Data and Models

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RWTH Aachen

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Outline

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1. Introduction
2. 3 Scenarios
   - Electron Microscopy
   - EELS Electron Energy Loss Spectroscopy
   - Climate Modeling

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2. 3 Scenarios
   - Electron Microscopy
   - EELS Electron Energy Loss Spectroscopy
   - Climate Modeling
3. Theoretical Performance Bounds
   - Nonparametric Estimation - A Sample Result

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What is it all about...

Objective:

...extract quantifiable information from corrupted, noisy data sets when

- off-the-shelf methods are not available

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Conceptual ingredients:

- adaptivity
- nonlinear recovery
- embedding into a proper continuous framework to exploit natural "problem metrics"

General “Philosophy”...

- devise mathematical model...possibly simplified...

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...has led to "unexpected" algorithmic structures...

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Precision in STEM Imaging scanning transmission electron microscopy

Collaborators: B. Berkels, N. Mevenkamp (AICES), Ernst-Ruska-Center Jülich, P. Voyles (University of Wisconsin), P. Binev, T. Vogt (Unisversity of South Carolina)

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Images/Models: distributions of intensities - stochastic processes

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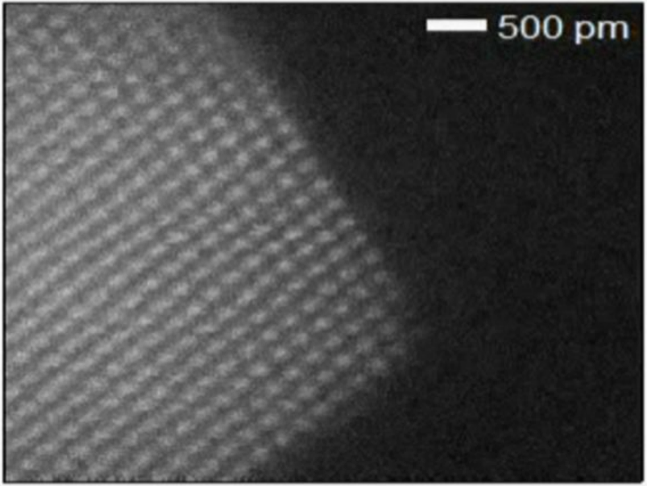
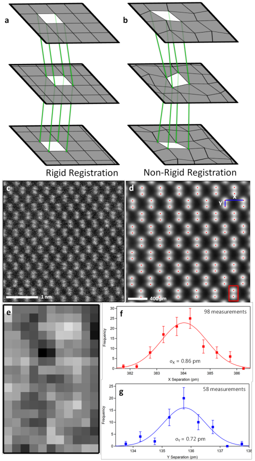
Obstructions:

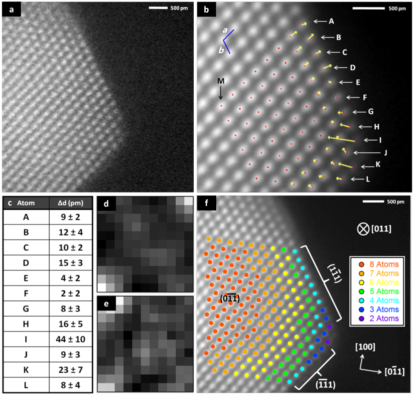
- high electron dose destroys specimen
- low electron dose causes low signal-to-noise ratio
- Poisson noise
- multiscale locally distorted movement of specimen

Pt nanocatalyst



Results - sub-picometer precision

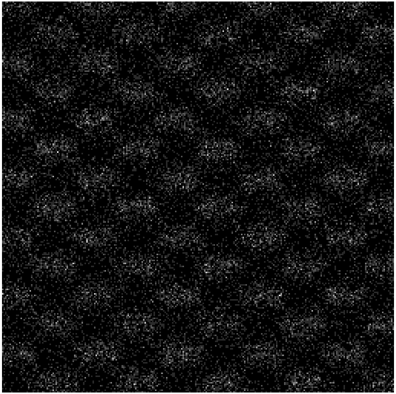


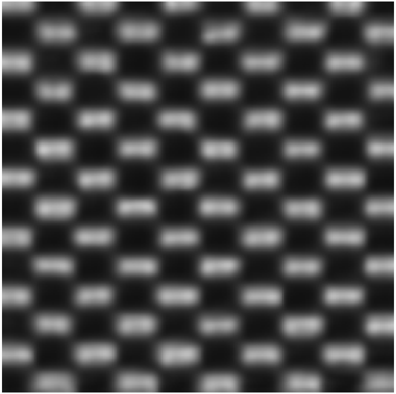


c Atom	Δd (pm)
A	9 ± 2
B	12 ± 4
C	10 ± 2
D	15 ± 3
E	4 ± 2
F	2 ± 2
G	8 ± 3
H	16 ± 5
I	44 ± 10
J	9 ± 3
K	23 ± 7
L	8 ± 4

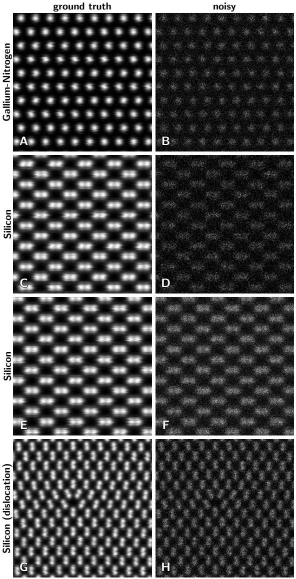
Result: improve precision by factors 5 to 10

...before and after...Perfect Silicon





...before and after...Perfect Silicon Gallium Nitride



Methods

Key ingredients:

- multilevel variational non-rigid registration scheme
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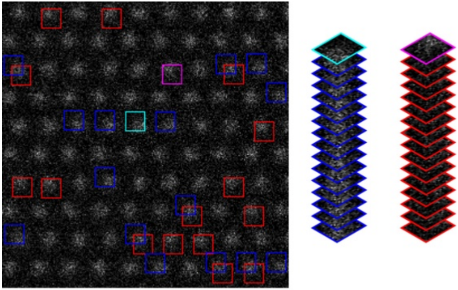
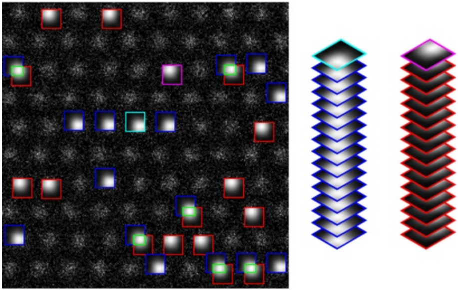
A. B. Yankovich, B. Berkels, W. Dahmen, P. Binev, S.I. Sanchez, S.A. Bradley, and P.M. Voyles, Picometer precision STEM imaging of Pt Nanocatalysts, Nature Communications 5, Article number: 4155 (2014) doi:10.1038/ncomms5155

N. Mevenkamp, P. Binev, W. Dahmen, P.M. Voyles, A.B. Yankovich, and B. Berkels, Poisson noise removal from high-resolution STEM images based on periodic block matching, Advanced Structural and Chemical Imaging, DOI 10.1186/s40679-015-0004-8



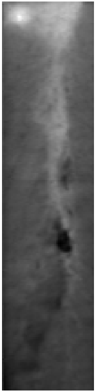


Outline

EELS-Images

electron energy loss spectroscopy ⇝ "function valued pixels"

Collaborations: B. Berkels (AICES), M. Duchamps (FZ Jülich), C. Bajaj, ICES, University of Texas at Austin



Example task: unmixing of materials

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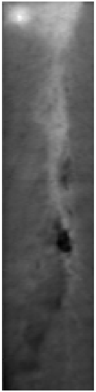

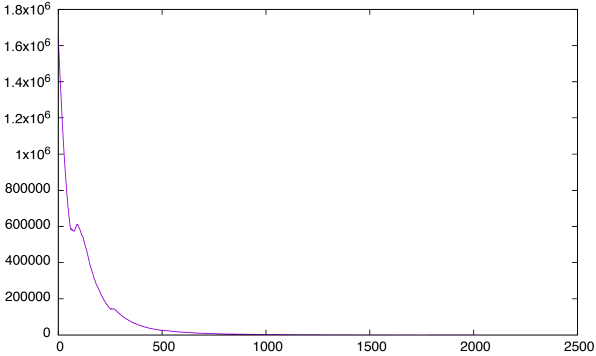

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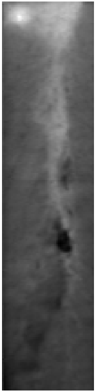

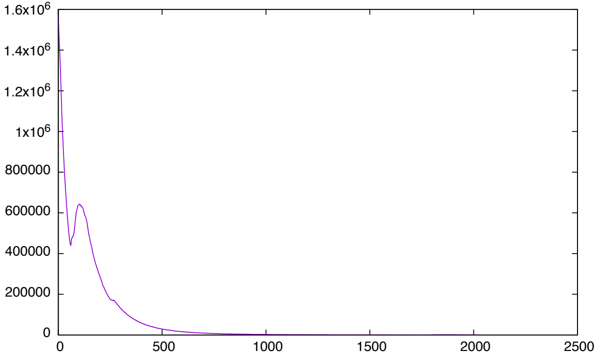

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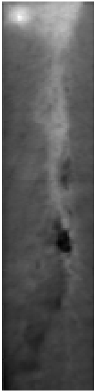

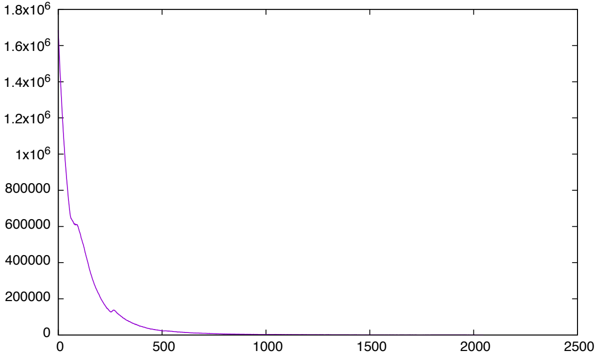

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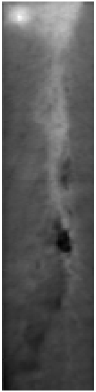

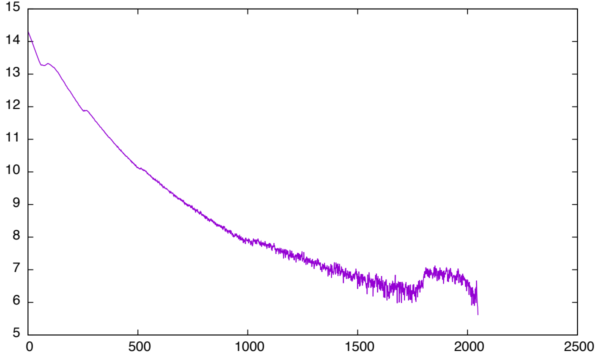

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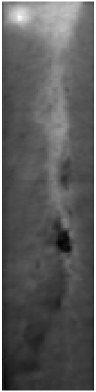

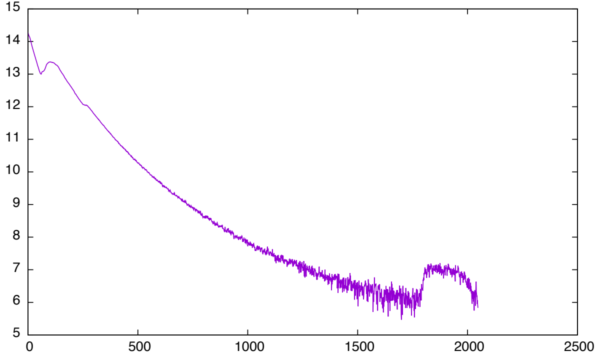

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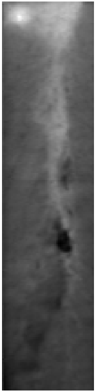

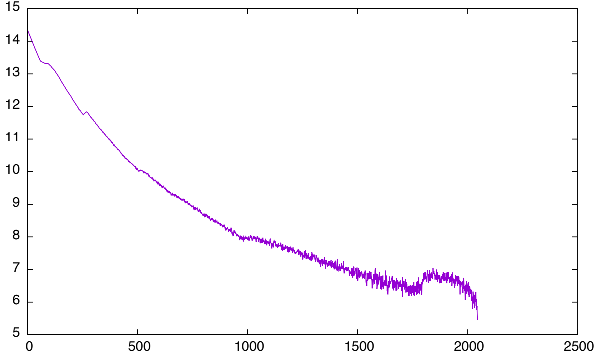

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Obstructions, Methods

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- very large, noisy data sets

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Methods:

- nonlocal means, BMD3-algorithm
- future: compressed sensing, dictionary learning, tensor methods,...

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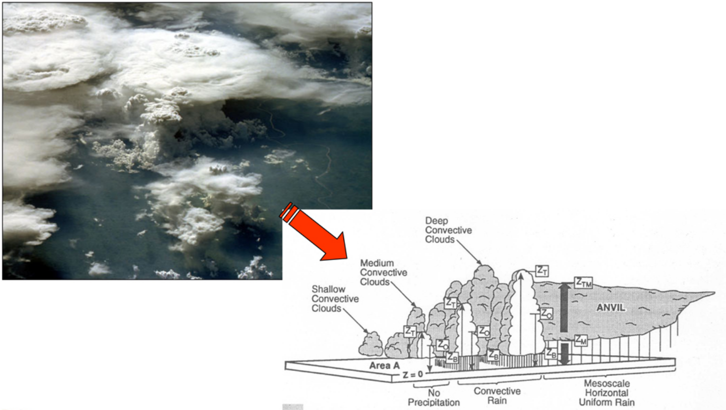
NCAR National Center of Atmospheric Research CAM Community Atmospheric Model

Collaborators: P. Binev, R. DeVore, P. Lamby, (M. Fox-Rabinowitz, V. Krasnopolsky)



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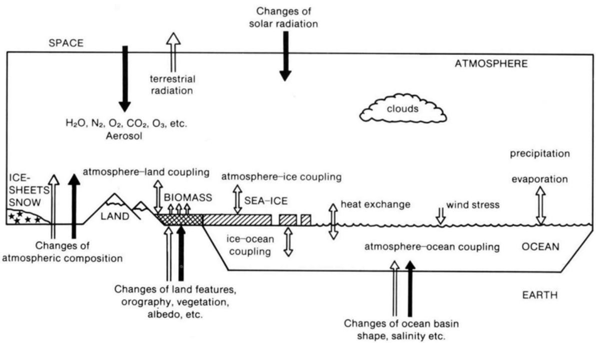

Figure 3.1: Schematic illustration of the components of the coupled atmosphere-ocean-ice-land climatic system. The full arrows are examples of external processes, and the open arrows are examples of internal processes in climatic change (from Houghton, 1984).

NCAR

igpm

NCAR Model general Circulation Model

$$d\overline{\mathbf{V}}/dt + fk \times \overline{\mathbf{V}} + \nabla\overline{\phi} = \mathbf{F}, \qquad \textit{(horizontal momentum)}$$

$$d\overline{T}/dt - \kappa\overline{T}\omega/p = Q/c_p, \qquad \textit{(thermodynamic energy)}$$

$$\nabla \cdot \overline{\mathbf{V}} + \partial\overline{\omega}/\partial p = 0, \qquad \textit{(mass continuity)}$$

$$\partial\overline{\phi}/\partial p + R\overline{T}/p = 0, \qquad \textit{(hydrostatic equilibrium)}$$

$$d\overline{q}/dt = S_q. \qquad \textit{(water vapor mass continuity)}$$

Harmless looking terms F, Q, and S_q $\Longrightarrow$ "physics"

NCAR CAM

General Circulation Model: fluid dynamics equation on the sphere

$$\partial_t \psi + D(\psi) = P(\psi)$$

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Bottleneck for numerical simulations: modeling physics/chemistry
Long Wave Radiation: 70% – 90% of total cost

Problem and Goal

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$\partial_t \psi + D(\psi) = P(\psi)$ "Learn" $P(\psi)$ from data

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$$\partial_t \psi + D(\psi) = P(\psi) \qquad \text{“Learn” } P(\psi) \text{ from data}$$

For LWR recovery $\rightsquigarrow$

$$f : X \subset \mathbb{R}^{220} \to \mathbb{R}^{33}$$

from data $\mathbf{z} = \{z^i = (x^i, y^i) : i = 1, \ldots, N\} \subset X \times Y$, where

$$N \sim 10^5$$

Inputs $x \in X$ consist of 10 vertical profiles of local physical properties and gas concentrations plus a surface characteristic.

Outputs y consist of a vertical profile of heating rates and some radiation fluxes

outputs $y = f(x)$ are computed via solving the physical model with input x

Key Issues

- Severe undersampling - Classical approximation schemes are not feasible
- Recover functions of many variables - curse of dimensionality

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  accuracy $\varepsilon \quad \leftrightarrow \quad$ computational work $O(\varepsilon^{-d/\alpha})$

- Meaningful results are only possible if the data are highly correlated - implicit lower dimensionality
- Key question: How much of the structure does an algorithm have to know in order to take advantage of it?

Procedural Definition of Function Recovery

learn f from $\mathbf{z} = \{(x^1, y^1), \ldots, (x^N, y^N)\}$

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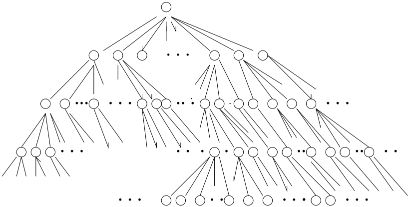
Candidates:

- kernel methods, artificial neural networks
- Recovery based on k nearest neighbor search
- Tree based schemes: random forests, sparse occupancy trees

Sparse Occupancy Trees

Hierarchy of nested partitions of X

$$X = \mathcal{P}_\emptyset \prec \mathcal{P}_0 \prec \mathcal{P}_1 \prec \cdots, \qquad X_{j,k} \in \mathcal{P}_j \rightsquigarrow X_{j,k} = \bigcup_{i \in \mathcal{I}_{j,k}} X_{j+1,i}$$



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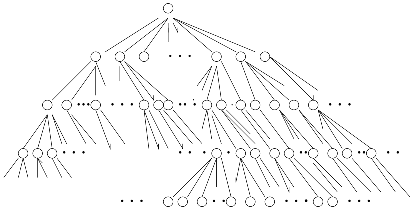

Cost Summary:

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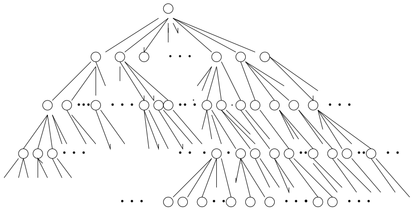

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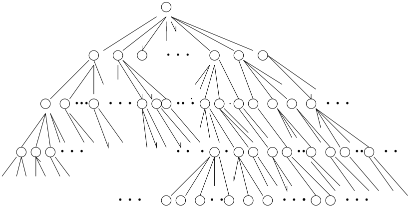

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- $O(N \log N)$ sorting operations of bitstreams of length $\leq Ld$

Simulation Results

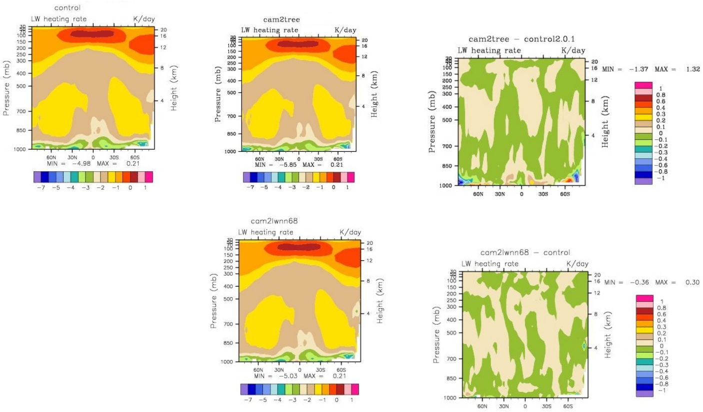

Figure: Comparison of the predicted annual zonal means of the LWR heating rates computed with the original parameterization (1 in 1. row), a tree based emulation (2, 3 in 1. row) and a neural network emulation (2. row). The right column plots the difference between the simulation and the control.

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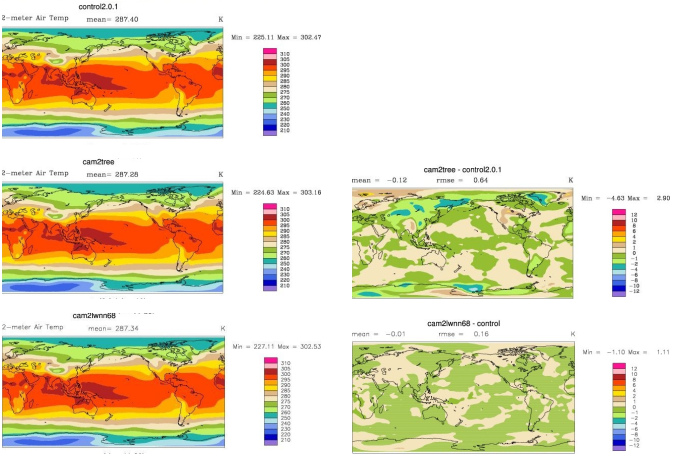

Figure: Comparison of the predicted annual means of the two meter air temperatures computed with the original parameterization (top row), a tree-based emulation (center row) and a neural network emulation (bottom row). The right column plots the difference between the simulation and the control.

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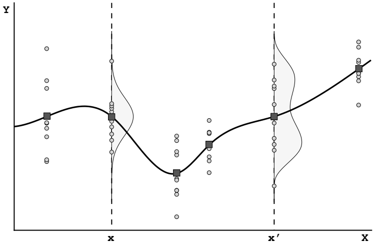
Setting - Model



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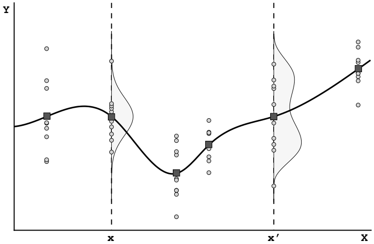

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$Z := X \times Y$

$d\rho(x, y) = d\rho(y|x)d\rho_X(x)$

$\mathrm{supp}\,\rho(\cdot|x) \subseteq [-M.M],\ x \in X$

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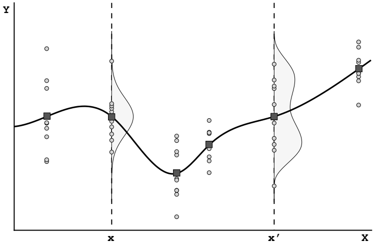

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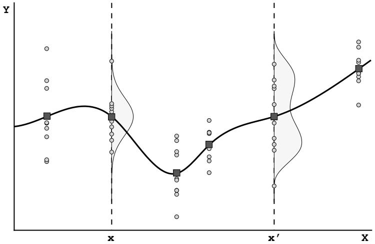

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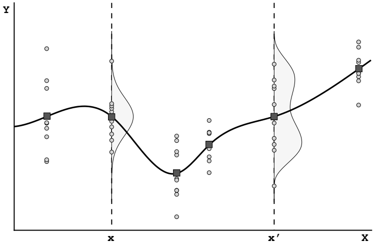
Risk functional: $\mathcal{E}(f) := \int_Z (y - f(x))^2 d\rho$

Setting - Model



ρ unknown measure on
$Z := X \times Y$
$d\rho(x,y) = d\rho(y|x)d\rho_X(x)$
$\operatorname{supp} \rho(\cdot|x) \subseteq [-M.M],\ x \in X$
Goal: estimate the regression function

$$f_\rho(x) := \int_Y y d\rho(y|x) = \mathbb{E}(y|x)$$

Risk functional: $\mathcal{E}(f) := \int_Z (y - f(x))^2 d\rho \rightsquigarrow$

$$\mathcal{E}(f) = \mathcal{E}(f_\rho) + \|f - f_\rho\|^2_{L_2(X,\rho_X)}, \quad \|\cdot\| := \|\cdot\|_{L_2(X,\rho_X)}$$

Estimators

Key issue: proper balance of bias and variance

- Adaptive Tree Partitioning
- Greedy algorithms

$\rightsquigarrow$ universality, i.e., realization of best rates without a priori knowledge about the searched regression function

A Performance Theorem

Bench mark: $f \in L_2(X, \rho_X) \rightsquigarrow \mathcal{T}(f, \eta)$ via $L_2(X, \rho_X)$- projections

$$|f|^p_{\mathcal{B}^s} := \sup_{\eta > 0} \eta^p \#(\mathcal{T}(f, \eta)), \quad \text{where } p := (s + 1/2)^{-1} \quad \rightsquigarrow$$

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If $f_\rho \in \mathcal{B}^s$ for some $s > 0$ then for $\beta > 0$ (arbitrary fixed), n samples, then

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$$\mathbb{E}(\|f_\rho - f_{\mathbf{z}}\|^2) \le C \left(\frac{d \log N}{N} \right)^{\frac{2s}{2s+1}}$$

Moreover, the scheme is universally consistent and need not know s.

Comments

- the convergence rates are best possible for a given "regularity" order $s > 0$;
- the smaller s the weaker the hypothesis, $\mathcal{B}^0 = L_2(X, \rho_X)$;
- to achieve this rate the algorithm does not need to know the property $f_\rho \in \mathcal{B}^s$ but automatically exploits such a property (adaptivity $\rightsquigarrow$ universality);
- for arbitrary densities ρ and piecewise polynomial estimators the estimates in probability hold only for piecewise constants, higher orders require restrictions on ρ, the rate in expectation holds for higher order piecewise polynomial estimators;
- analogous results are valid for tree based adaptive classifiers

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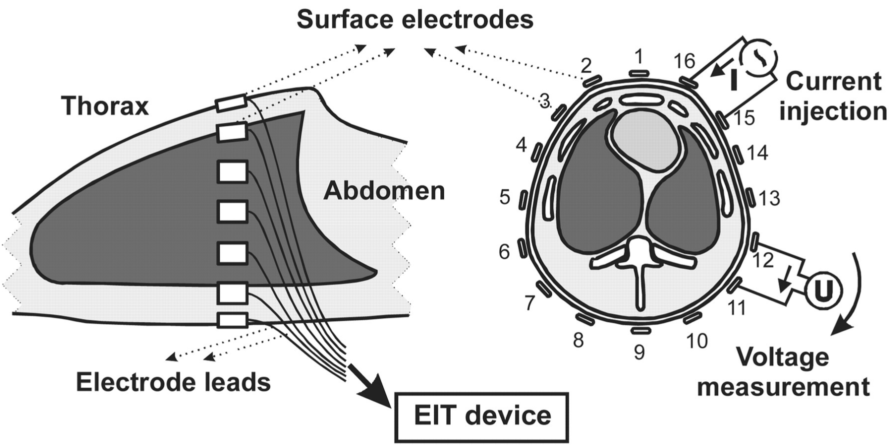
Example: Electron Impedance Tomography: “many parameters...”



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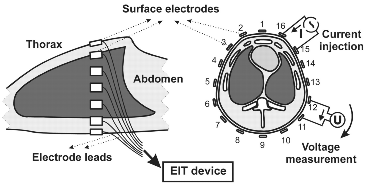

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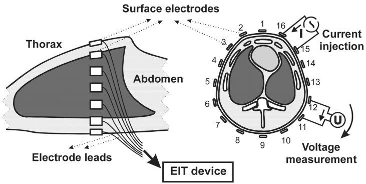

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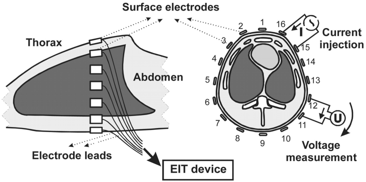

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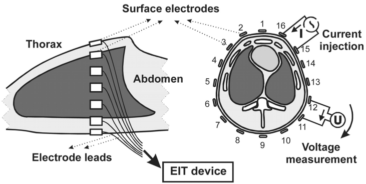

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Inverse problem: find $a(\omega, x) = a_0(x) + \sum_{j \in \mathbb{N}} y_j \psi_j(x) = a(y, x)$

Solution Manifold...

Find $u \in \mathcal{H}$, s.t.

$$F(u, y) = 0, \quad y \in \mathcal{Y} \quad \rightsquigarrow \mathcal{M} := \{u(y) \in \mathcal{H} : F(u(y), y) = 0\}$$

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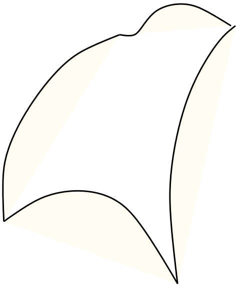
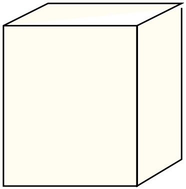


solution manifold $\mathcal{M}$



parameter domain $\mathcal{Y}$

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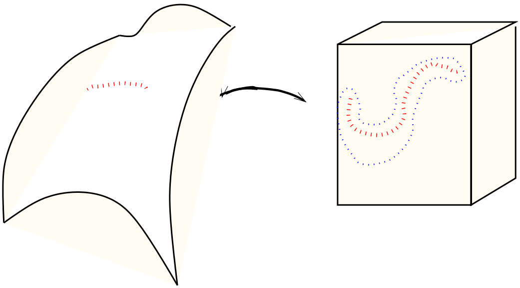

data: $d = \ell(u(y^*)) \in \mathbb{R}^d$ find the parameters $y^* \in \mathcal{Y}$

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