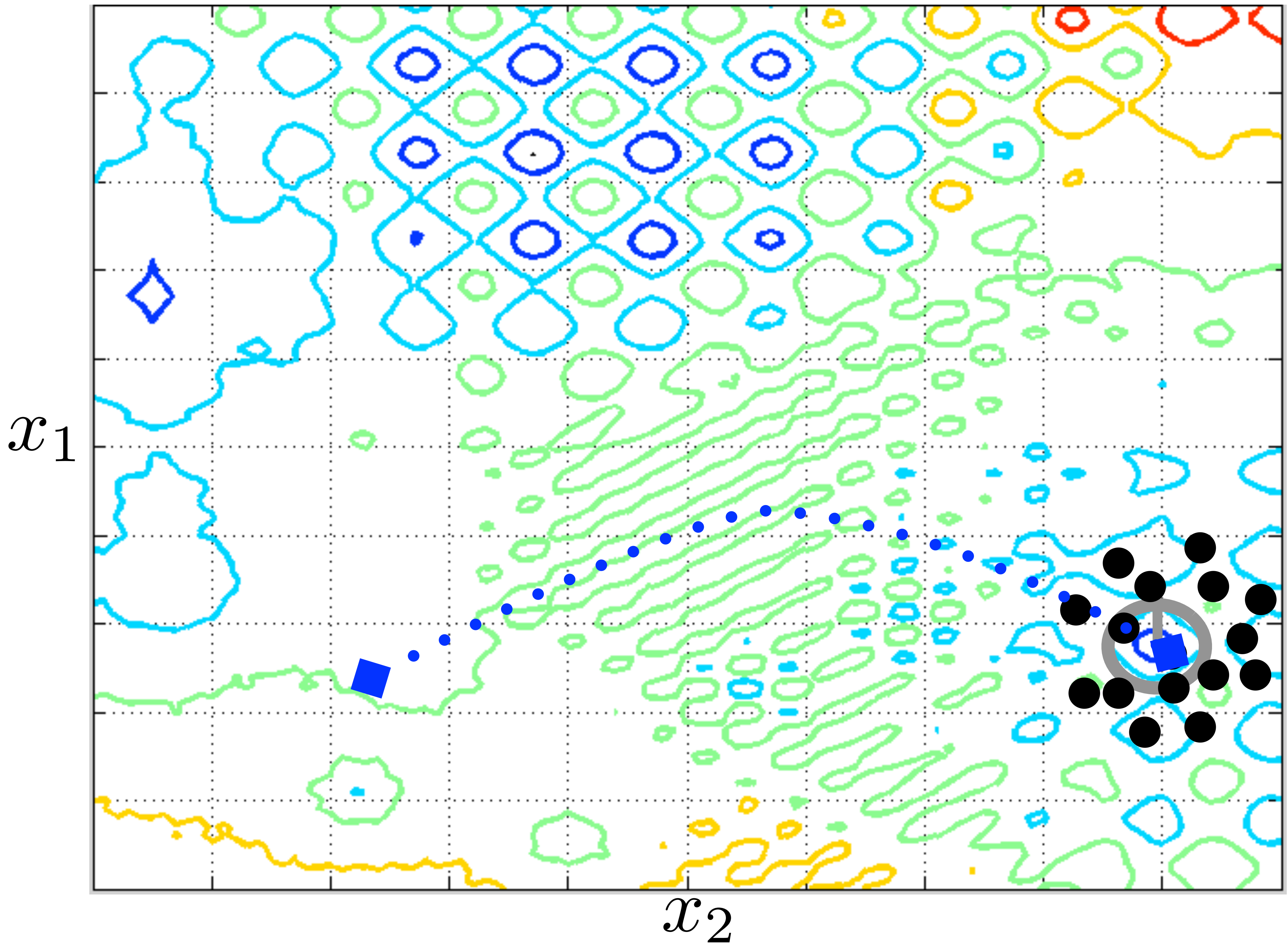

The ($\mu/\mu_w,\lambda$)-CMA-ES in mathematical terms

Sampling

$$\mathbf{x}_k^{(g+1)} \sim \mathbf{m}^{(g)} + \sigma^{(g)} \mathcal{N}\left(\mathbf{0}, \mathbf{C}^{(g)}\right) \quad \text{for } k = 1, \ldots, \lambda.$$

GRADIENT-FREE OPTIMIZATION WITH CMA-ES

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Evaluation

Calculate fitness of all λ individuals and sort them

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Selection

$$\mathbf{m}^{(g+1)} = \sum_{i=1}^{\mu} w_i \mathbf{x}_{i:\lambda}^{(g+1)} \qquad \sum_{i=1}^{\mu} w_i = 1, \quad w_1 \geq w_2 \geq \ldots \geq w_\mu > 0$$

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Recombination Adaptation

$$\mathbf{C}^{(g+1)} = (1 - c_{\text{cov}})\mathbf{C}^{(g)} + \frac{c_{\text{cov}}}{\mu_{\text{cov}}} \underbrace{\mathbf{p}_c^{(g+1)} \mathbf{p}_c^{(g+1)^T}}_{\text{rank-one-update}} + c_{\text{cov}} \left(1 - \frac{1}{\mu_{\text{cov}}}\right) \times \underbrace{\sum_{i=1}^{\mu} w_i \mathbf{y}_{i:\lambda}^{(g+1)} \left(\mathbf{y}_{i:\lambda}^{(g+1)}\right)^T}_{\text{rank-}\mu\text{-update}},$$

GRADIENT-FREE OPTIMIZATION WITH CMA-ES

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Recombination
Adaptation

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$$\sigma^{(g+1)} = \sigma^{(g)} \exp\left(\frac{c_\sigma}{d_\sigma}\left(\frac{||\mathbf{p}_\sigma^{(g+1)}||}{E||\mathcal{N}(\mathbf{0}, \mathbf{I})||} - 1\right)\right).$$

A NOTE ON DESIGN PRINCIPLES FOR OPTIMIZATION HEURISTICS

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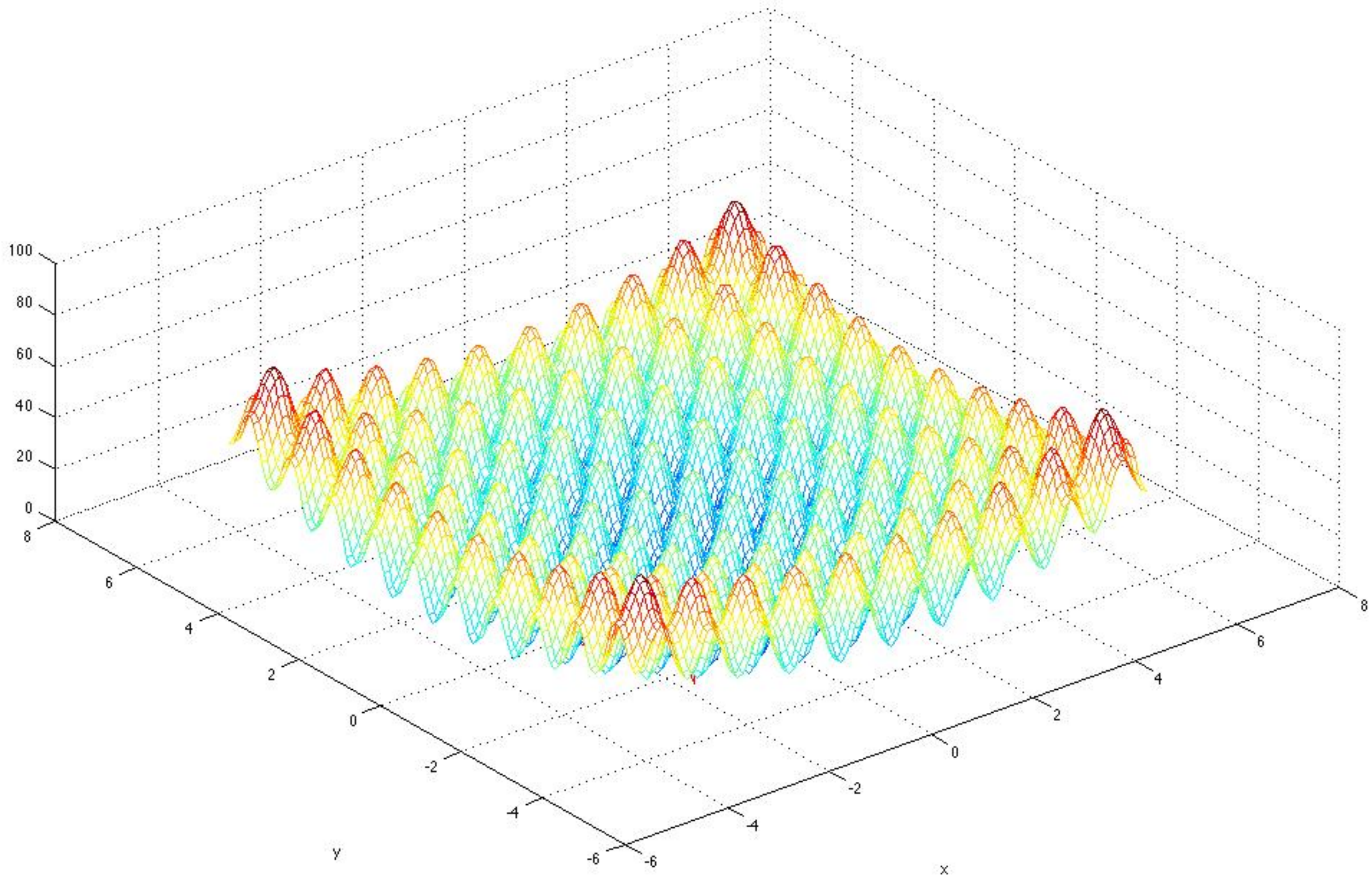
- Use invariance (symmetry) principles as much as possible
- CMA-ES is invariant to affine transformations of the domain
- CMA-ES is invariant to monotone transformations of the objective function

CMA-ES ON RASTRIGIN FUNCTION

Rastrigin's Function

$$f(\vec{x}) = 10 \times n + \sum_{i=1}^{n} \left(x_i^2 - 10 \times \cos(2\pi x_i) \right)$$



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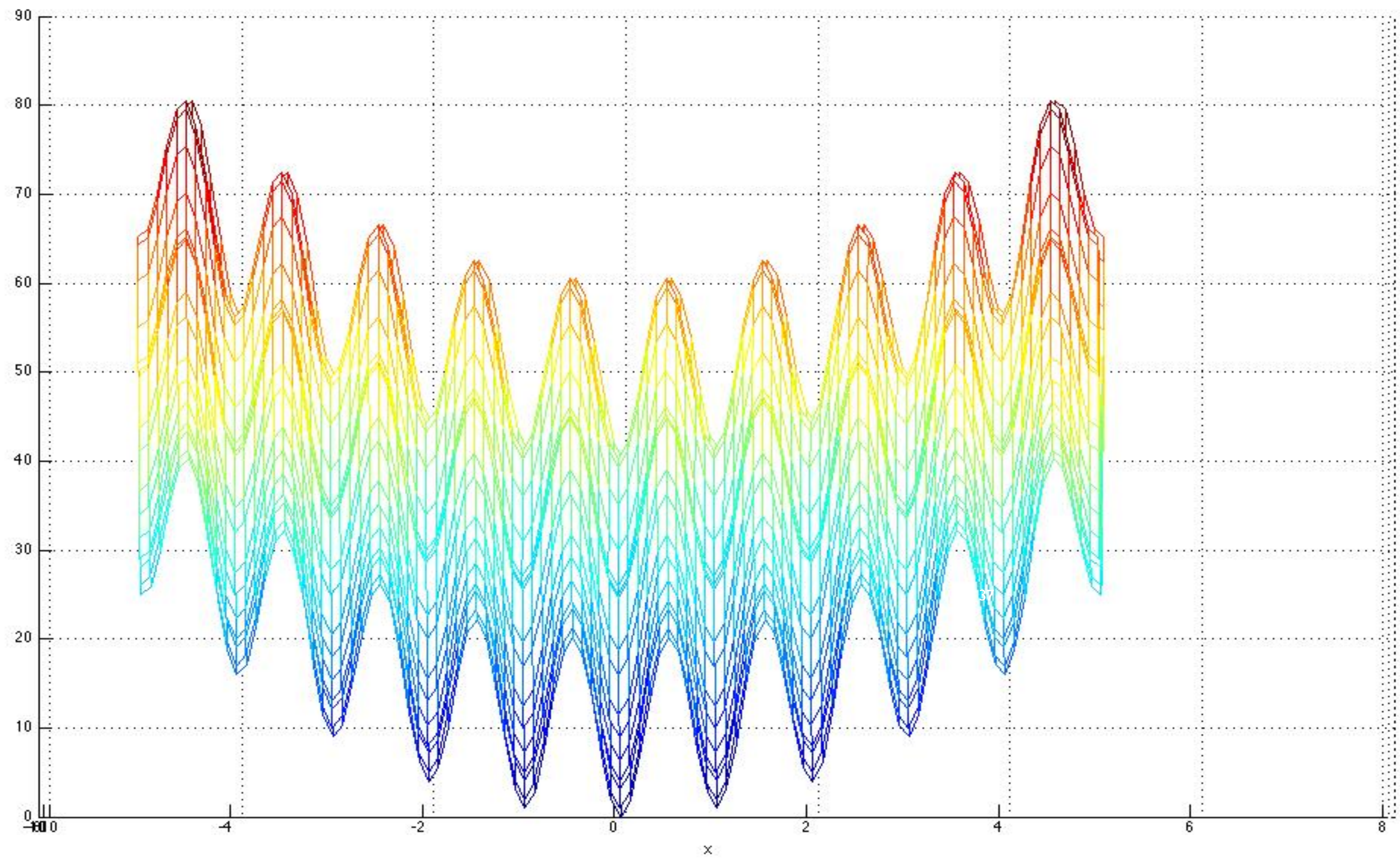

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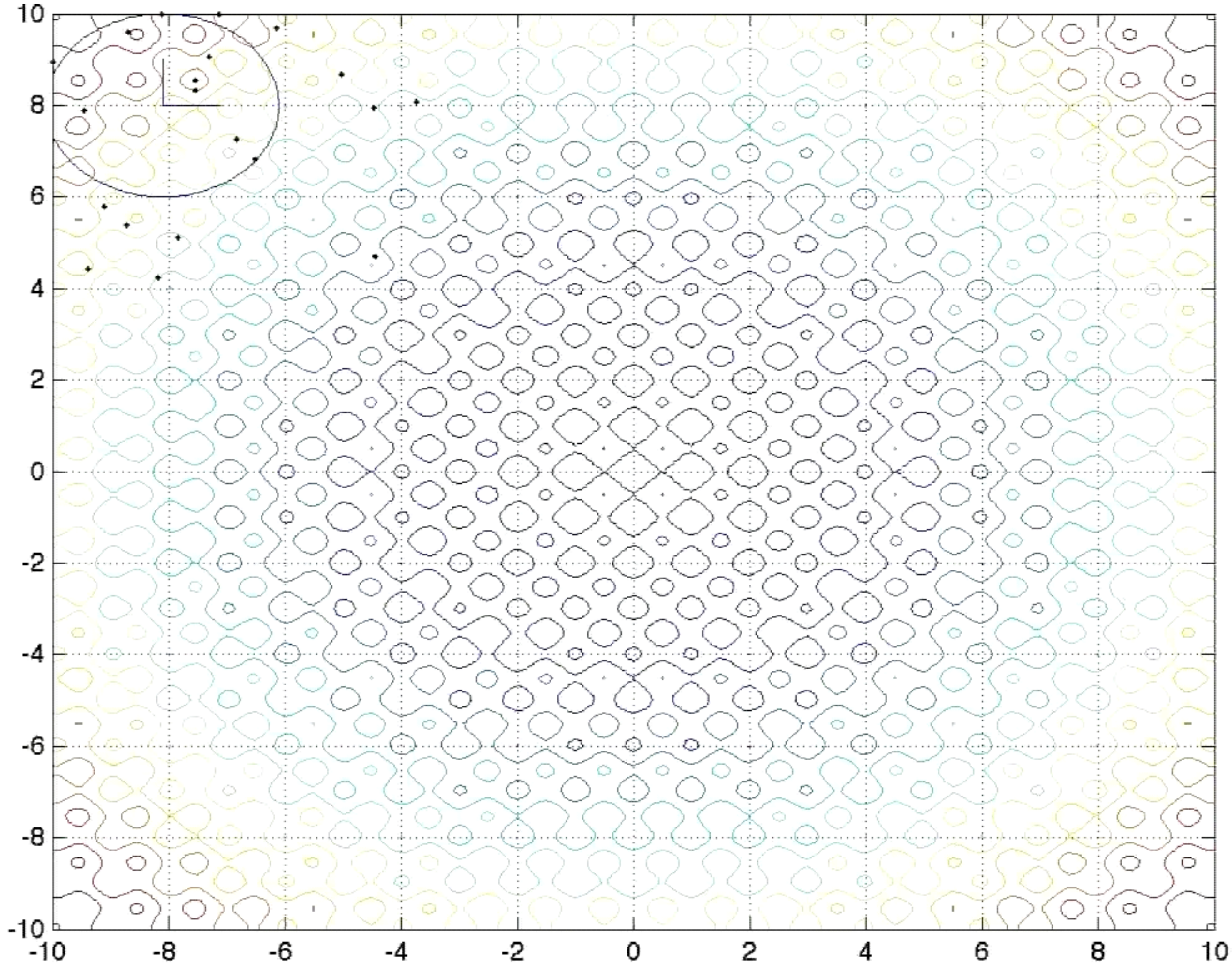

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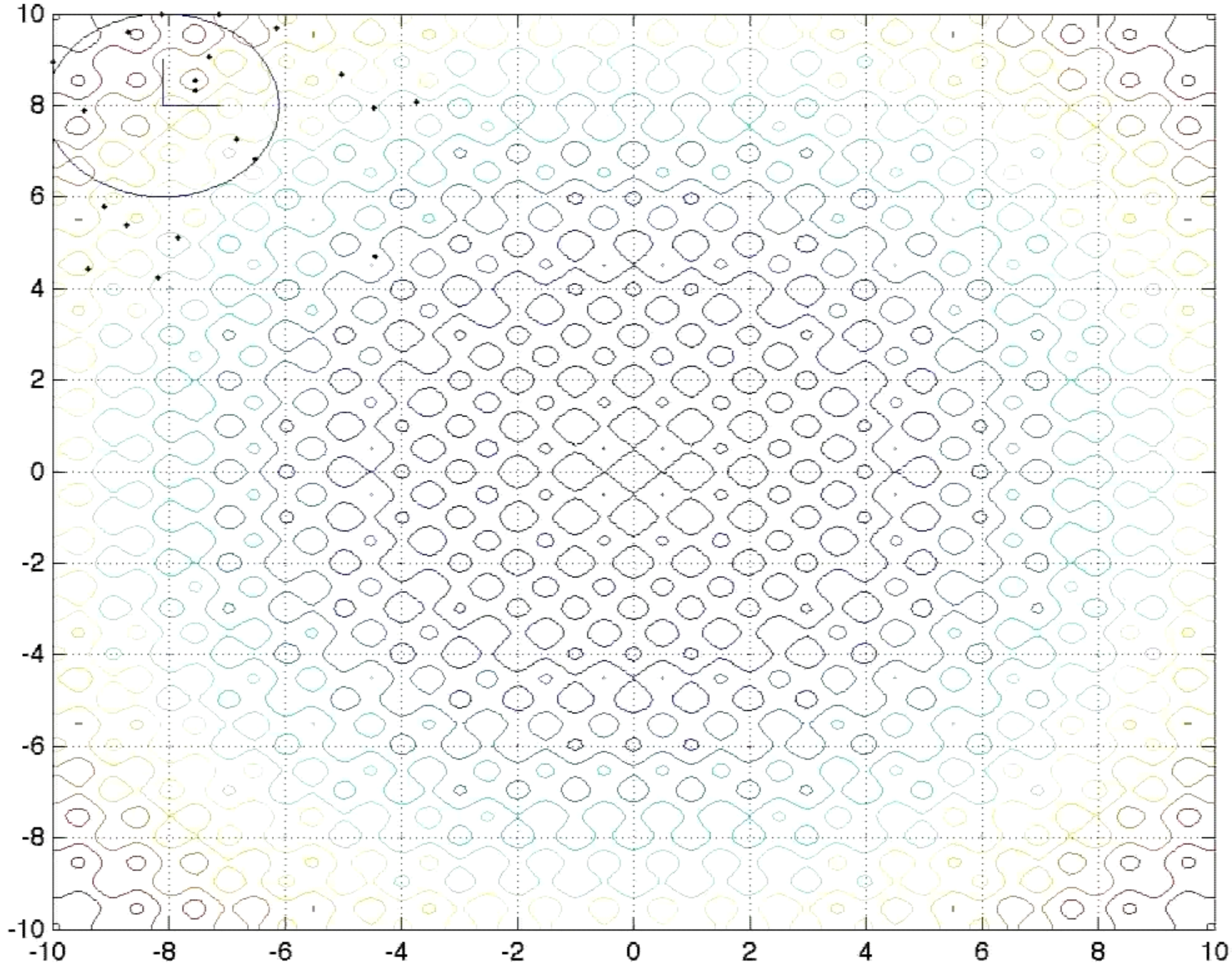
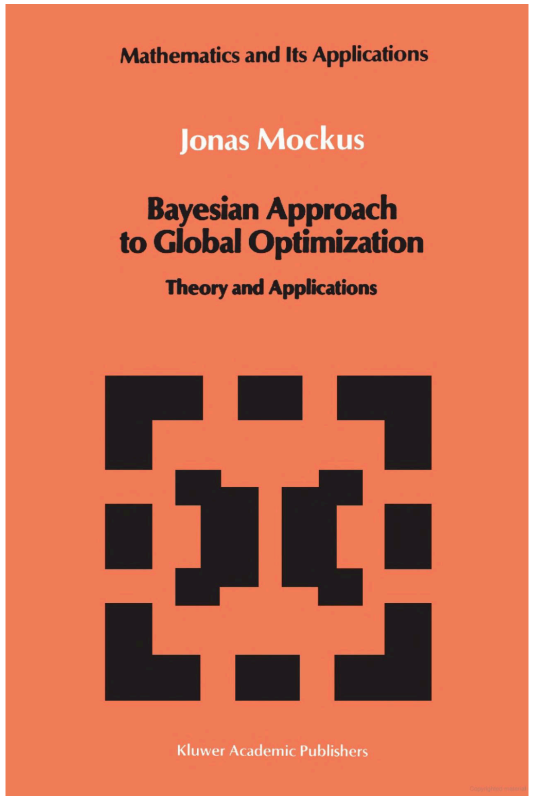


BAYESIAN OPTIMIZATION

- Bayesian optimization is a type of sequential design scheme
- An acquisition function guides the generation of a new function evaluation that balances exploration and exploitation
- Builds a surrogate model of the function (often with Gaussian Processes) (see Directed Evolution example)
- Use it when you know very little about the function and the function is **costly** and low-dimensional
- Input domain is simple, e.g. a hyper-cube



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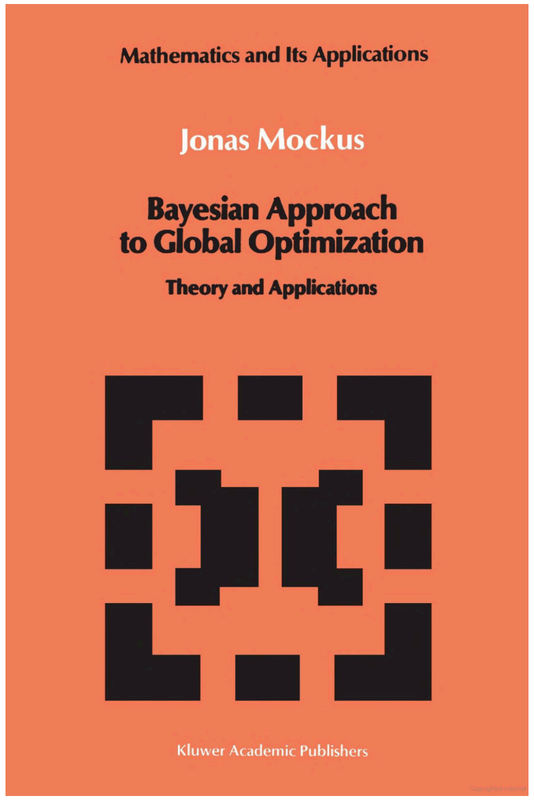

Practical Bayesian Optimization of Machine Learning Algorithms

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BAYESIAN OPTIMIZATION

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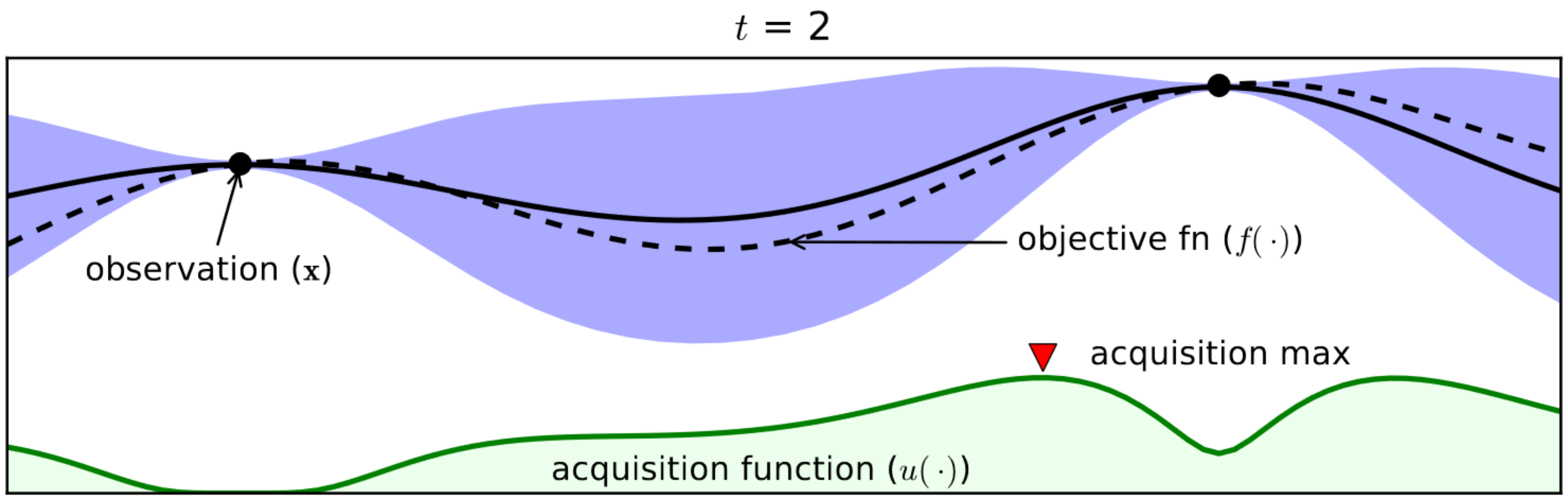

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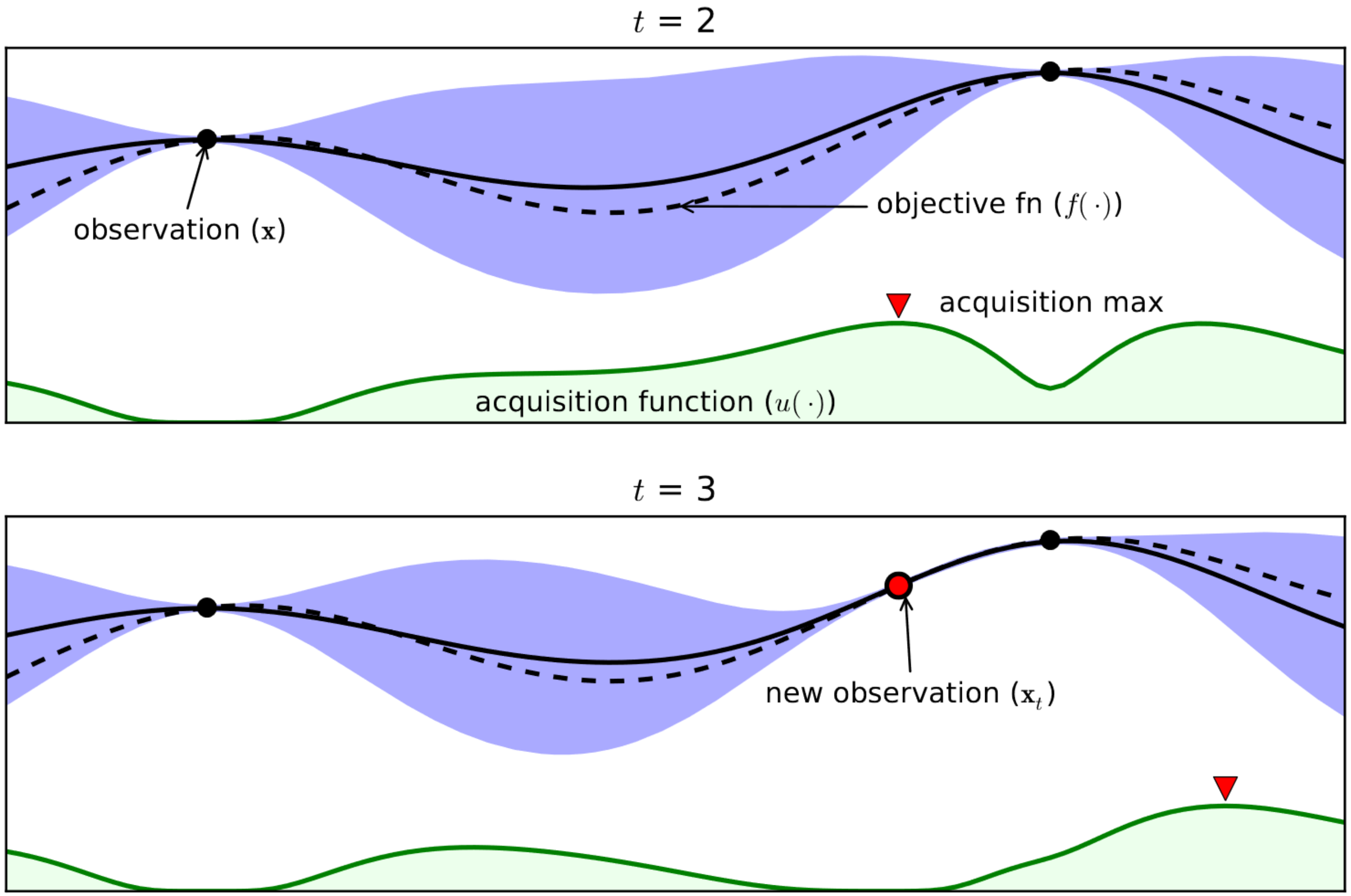

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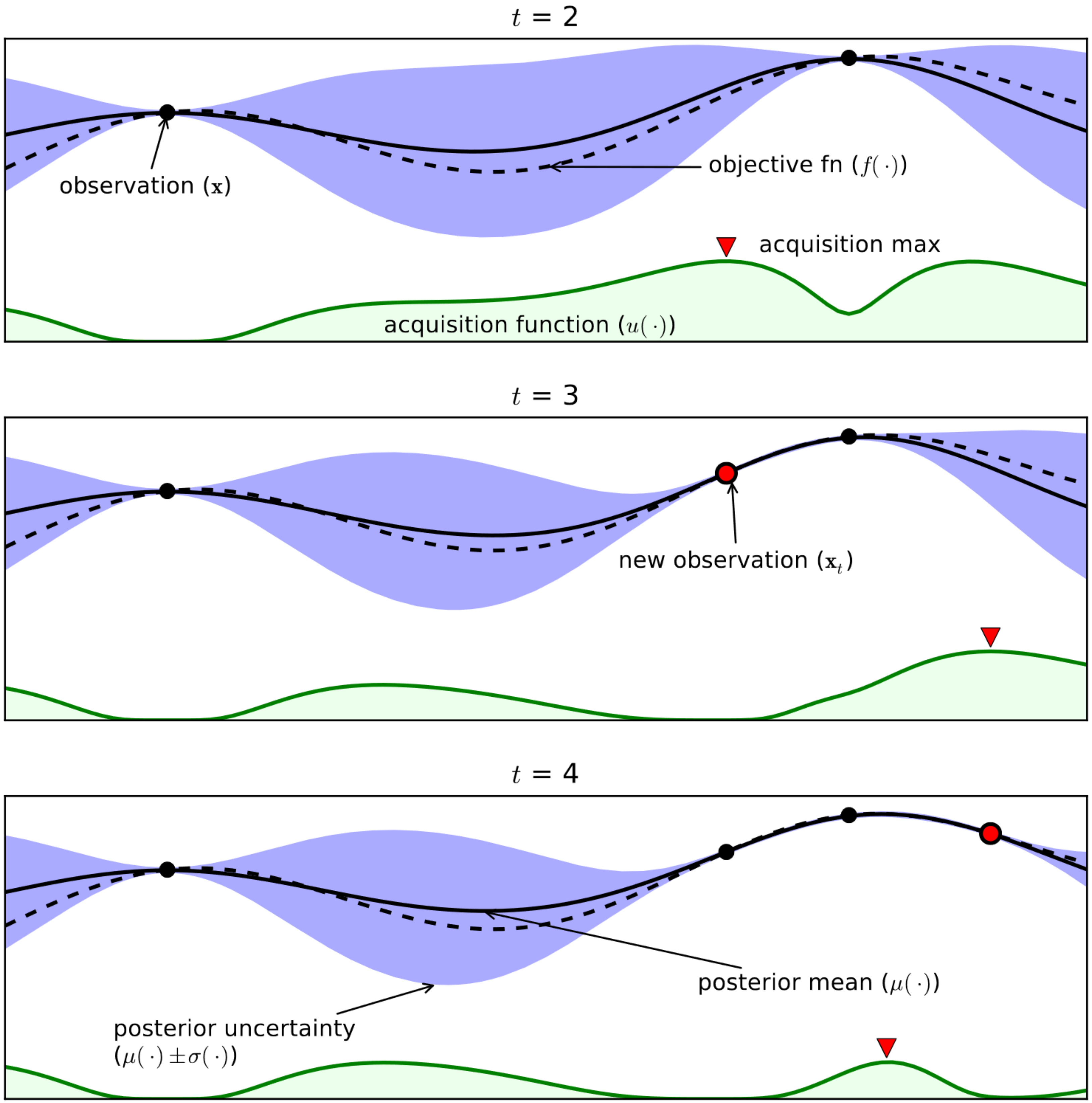

GRADIENT-BASED OPTIMIZATION

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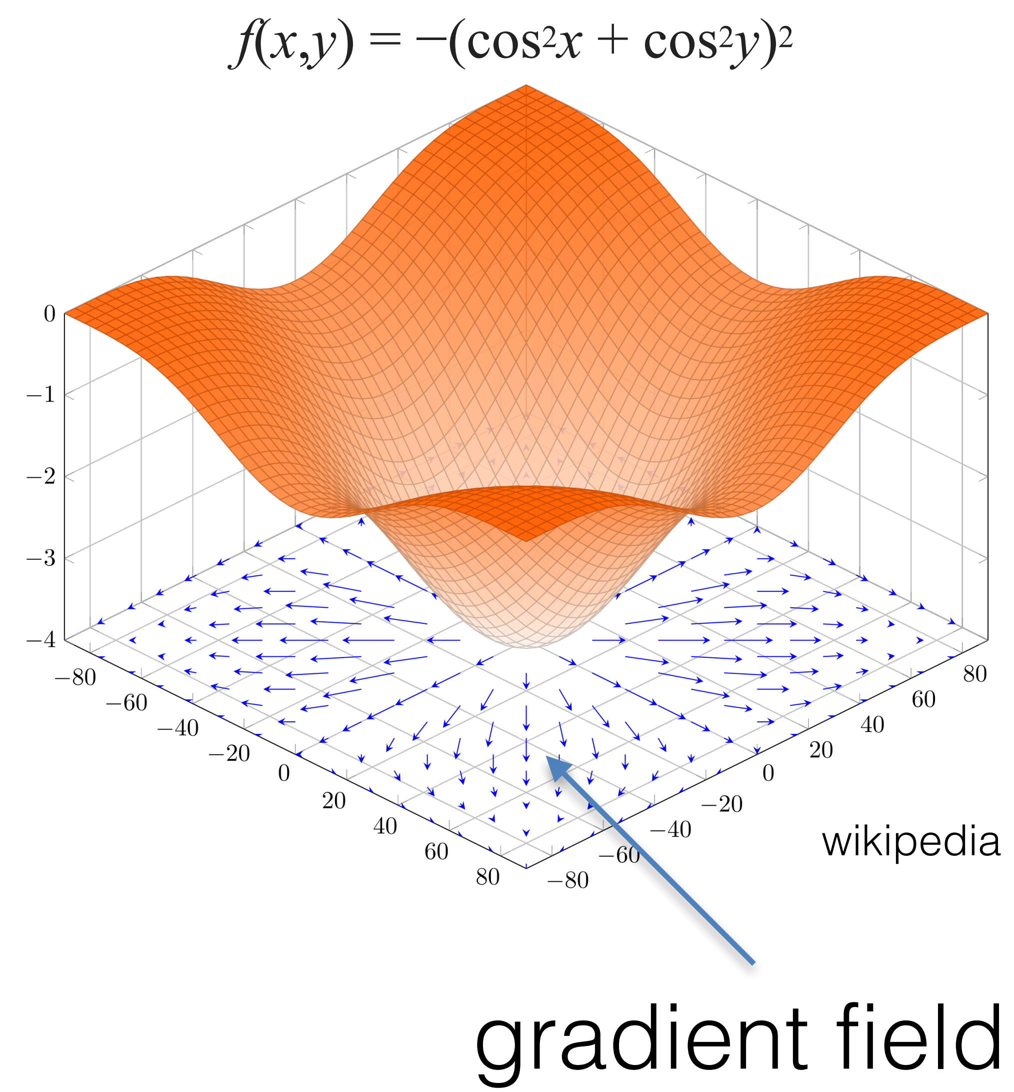

GRADIENT-BASED OPTIMIZATION

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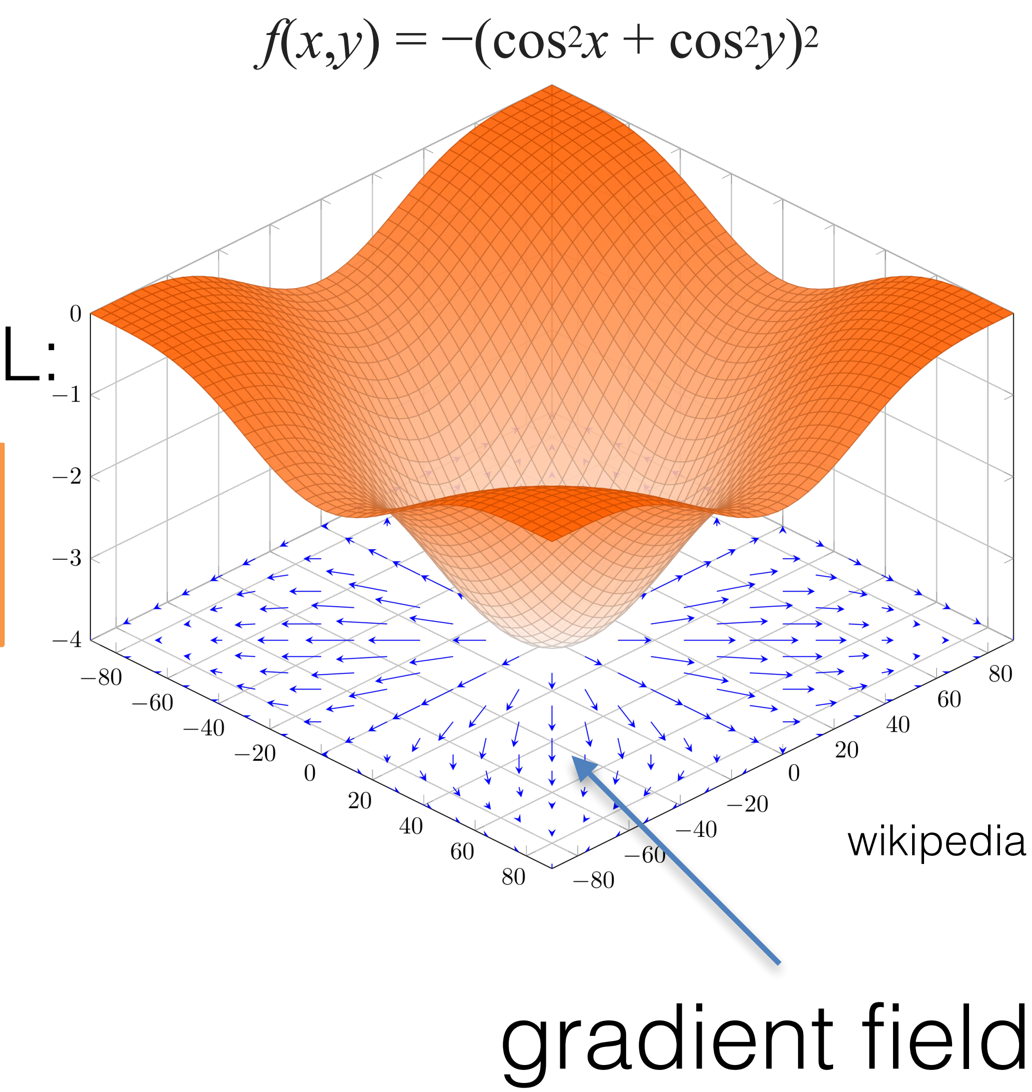
- The gradient of the function f is available
- The function can be high-dimensional
- The function is smooth with Lipschitz constant L:

$$f(\mathbf{y}) \leq f(\mathbf{x}) + \nabla f(\mathbf{x})^\top (\mathbf{y} - \mathbf{x}) + \frac{L}{2}\|\mathbf{x} - \mathbf{y}\|^2, \quad \forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^d.$$



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- Gradient descent:

Goal: Find $\mathbf{x} \in \mathbb{R}^d$ such that

$$f(\mathbf{x}) - f(\mathbf{x}^\star) \leq \varepsilon.$$

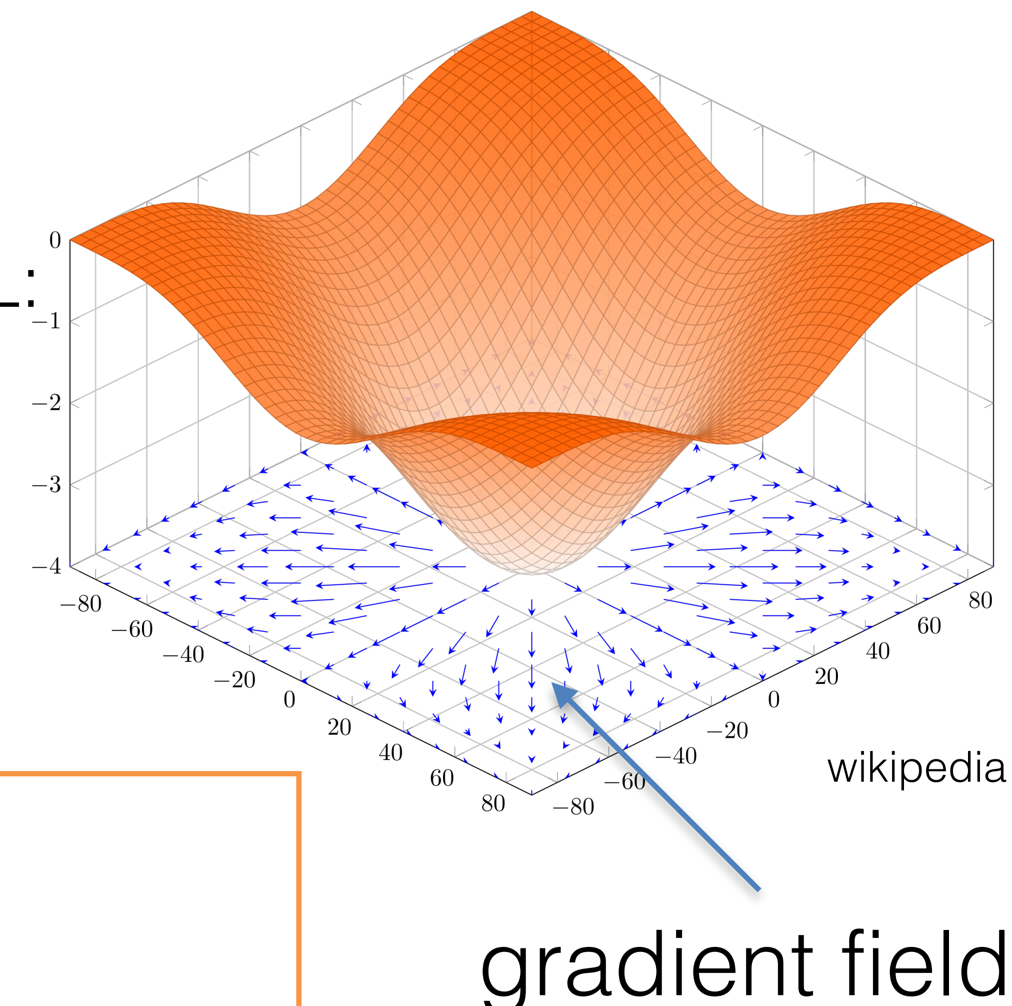
Note that there can be several minima $\mathbf{x}_1^\star \neq \mathbf{x}_2^\star$ with $f(\mathbf{x}_1^\star) = f(\mathbf{x}_2^\star)$.

Iterative Algorithm:

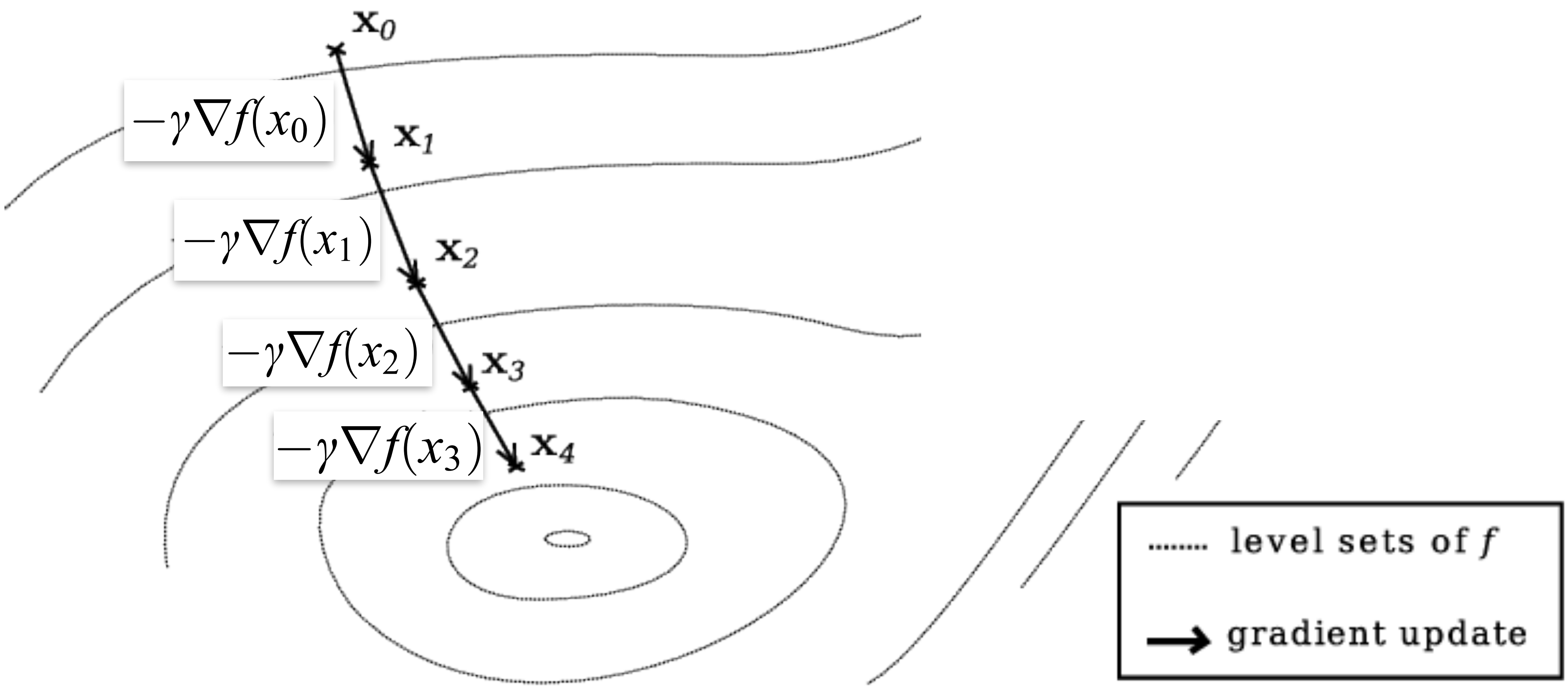
$$\mathbf{x}_{t+1} := \mathbf{x}_t - \gamma \nabla f(\mathbf{x}_t),$$

for **timesteps** $t = 0, 1, \ldots,$ and **stepsize** $\gamma \geq 0$.

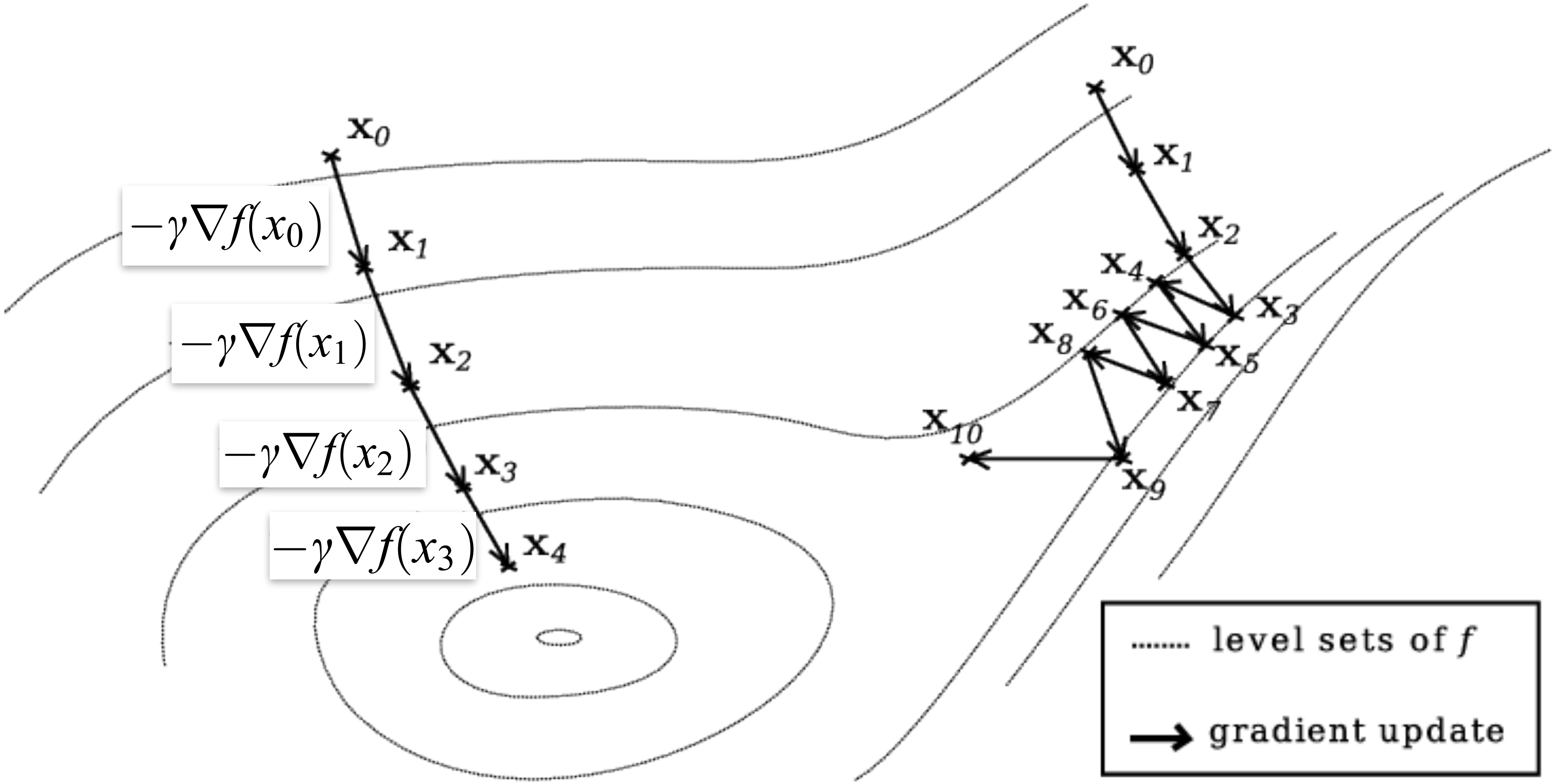
$f(x,y) = -(\cos^2 x + \cos^2 y)^2$



GRADIENT-BASED OPTIMIZATION



GRADIENT-BASED OPTIMIZATION



GRADIENT DESCENT RULES THE WORLD!!!

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- When the function is VERY high-dimensional, only stochastic gradients are computable (see Elad's talk)
- Adaptive gradient descent (ADAGRAD) or Nesterov acceleration is a standard workhorse in large-scale optimization in (online) machine learning
- Stochastic, batch, mini-batch gradient descent (with adaptive step sizes), such as ADAM, is the standard optimizer for Deep NN

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Journal of Machine Learning Research 12 (2011) 2121-2159 Submitted 3/10; Revised 3/11; Published 7/11

Adaptive Subgradient Methods for Online Learning and Stochastic Optimization*

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Published as a conference paper at ICLR 2015

ADAM: A METHOD FOR STOCHASTIC OPTIMIZATION

Diederik P. Kingma* University of Amsterdam, OpenAI dpkingma@openai.com
Jimmy Lei Ba* University of Toronto jimmy@psi.utoronto.ca

ABSTRACT

We introduce *Adam*, an algorithm for first-order gradient-based optimization of stochastic objective functions, based on adaptive estimates of lower-order moments. The method is straightforward to implement, is computationally efficient, has little memory requirements, is invariant to diagonal rescaling of the gradients, and is well suited for problems that are large in terms of data and/or parameters. The method is also appropriate for non-stationary objectives and problems with very noisy and/or sparse gradients. The hyper-parameters have intuitive interpretations and typically require little tuning. Some connections to related algorithms, on which *Adam* was inspired, are discussed. We also analyze the theoretical convergence properties of the algorithm and provide a regret bound on the convergence rate that is comparable to the best known results under the online convex optimization framework. Empirical results demonstrate that Adam works well in practice and compares favorably to other stochastic optimization methods. Finally, we discuss *AdaMax*, a variant of *Adam* based on the infinity norm.

GRADIENT-BASED OPTIMIZATION

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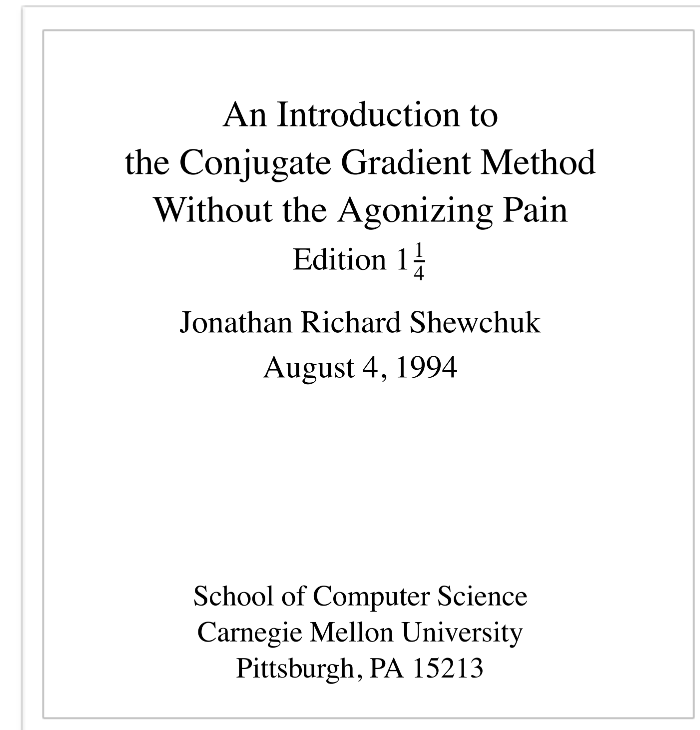
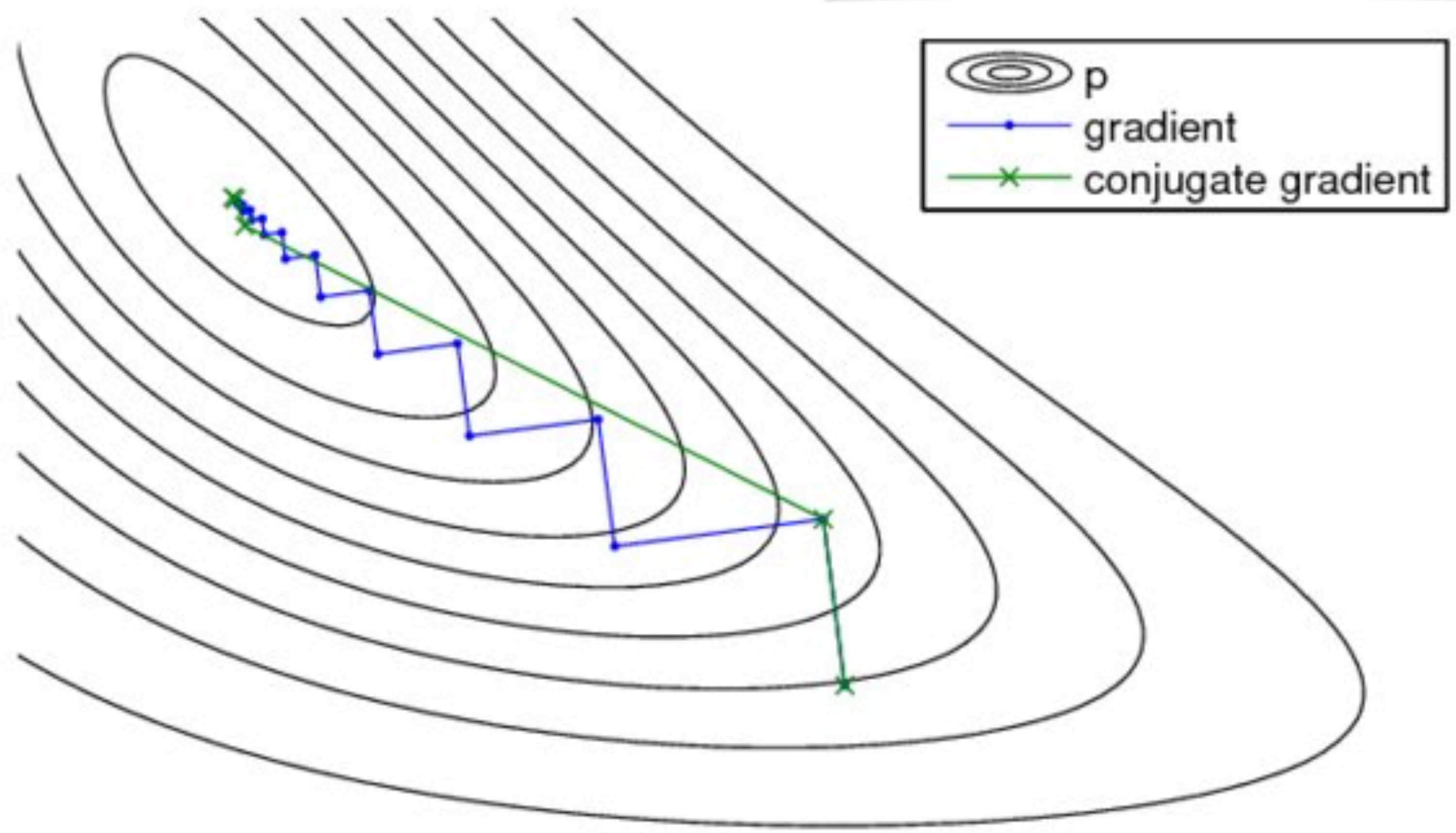
- Extension: **Nonlinear conjugate** gradient descent
- Use consecutive gradient directions to generate better search directions (conjugate directions)
- Use line search along the new search directions
- Keywords: Fletcher-Reeves, Polak–Ribière


An Introduction to
the Conjugate Gradient Method
Without the Agonizing Pain
Edition $1\frac{1}{4}$

Jonathan Richard Shewchuk
August 4, 1994

School of Computer Science
Carnegie Mellon University
Pittsburgh, PA 15213



SECOND-ORDER OPTIMIZATION

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- The gradient and the **Hessian** of the function f is available, i.e. local curvature information
- The function is moderately high-dimensional
- The function is smooth with Lipschitz constant L

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- The function is moderately high-dimensional
- The function is smooth with Lipschitz constant L
- Gradient descent:

General update scheme:

$$\mathbf{x}_{t+1} = \mathbf{x}_t - H(\mathbf{x}_t)\nabla f(\mathbf{x}_t),$$

where $H(\mathbf{x}) \in \mathbb{R}^{d\times d}$ is some matrix.

Newton's method: $H = \nabla^2 f(\mathbf{x}_t)^{-1}$.

Gradient descent: $H = \gamma I$.

Newton's method: "adaptive gradient descent", adaptation is w.r.t. the local geometry of the function at $\mathbf{x}_t$.

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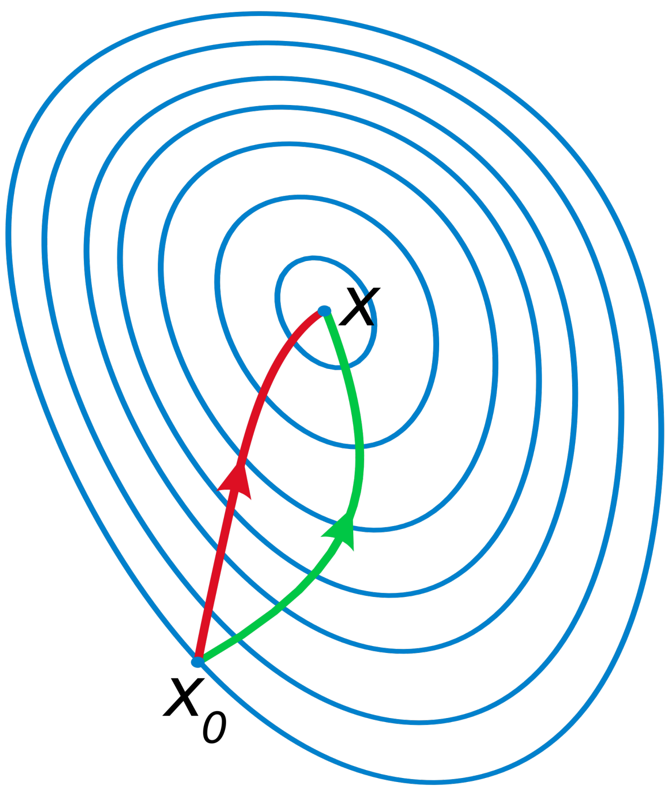

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SECOND-ORDER OPTIMIZATION AND APPROXIMATIONS

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- Second-order very useful when the dimension is not too high; otherwise storage of the Hessian becomes prohibitive ($O(n^2)$)
- When the function has many saddle-points, Newton's method needs to be modified
- Variable-metric methods provide an efficient alternative, e.g., BFGS (Broyden, Fletcher, Goldfarb, Shanno) and L-BFGS

SIAM J. OPTIMIZATION
Vol. 1, No. 1, pp. 1–17, February 1991

VARIABLE METRIC METHOD FOR MINIMIZATION*

WILLIAM C. DAVIDON†

Abstract. This is a method for determining numerically local minima of differentiable functions of several variables. In the process of locating each minimum, a matrix which characterizes the behavior of the function about the minimum is determined. For a region in which the function depends quadratically on the variables, no more than N iterations are required, where N is the number of variables. By suitable choice of starting values, and without modification of the procedure, linear constraints can be imposed upon the variables.

Key words. variable metric algorithms, quasi-Newton, optimization

AMS(MOS) subject classifications. primary, 65K10; secondary, 49D37, 65K05, 90C30

PDE-CONSTRAINT OPTIMIZATION

Complicated!

$$
\begin{aligned}
\underset{x}{\text{minimize}} \quad & f(x) \\
\text{subject to} \quad & g_i(x) \le 0, \quad i = 1, \ldots, m \\
& h_j(x) = 0, \quad j = 1, \ldots, p
\end{aligned}
$$

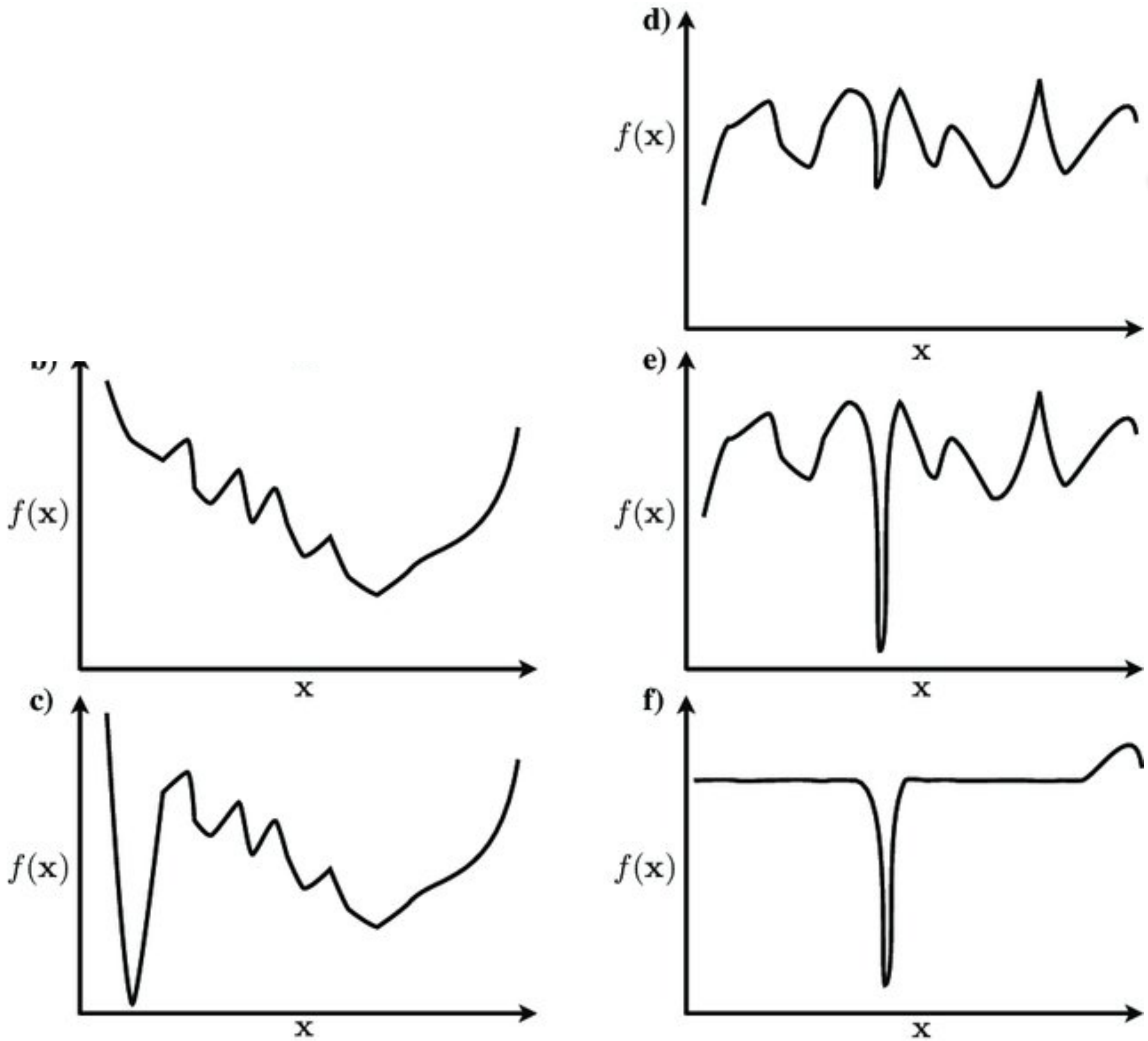
Solution of a (parameterized) partial differential equation!

- Arises in many optimal control problems
- Extremely costly is moderately high-dimensional
- Certain tricks allow efficient optimization (see Leslie's talk)

WHAT ARE GOOD FUNCTIONS?

Hard
but doable?!

Deceiving



Hopeless?

Stochastic Methods for Single Objective Global Optimization, Christian L. Müller, in: Computational Intelligence in Aerospace Sciences - Fundamental Concepts and Methods (2015) https://doi.org/10.2514/5.9781624102714.0063.0112

WHAT ARE GOOD FUNCTIONS?

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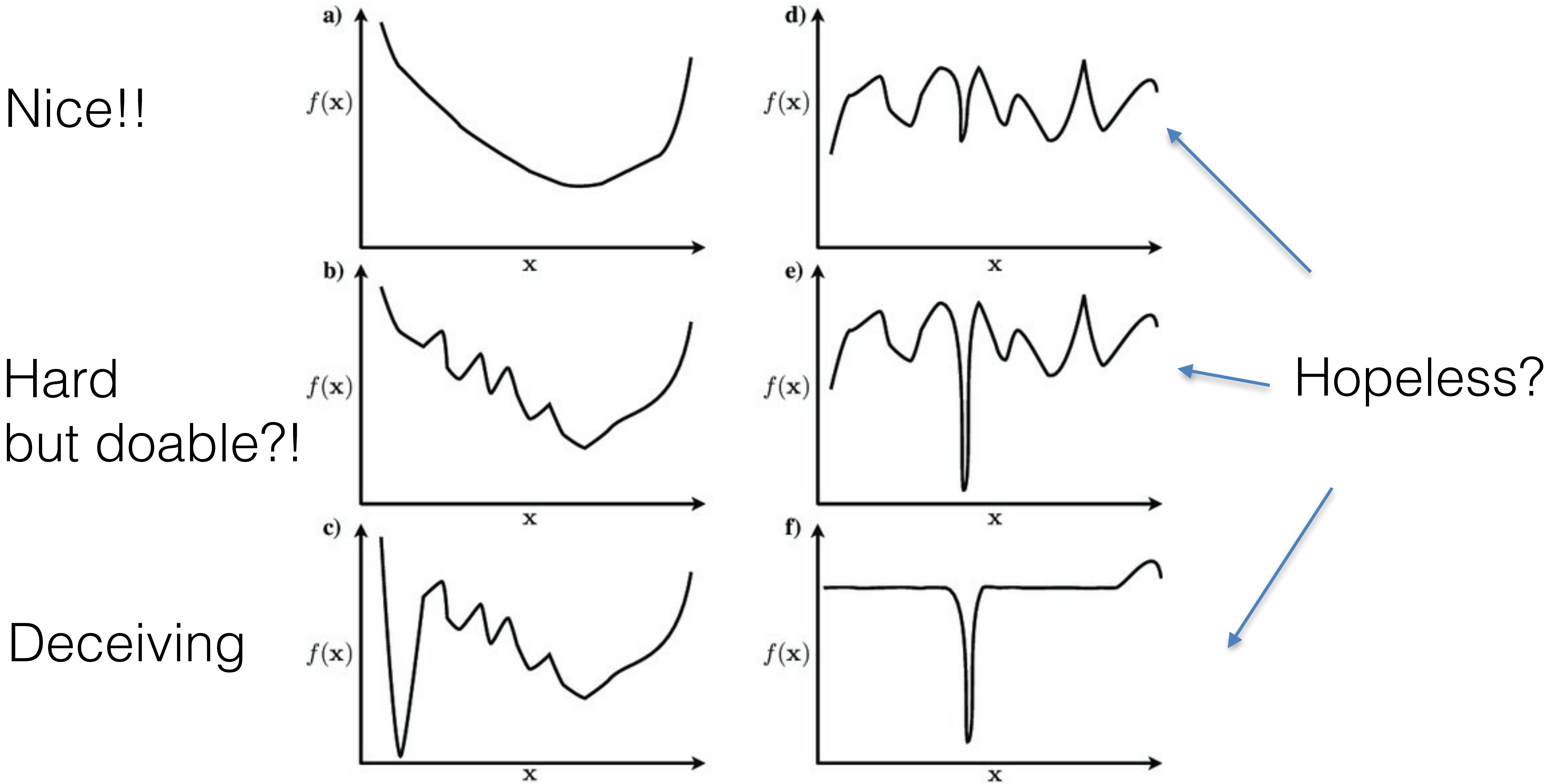

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CONVEX FUNCTIONS!

WHAT ARE GOOD FUNCTIONS?

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CONVEX FUNCTIONS!

"…in fact, the great watershed in optimization isn't between linearity and nonlinearity, but convexity and nonconvexity."
- R. Tyrrell Rockafellar, in SIAM Review, 1993

WHAT ARE GOOD FUNCTIONS?

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CONVEX FUNCTIONS!

“…in fact, the great watershed in optimization isn't between linearity and nonlinearity, but convexity and nonconvexity.”
- R. Tyrrell Rockafellar, in SIAM Review, 1993

“if it’s not convex, it’s not science”
- attributed to Emmanuel Candes, undated

CONVEX OPTIMIZATION

A convex optimization problem is said to be in the *standard form* if it is written as

$$\begin{aligned} \underset{\mathbf{x}}{\text{minimize}} \quad & f(\mathbf{x}) \\ \text{subject to} \quad & g_i(\mathbf{x}) \leq 0, \quad i = 1, \ldots, m \\ & h_i(\mathbf{x}) = 0, \quad i = 1, \ldots, p, \end{aligned}$$

where $x \in \mathbb{R}^n$ is the optimization variable, the functions $f, g_1, \ldots, g_m$ are convex, and the functions $h_1, \ldots, h_p$ are affine.

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Let X be a convex set in a real vector space and let $f : X \to \mathbb{R}$ be a function.

- f is called **convex** if:

$$\forall x_1, x_2 \in X, \forall t \in [0, 1] : \qquad f(tx_1 + (1-t)x_2) \leq tf(x_1) + (1-t)f(x_2)$$

- f is called **strictly convex** if:

$$\forall x_1 \neq x_2 \in X, \forall t \in (0, 1) : \qquad f(tx_1 + (1-t)x_2) < tf(x_1) + (1-t)f(x_2)$$

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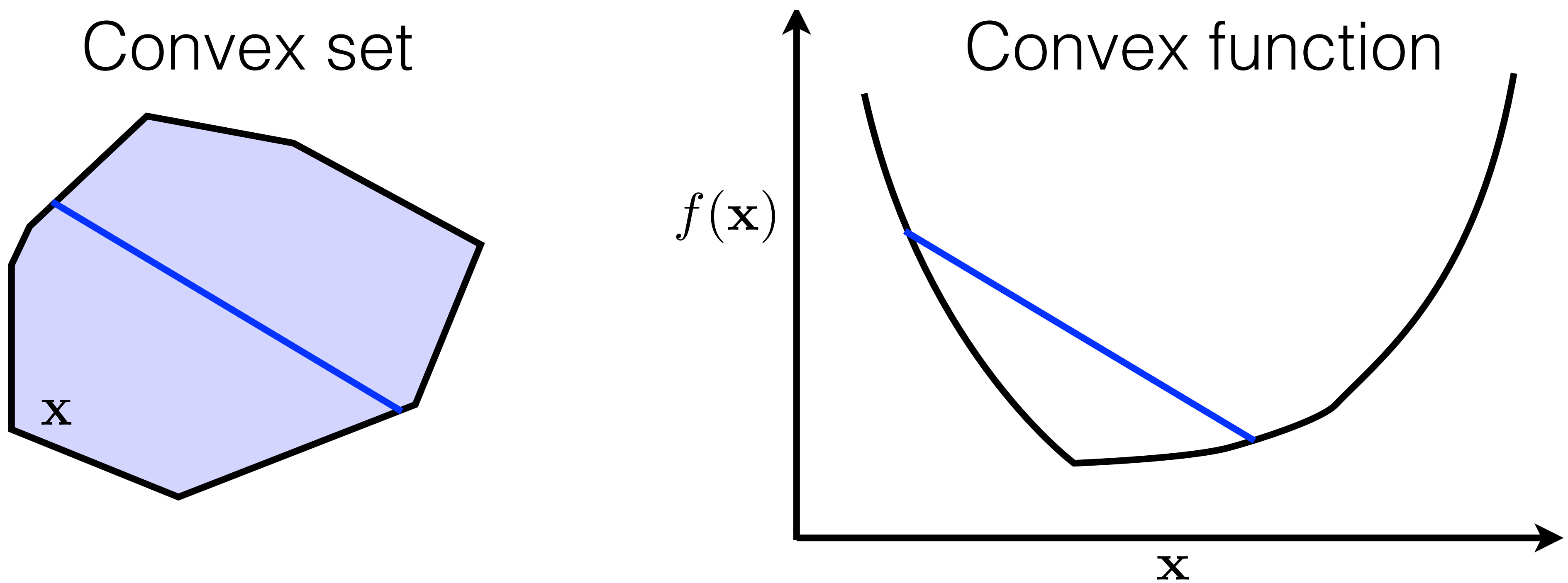

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  $\forall x$ …

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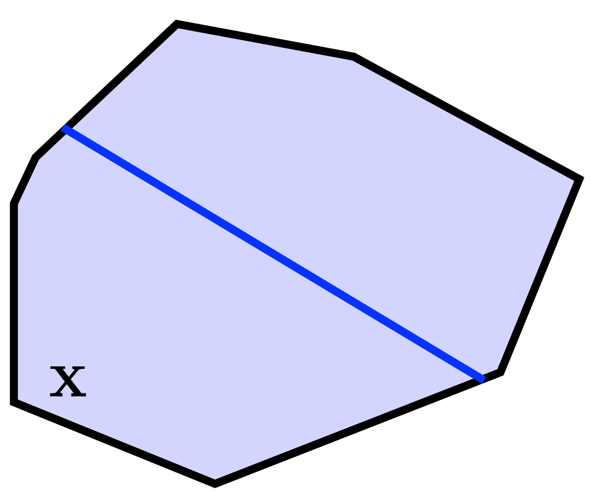
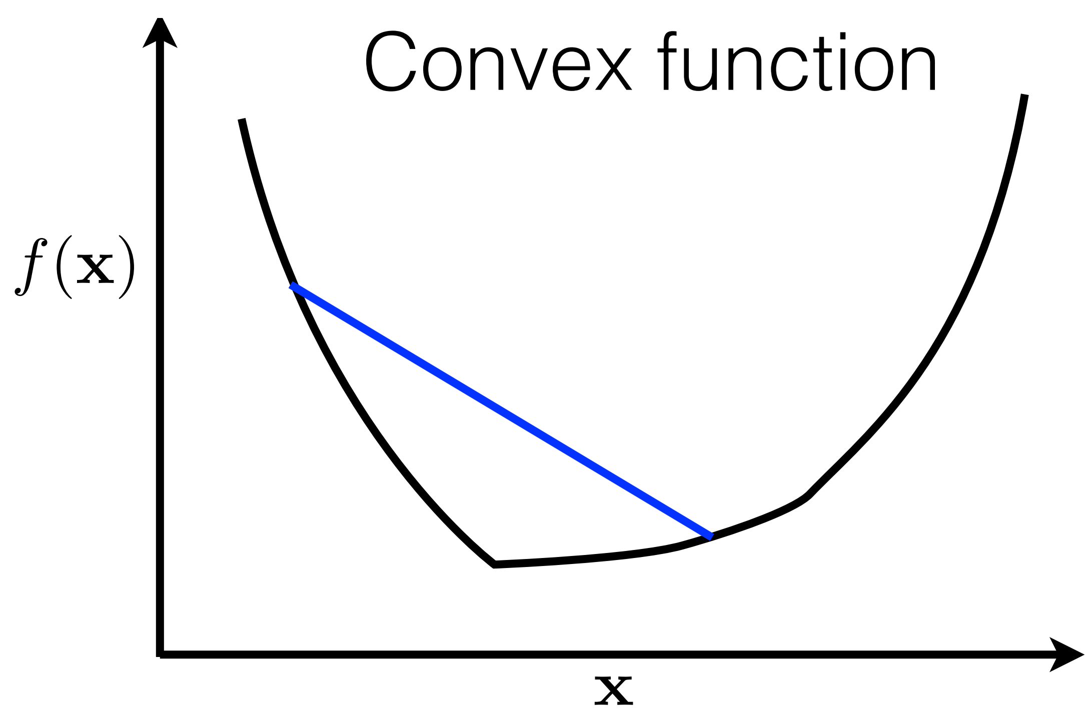
Every local minimum is a global minimum!

Convex set



Convex function



CONVEX OPTIMIZATION WITH CONVEX CONSTRAINTS

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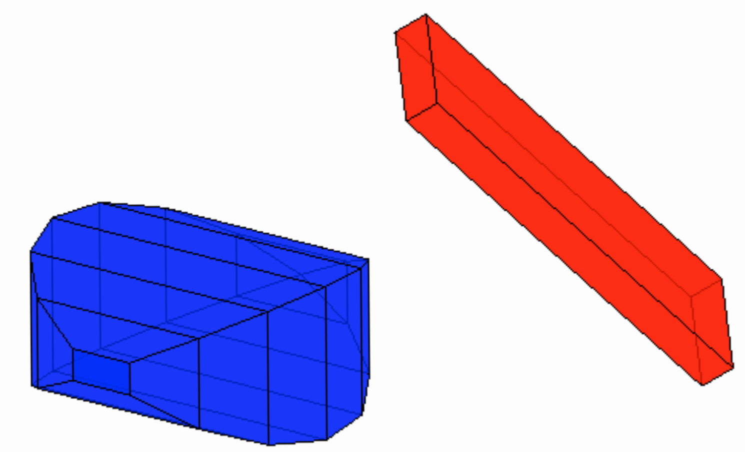
$$\min_{\mathbf{x} \in \mathbb{R}^n} \quad f(\mathbf{x})$$
$$\text{s.t.} \quad \mathbf{A}\mathbf{x} \leq \mathbf{b}\,.$$



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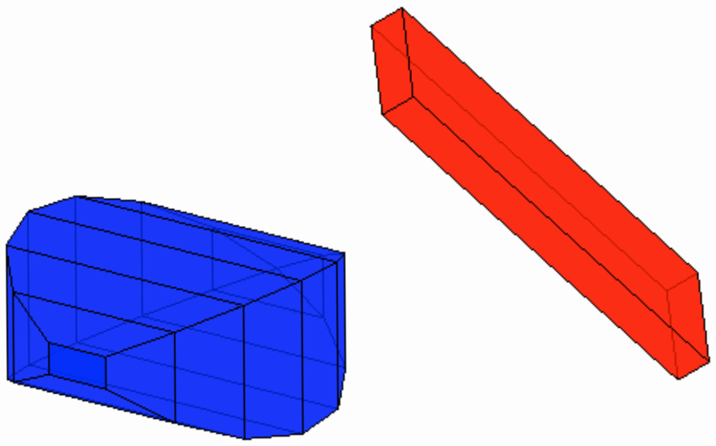
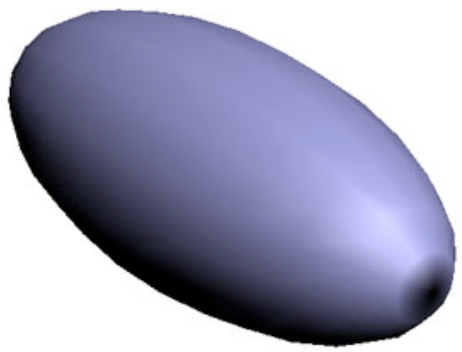


$$\text{s.t.} \quad \mathbf{x}^T\mathbf{A}\mathbf{x} \leq 1\,.$$



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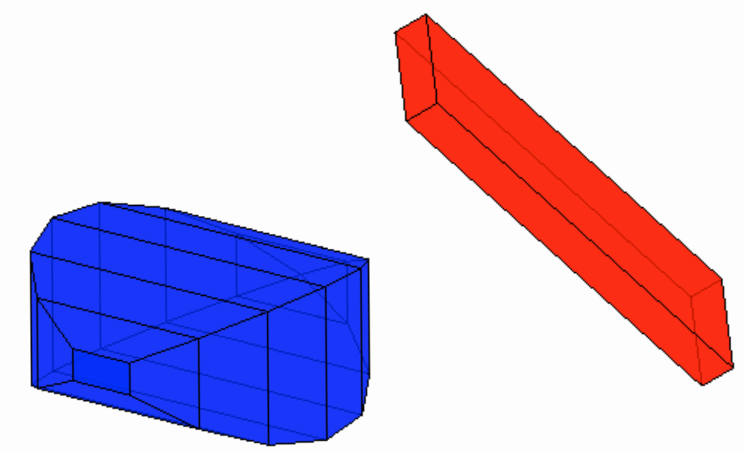

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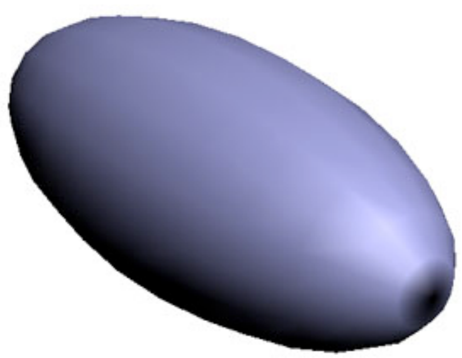
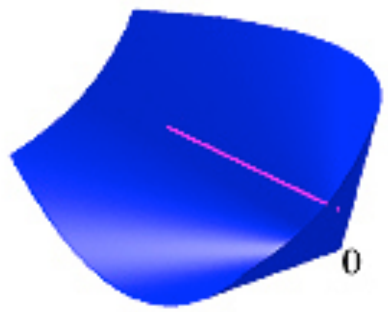


$$\text{s.t.} \quad \mathbf{A}_0 + x_1\mathbf{A}_1 + \ldots + x_n\mathbf{A}_n \preceq 0\,.$$



CONVEX ANALYSIS/MODELING

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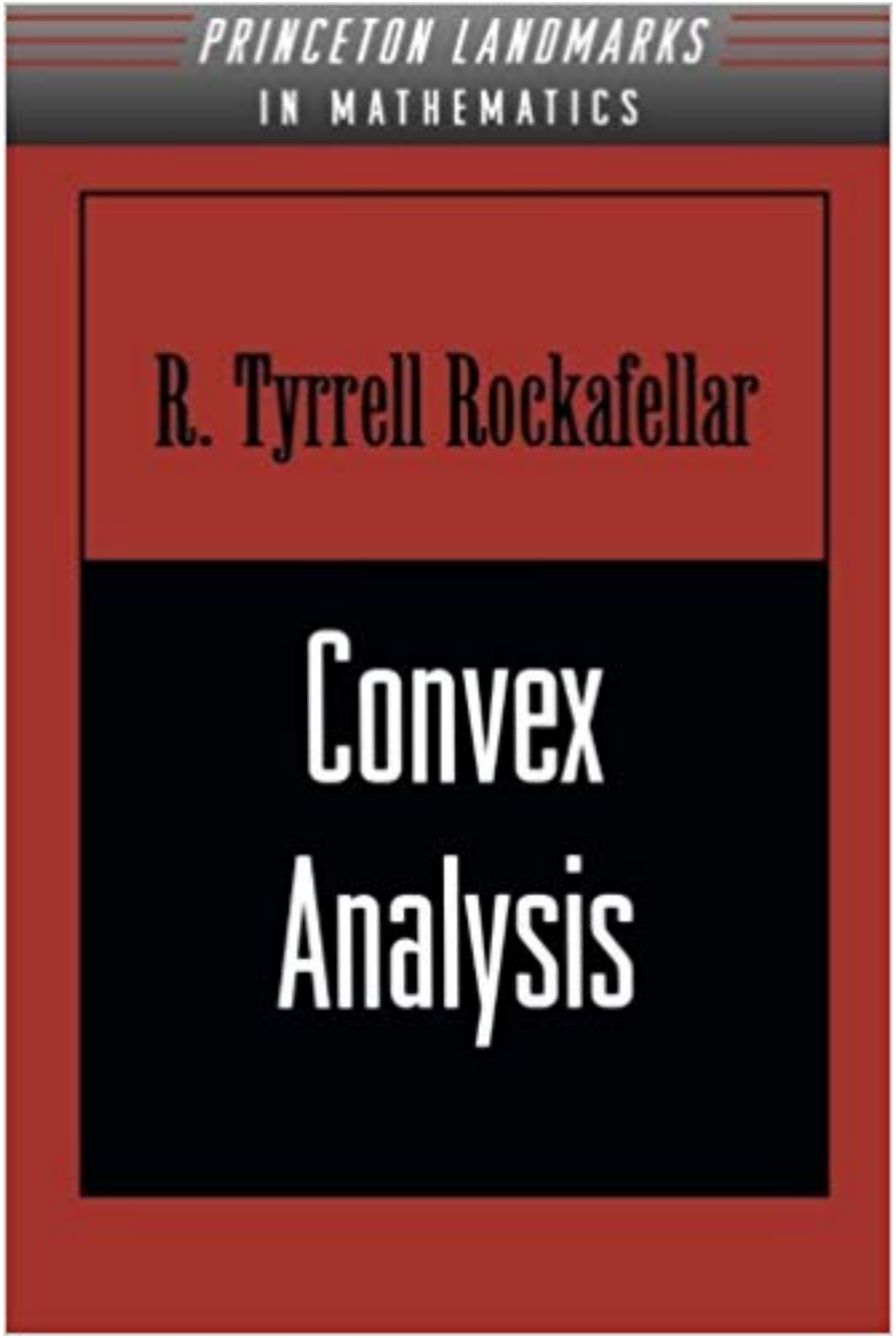

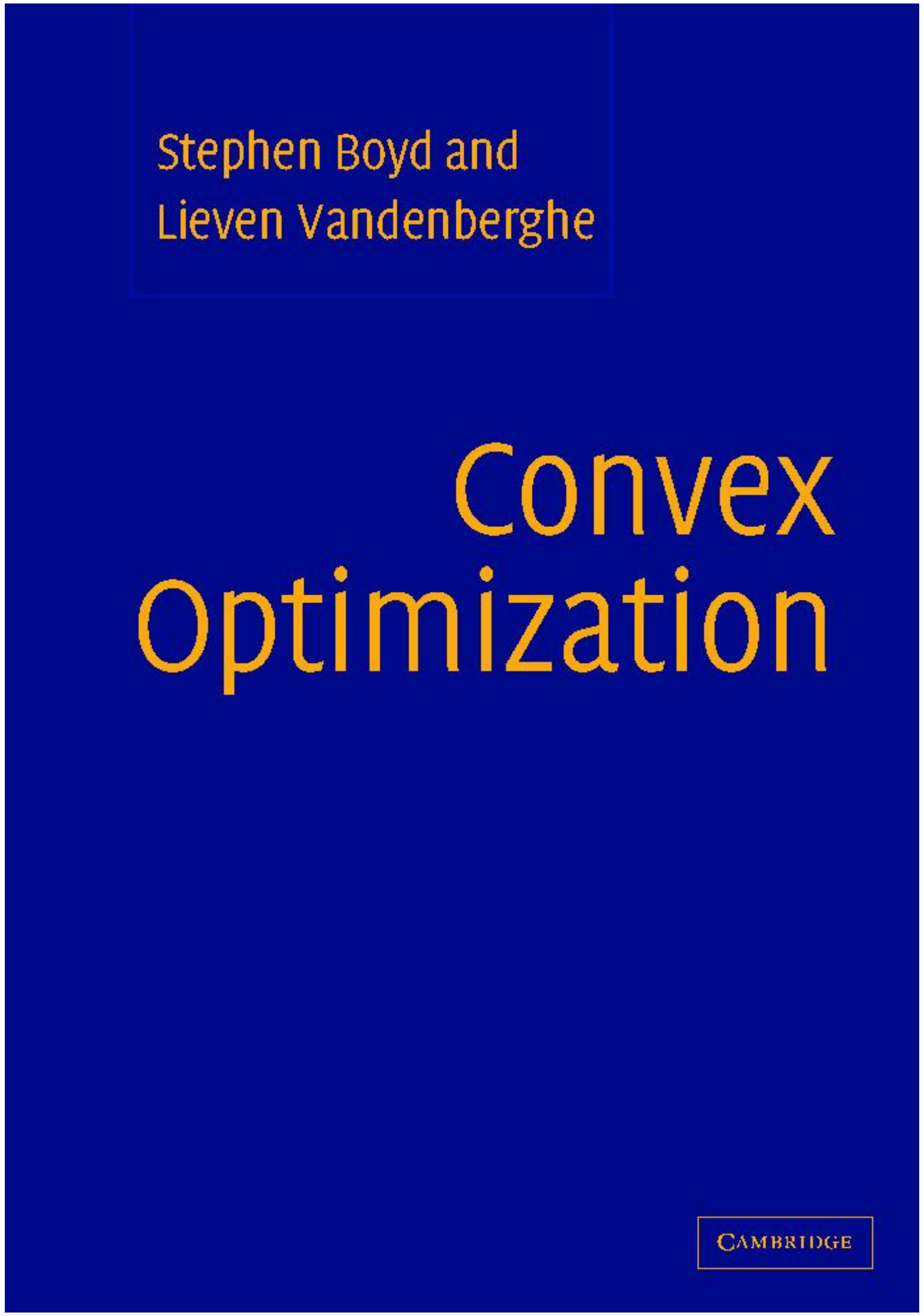

THE HIERARCHY OF CONVEX PROGRAMS

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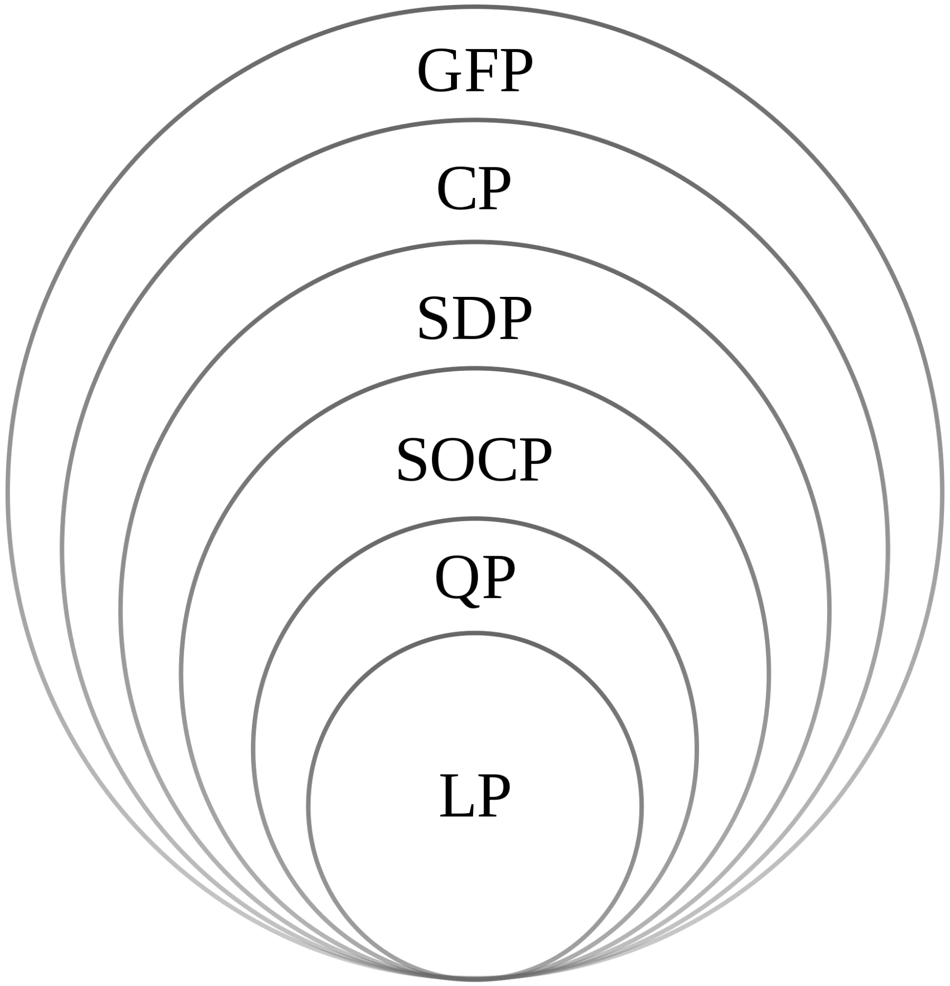
- Each category has a standard form and associated **generic solvers**
- Many engineering problems can be formulated as one of these problems and efficiently solved with theoretical guarantees
- Convergence guarantees and rates can be proven under certain conditions
- Interior-point methods as fundamental breakthrough



LP: linear program
QP: quadratic program
SOCP second-order cone program
SDP: semidefinite program
CP: cone program
GFP: graph form program

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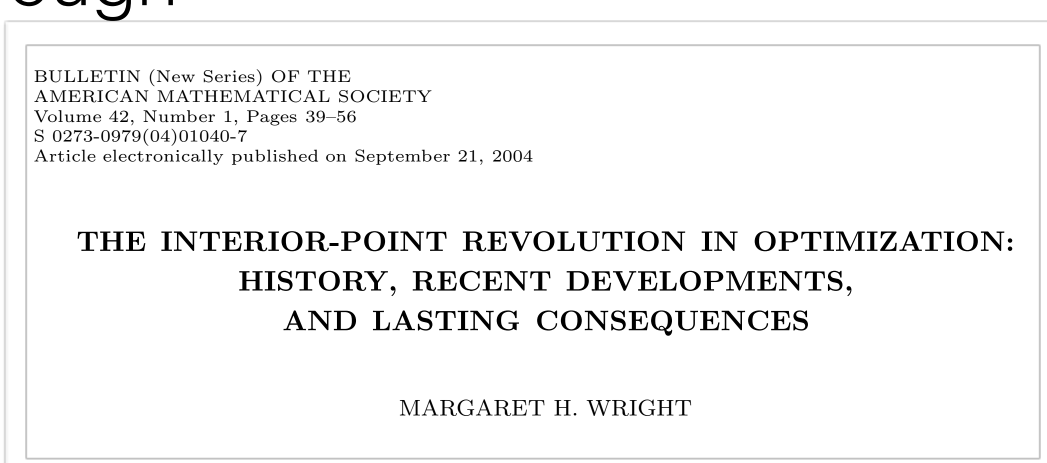

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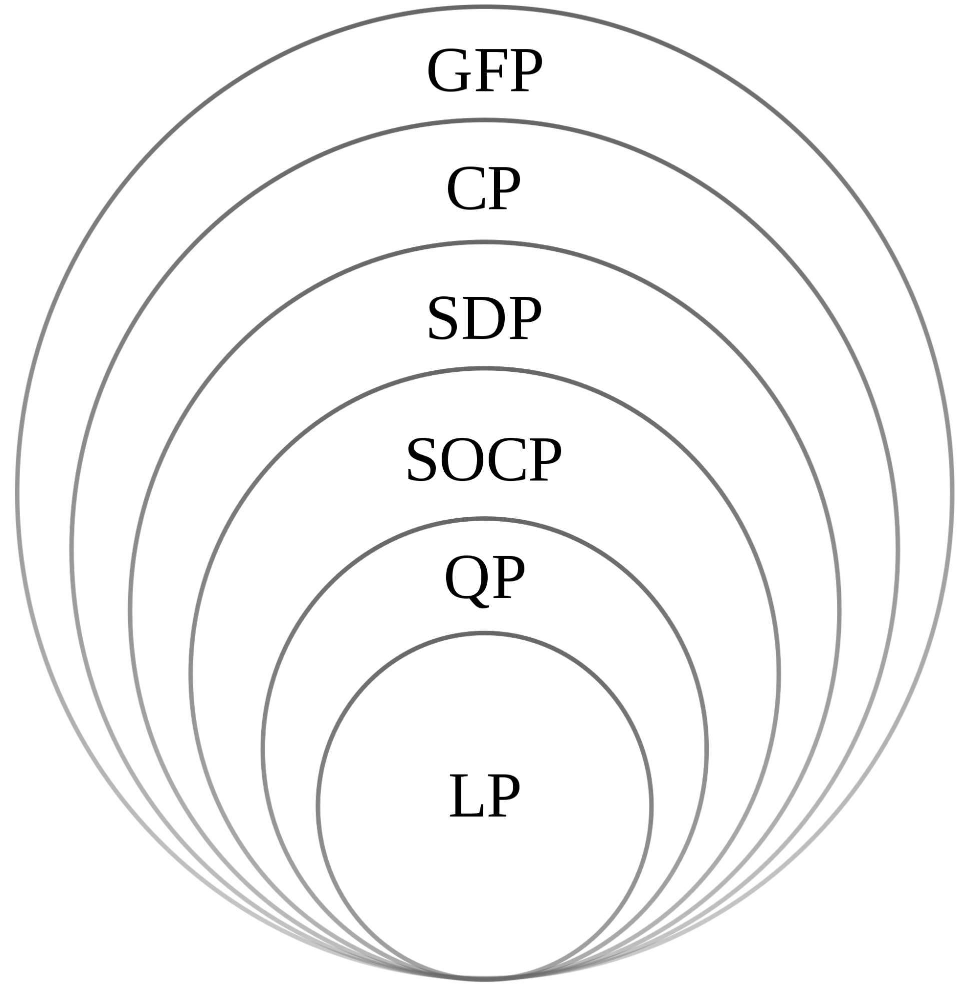
Volume 42, Number 1, Pages 39–56
S 0273-0979(04)01040-7
Article electronically published on September 21, 2004

THE INTERIOR-POINT REVOLUTION IN OPTIMIZATION: HISTORY, RECENT DEVELOPMENTS, AND LASTING CONSEQUENCES

MARGARET H. WRIGHT



LP: linear program
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SOCP second-order cone program
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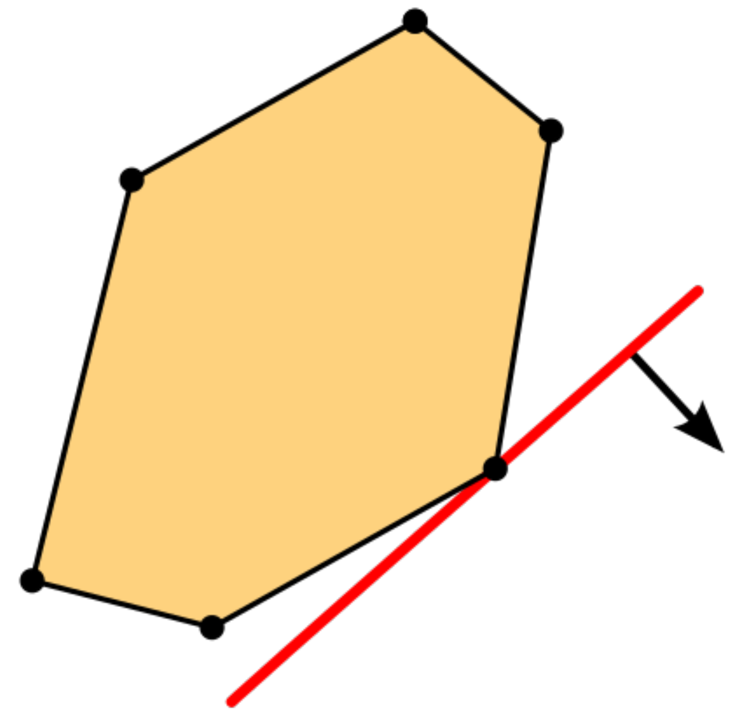
LINEAR PROGRAMS

$$\begin{array}{ll} \text{Maximize} & \mathbf{c}^{\mathrm{T}}\mathbf{x} \\ \text{subject to} & A\mathbf{x} \leq \mathbf{b} \\ \text{and} & \mathbf{x} \geq \mathbf{0} \end{array}$$



- Dantzig's simplex algorithm popular in practice (but exponential runtime in worst case)
- Khachiyan's ellipsoidal algorithm and Karmarkar's projective algorithm give polynomial-time guarantees

PROPERTIES OF CONVEX FUNCTIONS AND OPTIMIZATION

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- Choice, run time, and applicability of different methods depend on the **specific properties** of the convex functions and the constraints
- Keywords: Strongly convex, smooth, non-smooth, constrained, unconstrained,…
- Optimal convergence rates (in function value and iterates) can be proven for many algorithms for specific classes of convex function

RECENT NICE EXAMPLE

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- Gradient descent with adaptive step size

Revisiting the Polyak step size

Elad Hazan *† Sham M. Kakade *‡

	convex	β-smooth	α-strongly convex	(α, β)-well conditioned
error	$\frac{1}{\sqrt{T}}$	$\frac{\beta}{T}$	$\frac{1}{\alpha T}$	$e^{-\frac{\beta}{\alpha}T}$
step size	$\frac{1}{\sqrt{T}}$	$\frac{1}{\beta}$	$\frac{1}{\alpha T}$	$\frac{1}{\beta}$

RECENT NICE EXAMPLE

Flatiron Institute — Center for Computational Mathematics

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step size	$\frac{1}{\sqrt{T}}$	$\frac{1}{\beta}$	$\frac{1}{\alpha T}$	$\frac{1}{\beta}$

Algorithm 1 GD with the Polyak stepsize

1: Input: time horizon T, x_0
2: **for** $t = 0, \ldots, T-1$ **do**
3: Set $\eta_t = \frac{h_t}{\|\nabla_t\|^2}$
4: $\mathbf{x}_{t+1} = \mathbf{x}_t - \eta_t \nabla_t$
5: **end for**
6: Return $\bar{\mathbf{x}} = \operatorname{argmin}_{\mathbf{x}_t} \{f(\mathbf{x}_t)\}$

PROXIMAL ALGORITHMS FOR NON-SMOOTH CONVEX OPTIMIZATION

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- Many high-dimensional statistics problems are non-smooth convex problems (e.g., Lasso, structured sparsity, …)
- Proximity operator as fundamental building block
- Efficient schemes and exact convergence guarantees

Chapter 10
Proximal Splitting Methods in Signal Processing

Patrick L. Combettes and Jean-Christophe Pesquet

Foundations and Trends® in Optimization
Vol. 1, No. 3 (2013) 123–231

DOI: xxx

now
the essence of knowledge

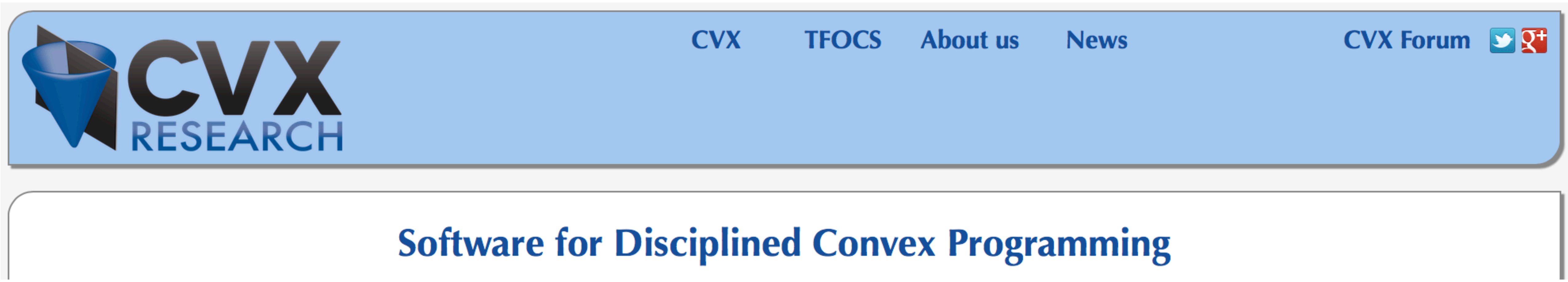
Proximal Algorithms

Neal Parikh
Department of Computer Science
Stanford University
npparikh@cs.stanford.edu

Stephen Boyd
Department of Electrical Engineering
Stanford University
boyd@stanford.edu

NEXT TALK

OPTIMIZATION SOFTWARE



$$\begin{array}{ll} \text{minimize} & \|Ax - b\|_2 \\ \text{subject to} & Cx = d \\ & \|x\|_\infty \leq e \end{array}$$

```
m = 20; n = 10; p = 4;
A = randn(m,n); b = randn(m,1);
C = randn(p,n); d = randn(p,1); e = rand;
cvx_begin
    variable x(n)
    minimize( norm( A * x - b, 2 ) )
    subject to
        C * x == d
        norm( x, Inf ) <= e
cvx_end
```

OPTIMIZATION SOFTWARE

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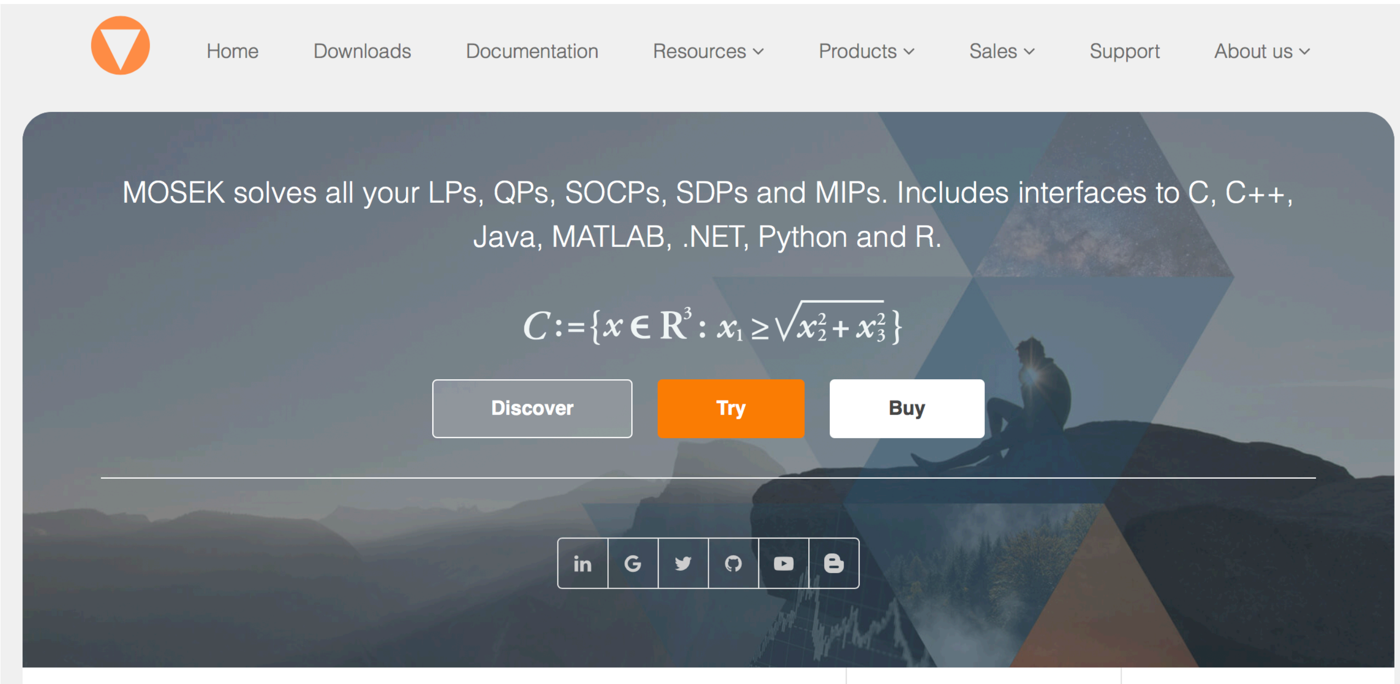

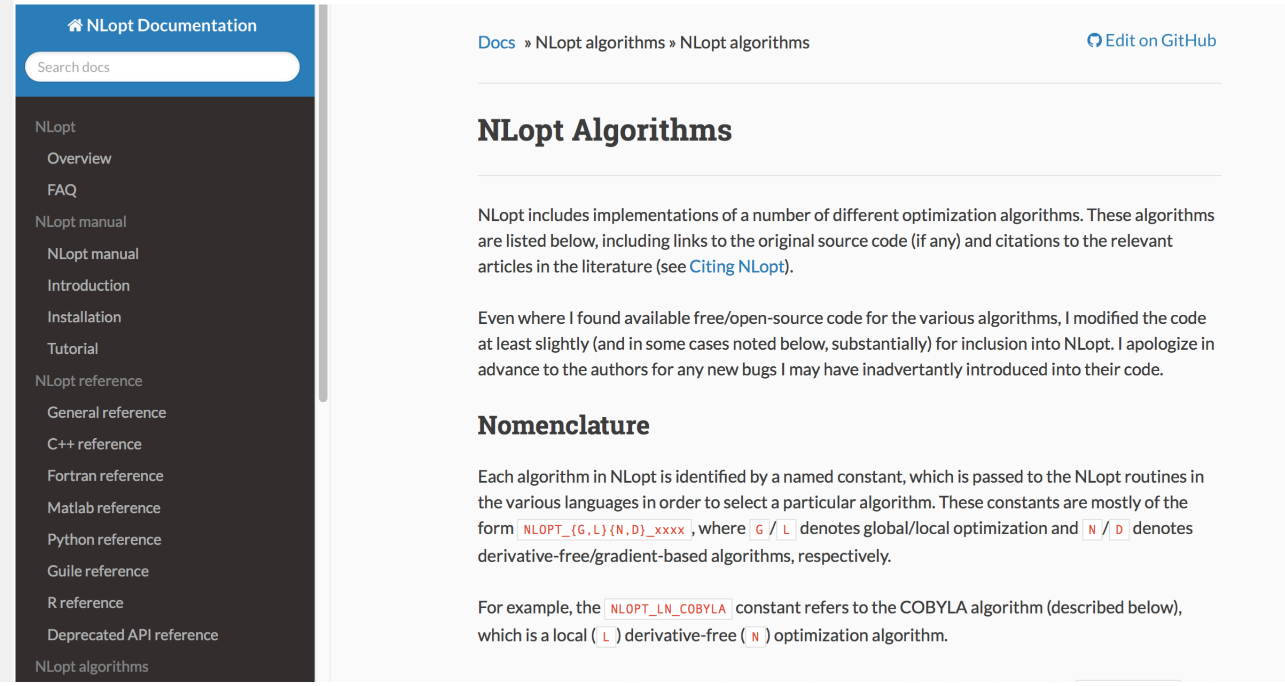

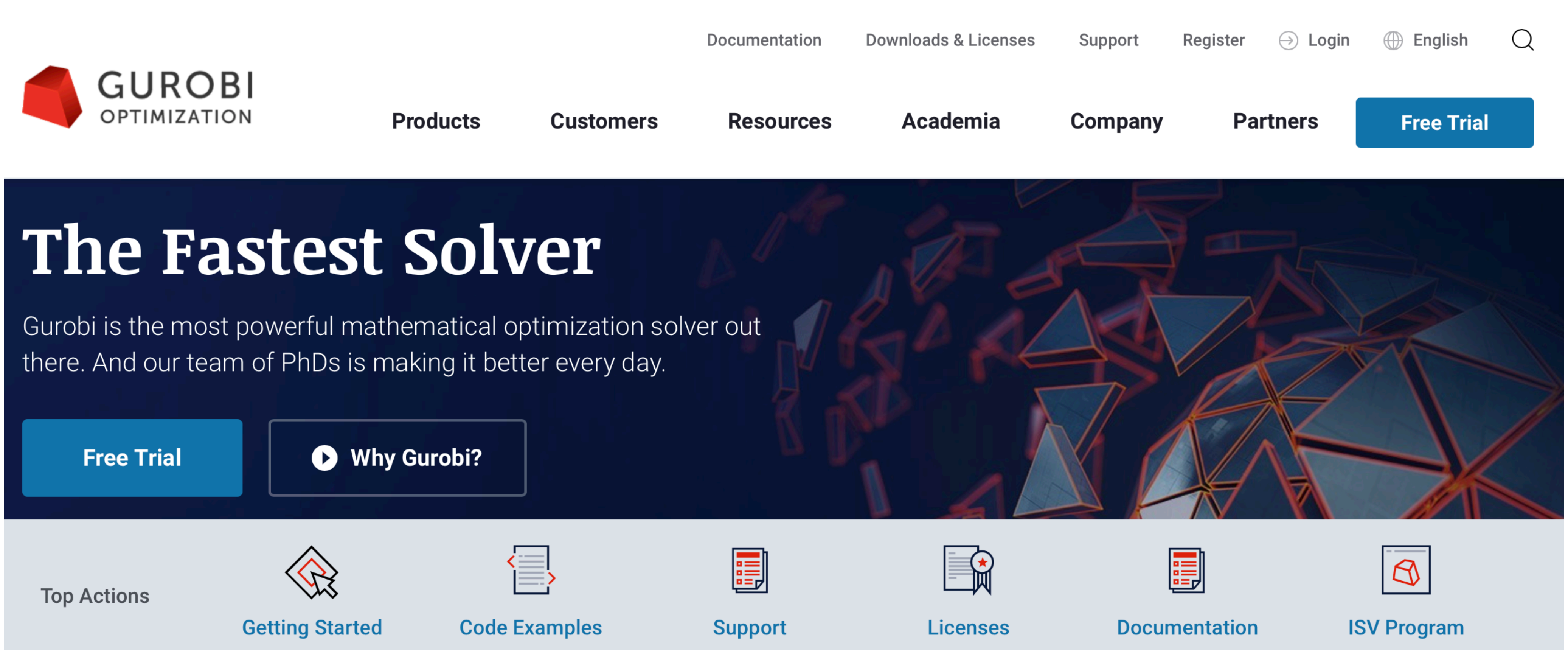

OUTLOOK - DNN LANDSCAPES

FLATIRON INSTITUTE
Center for Computational Mathematics

Towards Understanding Generalization of Deep Learning: Perspective of Loss Landscapes

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Large Scale Structure of Neural Network Loss Landscapes

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Abstract

There are many surprising and perhaps counter-intuitive properties of optimization of deep neural networks. We propose and experimentally verify a unified phenomenological model of the loss landscape that incorporates many of them. High dimensionality plays a key role in our model. Our core idea is to model the loss landscape as a set of high dimensional *wedges* that together form a large-scale, inter-connected structure and towards which optimization is drawn. We first show that hyperparameter choices such as learning rate, network width and L_2 regularization, affect the path optimizer takes through the landscape in a similar ways, influencing the large scale curvature of the regions the optimizer explores. Finally, we predict and demonstrate new counter-intuitive properties of the loss-landscape. We show an existence of low loss subspaces connecting a set (not only a pair) of solutions, and verify it experimentally. Finally, we analyze recently popular ensembling techniques for deep networks in the light of our model.

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Visualizing the Loss Landscape of Neural Nets

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Abstract

Neural network training relies on our ability to find "good" minimizers of highly non-convex loss functions. It is well-known that certain network architecture designs (e.g., skip connections) produce loss functions that train easier, and well-chosen training parameters (batch size, learning rate, optimizer) produce minimizers that generalize better. However, the reasons for these differences, and their effect on the underlying loss landscape, are not well understood. In this paper, we explore the structure of neural loss functions, and the effect of loss landscapes on generalization, using a range of visualization methods. First, we introduce a simple "filter normalization" method that helps us visualize loss function curvature and make meaningful side-by-side comparisons between loss functions. Then, using a variety of visualizations, we explore how network architecture affects the loss landscape, and how training parameters affect the shape of minimizers.

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Spurious Valleys in One-hidden-layer Neural Network Optimization Landscapes

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OUTLOOK

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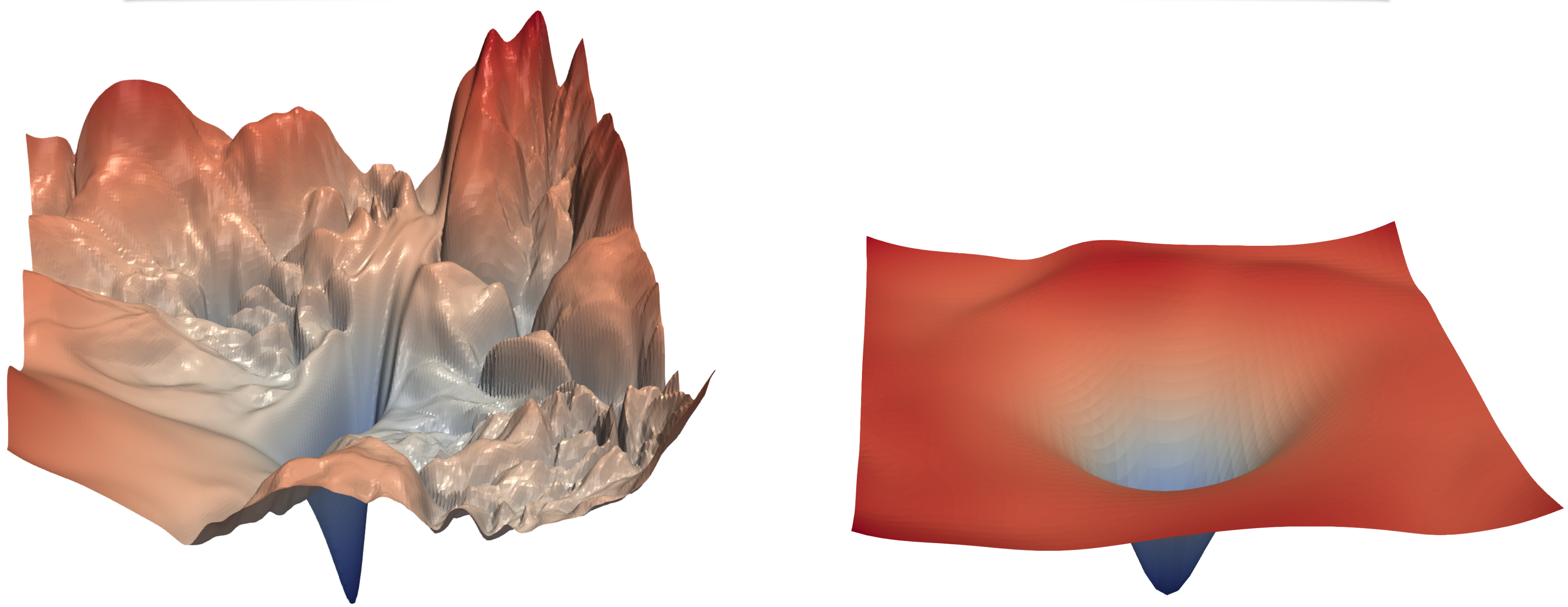

(a) without skip connections (b) with skip connections

Figure 1: The loss surfaces of ResNet-56 with/without skip connections. The proposed filter normalization scheme is used to enable comparisons of sharpness/flatness between the two figures.

Thank you for your time! Questions?

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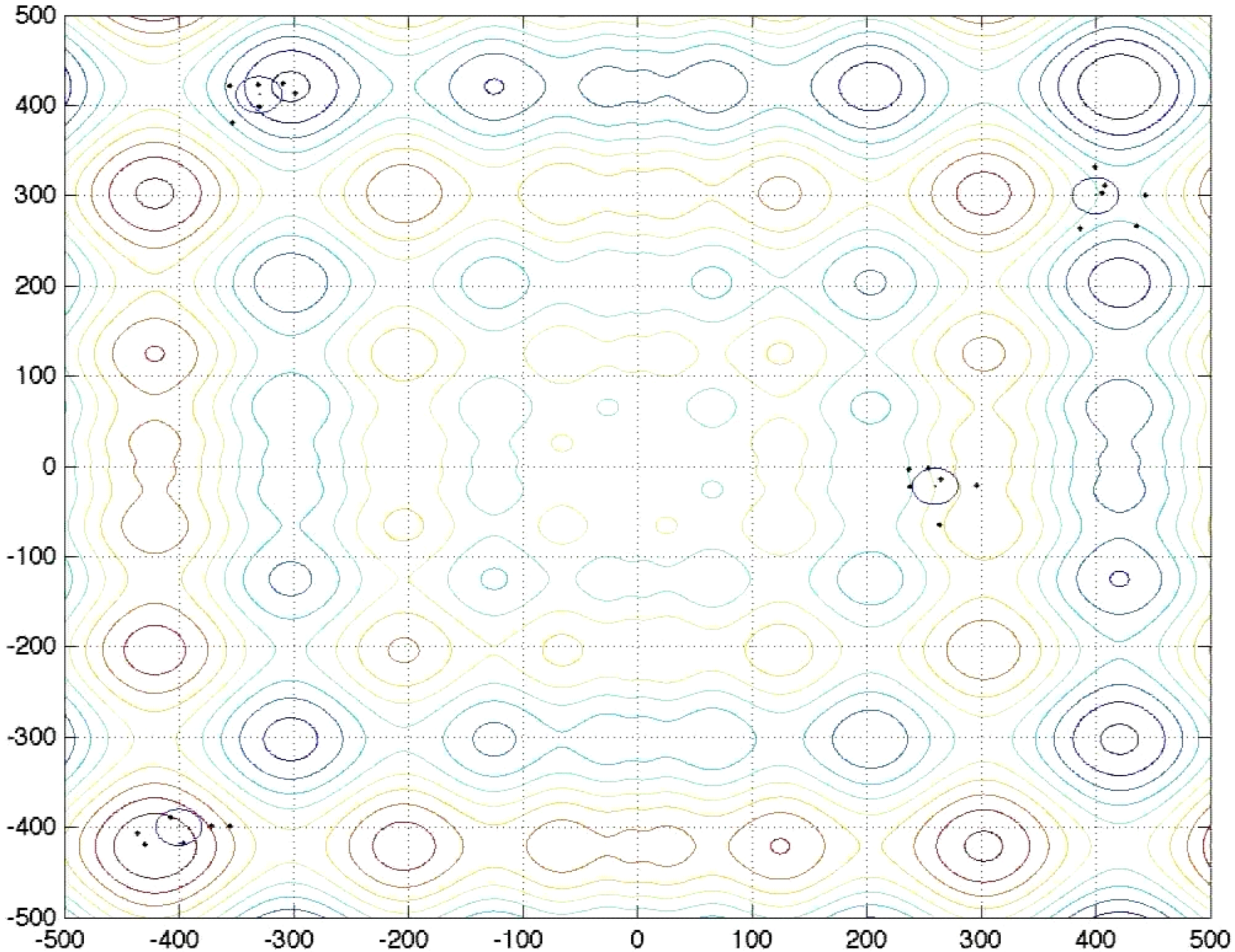

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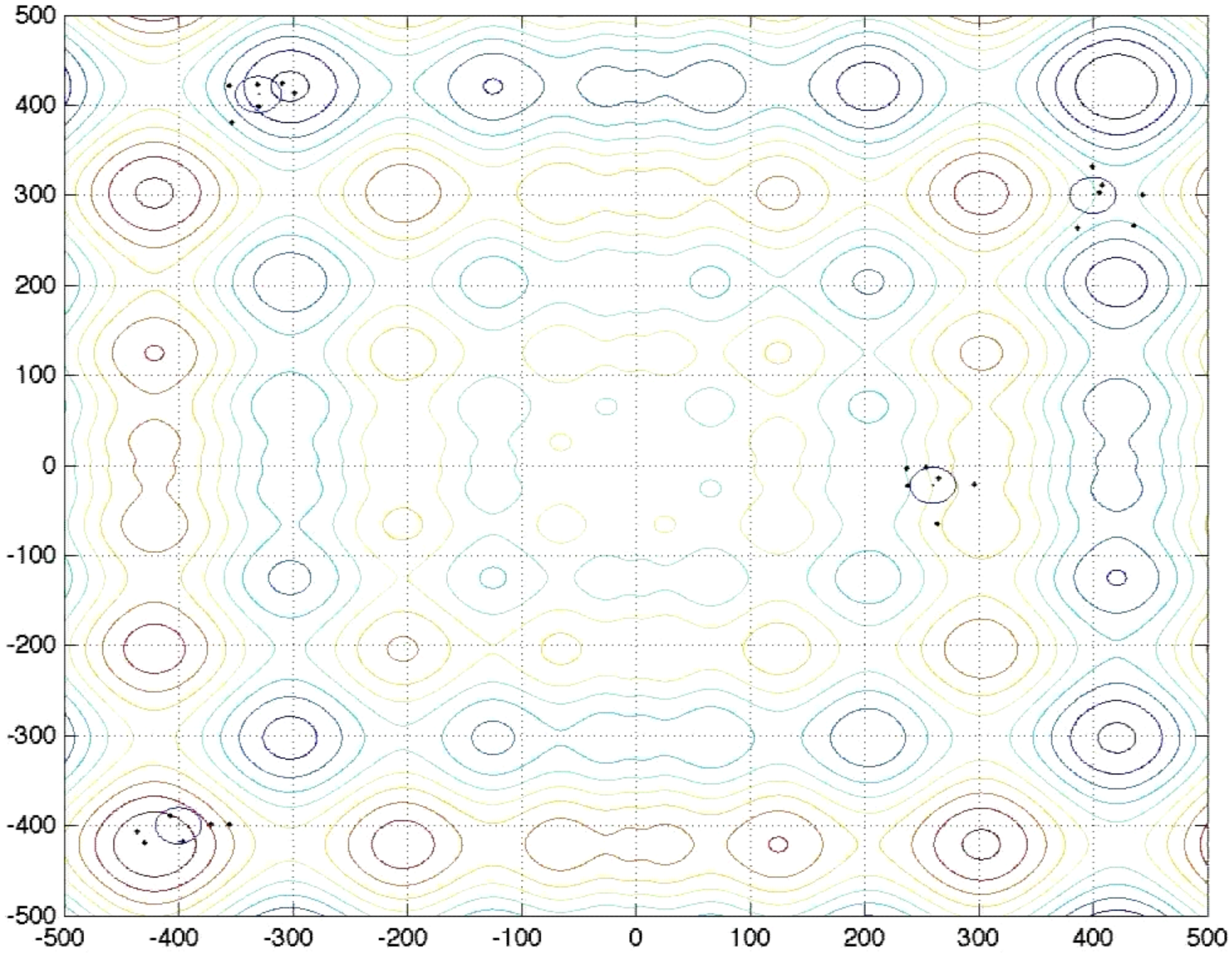

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