Knowledge- and data-driven modeling for inverse problems

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$$y = A(x_{\mathsf{true}}) + e.$$

• $y \in Y$ Data

• $x_{\mathsf{true}} \in X$ Image

ullet $\mathcal{A}:X o Y$ Forward operator

• $e \in Y$ Noise

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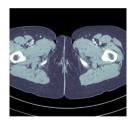
Image

• $x_{\mathsf{true}} \in X$ • $A: X \to Y$

Forward operator

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Noise





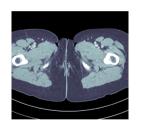
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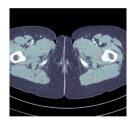
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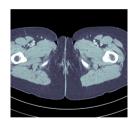
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Knowledge-driven: Model is prescribed beforehand using reductionistic approach, data is used to calibrate model.

- + Model design strongly guided by first principles (explicit laws and dependencies encoded by equations) that can be tested and validated independently.
- + Rather moderate data requirements.
- + Provides conceptual simplification aiding understanding.
- + Highly successful in natural and engineering sciences.

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- + Highly successful in natural and engineering sciences.
- Requires explicitly describing all causal relations, so less successful when first principles are unavailable or unreliable (life sciences, social and behavioral sciences, finance, ...).
- Difficult to account for statistical properties in data (uncertainty quantification).

Data-driven: Model is learnt from data without resorting to any first principles using assumptions about its statistical properties.

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- Can capture complicated causal relations without making strong limiting assumptions.
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- + Requires a lot of sufficiently informative data.
- Can capture complicated causal relations without making strong limiting assumptions.
- + Based from outset on a model for statistical properties in data.
- Does not provide any conceptual simplification.
- Not easy to incorporate a priori knowledge.

Knowledge driven modelling

- Analytic pseudoinverse (FBP, FDK) $x = A^{\dagger}(y)$
- Iterative methods (ART, SART)

$$x_{i+1} = x_i - \omega \mathcal{A}^* (\mathcal{A}(x_i) - y)$$

Variational methods (TV, TGV, Huber)

$$x = \arg\min_{x} ||\mathcal{A}(x) - y||_{Y}^{2} + \lambda ||\nabla x||_{1}$$

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Pseudo-inverse methods are analytic (e.g.) one-pass methods. For example, if \mathcal{A} is an invertible matrix, an analytic inverse is simply the matrix inverse.

Problem 1: For many problems an inverse does not exist or is not unique.

Solution 1: We can use a pseudo-inverse $\mathcal{R}=\mathcal{A}^{\dagger}$

Problem 2: For many problems an inverse exists but it is not bounded! Example $A: \ell^2 \to \ell^2$

$$\mathcal{A}([x_1, x_2, x_3, \dots]) = [x_1, x_2/2, x_3/3, \dots]$$

$$\mathcal{A}^{-1}([y_1, y_2, y_3, \dots]) = [y_1, 2y_2, 3y_3, \dots]$$

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What are iterative methods?

Iterative methods define a sequence of iterates

 x_1, x_2, \dots

Example: Landwebers method (ART, SIRT)

$$x_{i+1} = x_i - \omega \mathcal{A}^* (\mathcal{A}(x_i) - y)$$

 \mathcal{A}^* is the *adjoint* operator

$$\langle \mathcal{A}(x), y \rangle_Y = \langle x, \mathcal{A}^*(y) \rangle_X$$

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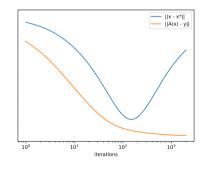
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What are variational methods?

Variational methods are methods based on the calculus of variations. They are formulated as minimization problems, for inverse problems typically of the form

$$\min_{f} \left[D(f;g) + R(f) \right]$$

with

- given data g according to a forward model,
- data discrepancy functional $D(\cdot; g)$,
- regularization functional R

Typical example: Total Variation (TV) regularization with L^2 data term:

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Optimization example: linearized ADMM

Example: The Alternating Direction Method of Multipliers (ADMM) is a popular method for the solution of problems

$$\min_{f} \left[F(f) + G(Lf) \right]$$

with convex functionals F and G and a linear operator L. The linearized variant uses the following iteration (τ and σ are parameters, $z^{(0)} = u^{(0)} = 0$):

$$f^{(k+1)} = \operatorname{prox}_{\tau F} \left[f^{(k)} - \frac{\tau}{\sigma} L^* \left(L f^{(k)} + u^{(k)} - z^{(k)} \right) \right]$$

$$z^{(k+1)} = \operatorname{prox}_{\sigma G} \left[L f^{(k+1)} + u^{(k)} \right]$$

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Here, prox is the proximal operator of a functional

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Implementation of linearized ADMM

```
def admm_linearized(f, F, G, L, tau, sigma, niter):
     z = u = L.range.zero()
     for i in range(niter):
           f[:] = F.proximal(tau)(f - tau / sigma * L.adjoint(L(f) + u - z))
           z = G.proximal(sigma)(L(f) + u)
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        z = G.proximal(sigma)(L(f) + u)
        u = L(f) + u - z
```

Notable:

- Implementation uses ODL, a Python framework for inverse problems
- L is an Operator that can be queried for its domain and range (actually codomain).
- F and G are Functionals that can be queried for their proximal operators.
- L.adjoint is again an Operator.

Task: Does the image contain a rabbit?

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Knowledge driven modelling:

Connected structure consisting of fused ellipsoids, two specific elongated structures near each other (ears), fibre-like texture (fur) with specific range of colours, ... then it is a rabbit!

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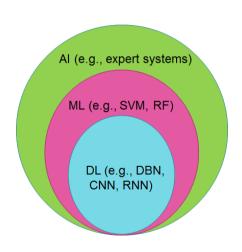
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- Artificial Intelligence (AI): Any technique that enables computers to mimic human intelligence
- Machine learning (ML): A subset of AI using statistical techniques to enable machines to learn from data
- Deep Learning (DL): A subset of ML where complicated tasks are performed by breaking them down into several layers



Data-driven modeling Machine learning: History

- Early history (1950–1990)
 - First artificial neural network computational machines in 1954
 - The perceptron for pattern recognition introduced in 1958.
 - First functional networks with many layers introduced in 1965.

Stagnation: Basic perceptrons cannot process the exclusive-or circuit (1969) and computers not powerful enough.

- Deep convolutional neural networks (2000)
 Series of papers in early 2000s showing state-of-the-art results for many tasks.
 Key aspects
 - Many network layers & huge amount of training data.
 - Massively paralleled GPU based implementations.
 - Optimisation algorithms (effective initializations & stochastic gradient descent).

Data-driven modeling Machine learning: History

- Applications: Began with written digit recognition (classification), moving towards tasks associated with vision, speech recognition & natural language processing.
 - Denoising: BM2D performed better than any known image denoising algorithm in 2012.
 - Single image super-resolution
 - Demosaicing
 - Deblurring
 - Segmentation
 - Image annotation
 - Face recognition
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Deep learning currently addresses many image processing tasks with unsurpassed results.

Data-driven modeling Machine learning: In the news



Tech

11,281 VIEWS FEB 19, 2015 @ 01:06 PM

Microsoft's Deep Learning Project **Outperforms Humans** In Image Recognition



Google's DeepMind Achieves **Speech-Generation Breakthrough**

by Jaramy Kahn

September 9, 2016 - 7:29 AM EDT

MIT **Technology** Review

Deep Learning Machine Beats Humans in IQ Test

Computers have never been good at answering the type of verbal reasoning questions found in IQ tests. Now a deep learning machine unveiled in China is changing that.

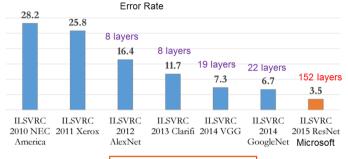
June 12, 2015



Historic Achievement: Microsoft researchers reach human parity in conversational speech recognition

October 18, 2016

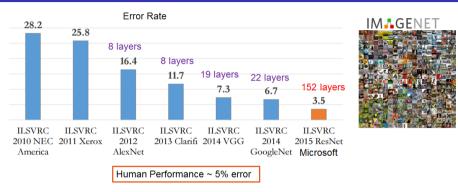
Data-driven modeling Machine learning: In the news



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Human Performance ~ 5% error

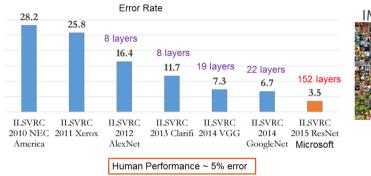
Data-driven modeling Machine learning: In the news



Achievements obtained without theoretical understanding:

- Optimisation solved during learning is highly non-convex and seems intractable from a theoretical viewpoint.
- Unclear what characterises good training data.
- Stability properties of network architectures (adversarial attacks).

Data-driven modeling Machine learning: In the news



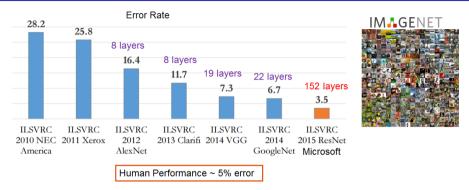


Success stories of deep learning this far confined to tasks that do not require knowledge about how data is generated.

Entirely data-driven tomographic image reconstruction is unfeasible.

As an example, a typical 3D CB-CT problem (512 \times 512 \times 512 voxel) requires a network with at least $\approx 2 \cdot 10^{16}$ connections!!

Data-driven modeling Machine learning: In the news



Hybrid: Combine elements of knowledge- and data-driven approaches for modelling.

Can a hybrid approach be useful for solving ill-posed inverse problems? In particular, can one incorporate the knowledge of a forward operator when designing a neural network for reconstruction?

