Solving Inverse Problems via Joint Modeling with Forward Process Improves Fidelity

Krishnanunni C G
Machine Intelligence Group
Kowshik Thopalli, Yamen Mubarka, Vivek Narayanaswamy, Jayaraman J. Thiagarajan

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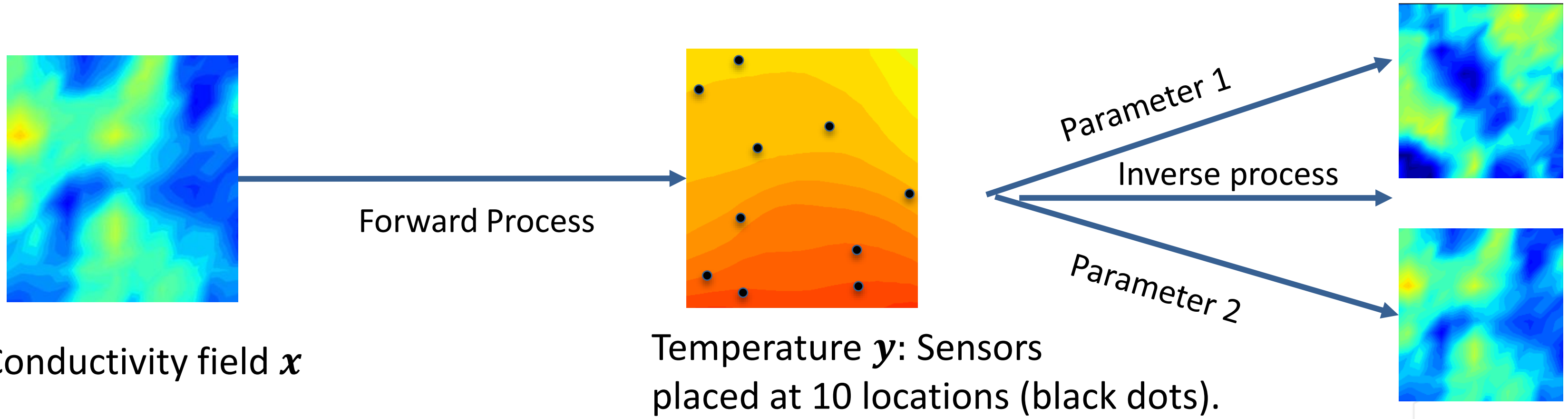
Transformer Architectures Provide a Unique Opportunity to Solve Inverse Problems

Inverse Problems:

Given only partially observed outputs can we recover the inputs that caused them?



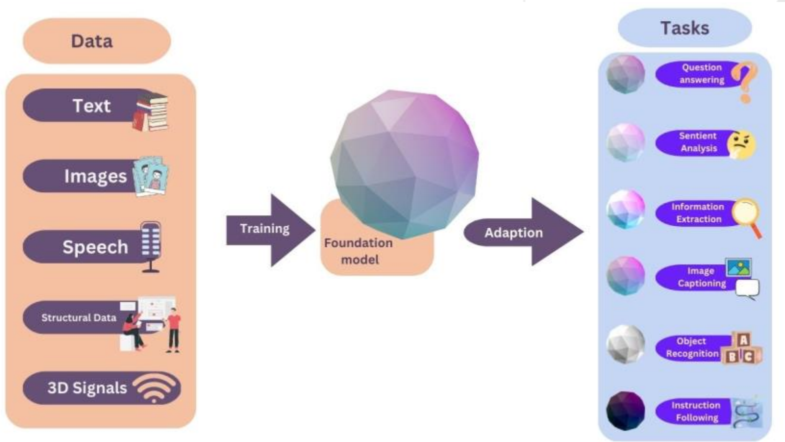
Conductivity field $\boldsymbol{x}$

Temperature $\boldsymbol{y}$: Sensors placed at 10 locations (black dots).

Solution: Determine parameter distribution $q(\boldsymbol{x}|\boldsymbol{y})$ instead of inverse function (which does not exist).

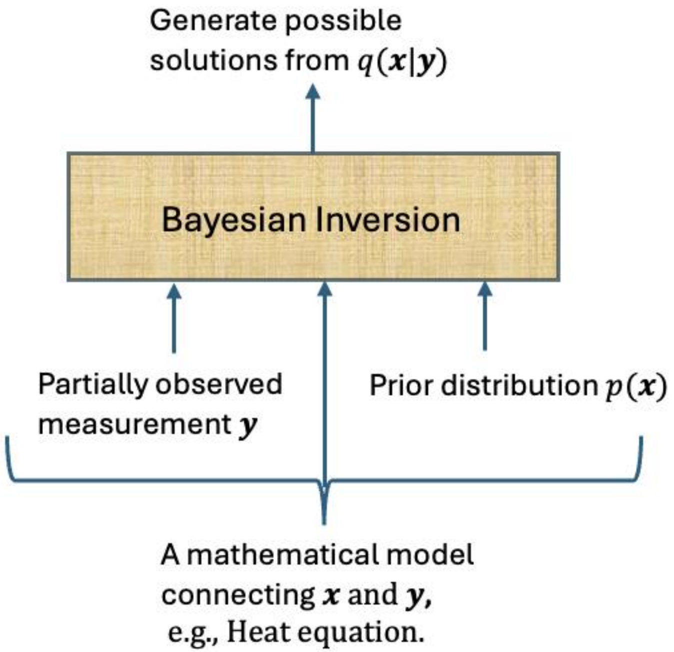
Current deep learning based solutions do not model the forward and inverse processes jointly thus posing fidelity risks.

Transformer architectures which act as unified architectures to map between sequences.

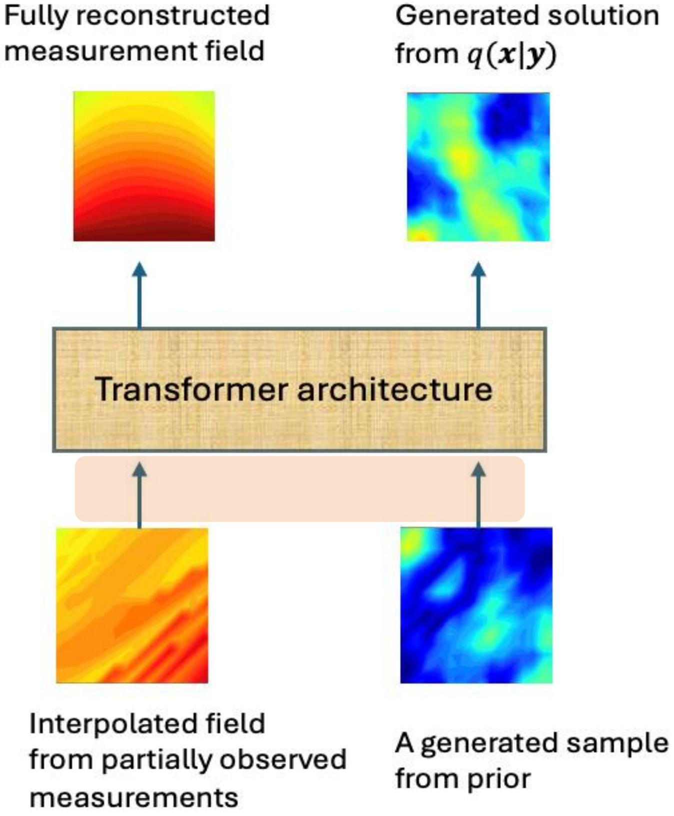


Regression Transformers For Posterior Inference

- Our transformer* architecture takes conductivity field and partially observed temperature field jointly as inputs:
  - a) Interpolated measurement (based on 10 measurements); and b) A generated sample from the prior $p(\boldsymbol{x})$.



Prior $p(\boldsymbol{x})$ may be determined from experience, such as previous experiments.



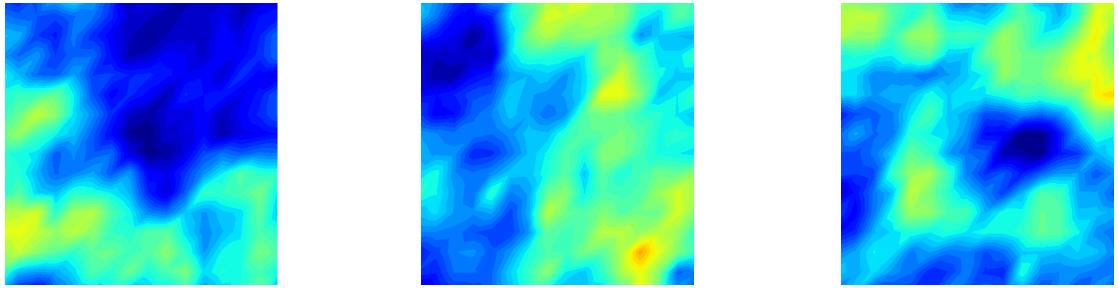
- Output of the transformer:
  - Generated solutions to the inverse problem,
  - Fully reconstructed measurement field.
- *Joint modeling* of prior sample and interpolated measurement to generate a solution.
- We designed novel loss functions to train this unified architecture.
- Once trained, our framework can generate all possible inverse solutions (conductivity fields) for any partially observed temperature field $\boldsymbol{y}$.

Born Jannis, Matteo Mancia. “Regression transformer enables concurrent sequence regression and generation for molecular language model”, Nature Machine Intelligence 5.4 (2023):432-444.

Numerical Results For Conductivity Field Inversion in a 2D Heat Equation

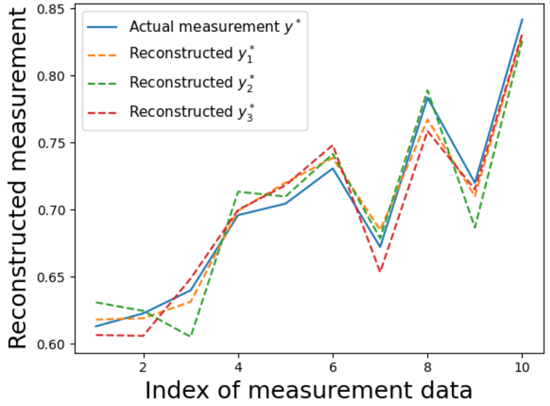
Solved Simultaneously

Solution to the inverse problem: Generated conductivity fields for a particular test measurement input



Solution 1 Solution 2 Solution 3

Let's check if our generated solutions are consistent!



We see that all the solutions produces back the same partially observed temperature field!

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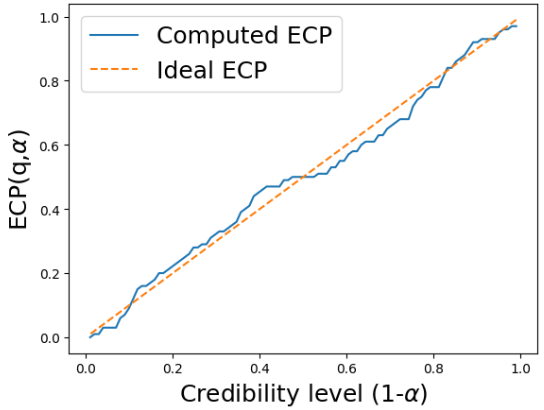
Showing that we can recover all solutions (conductivity field) by our approach!

Solution to the forward problem: Full temperature field reconstruction from generated conductivity fields

Ground truth GPR/Kriging Proposed approach

Black dots measured MSE: 0.0048 MSE: 0.00043



Expected coverage probability (Lemos et al.)
Our method consistently produces accurate solutions