Seminar Series Kickoff

Various Remarks, “Data & Modeling”

Conor Rowan

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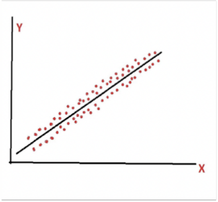
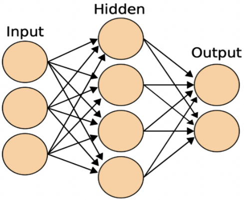
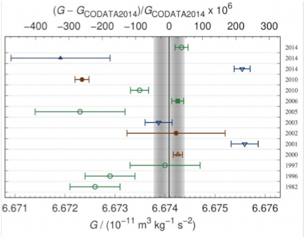
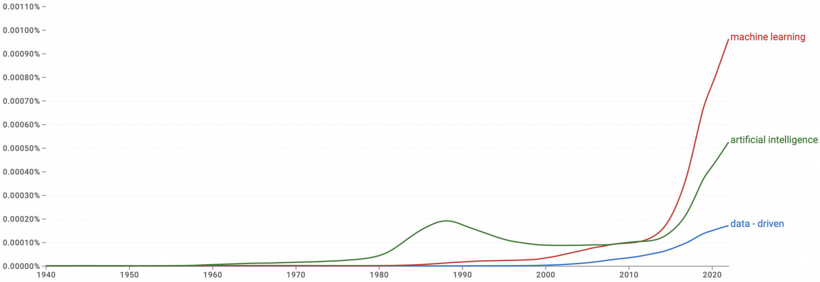






The Data Revolution



- "Big data" has emerged as a new paradigm in science

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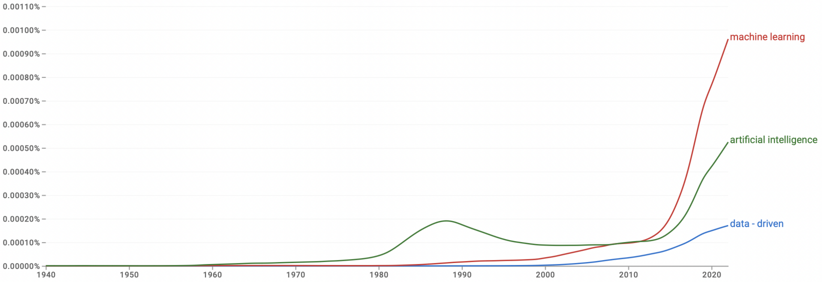

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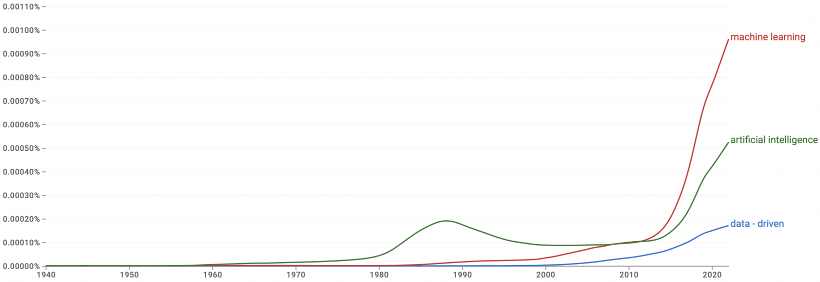

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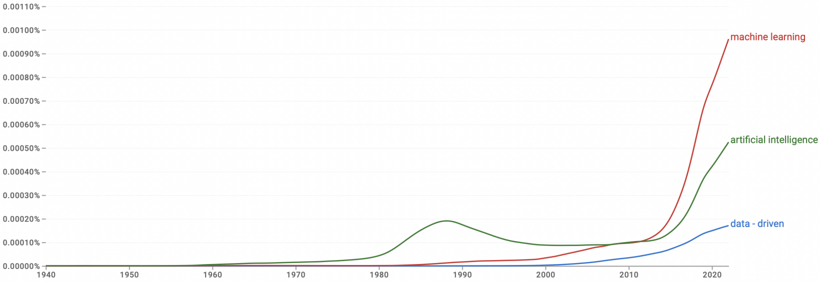

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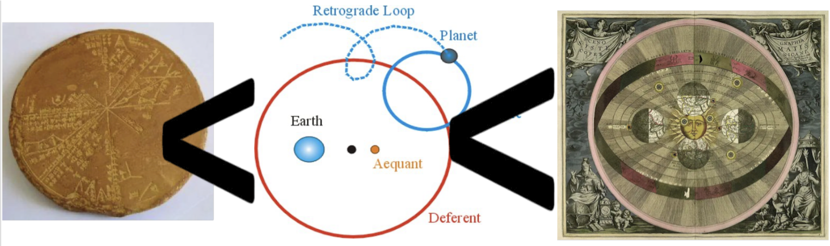
- Lots of success stories: AlphaFold, AlphaGo, DeepBlue, ChatGPT, etc.
- Data-driven models are often contrasted with more traditional rule- and physics-based methods–**does this make sense?**
- Bertrand Russell: "the point of philosophy is to start with something so simple as to seem not worth stating, and to end with something so paradoxical that no one will believe it."

Data-driven, as opposed to what?



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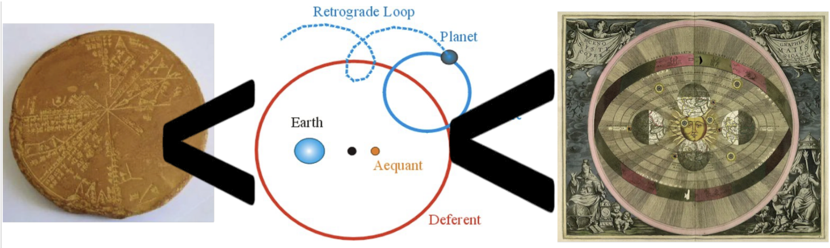

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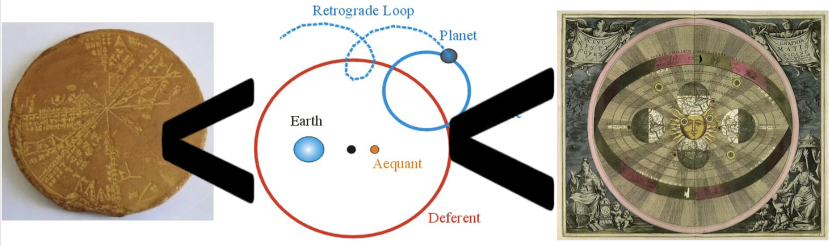

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- Obviously data contributes to the development of basic theory
- Kuhn on theory construction: *"In the absence of a paradigm . . . all of the facts that could possibly pertain to the development of a given science are likely to seem equally relevant. As a result, early fact gathering is a far more nearly random activity than the one that subsequent scientific development makes familiar."* [1]

Theories & data

Egyptian myth

"When bodies were placed in sarcophagi the flesh disappeared, leaving only the bones: so the body was thought to have been absorbed, or eaten, by the stone . . . this is an interesting case of a generalized observation serving as evidence for a magical or mythical view." [2]

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Medieval challenges to Greek science

"[The] attack on science took the form of 'occasionalism'–the doctrine that whatever happens is a singular occasion, governed not by any laws of nature but directly by the will of God." [4]

Assume we have a (good) theory

- For the sake of argument, assume that the theory/model is "correct" (e.g. gravity is an inverse square law, continuum mechanics is the right way to model matter, etc.)

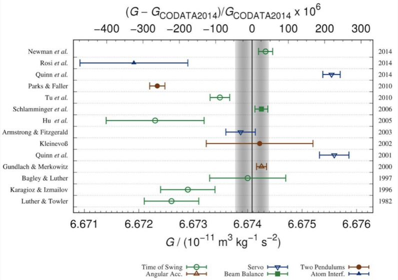

Figure: Measuring the gravitational constant G in $F = GMm/r^2$

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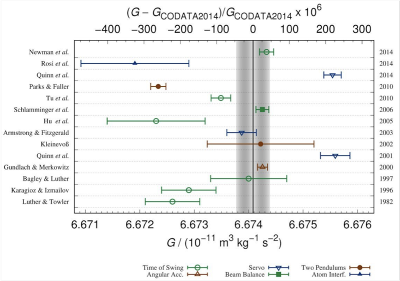

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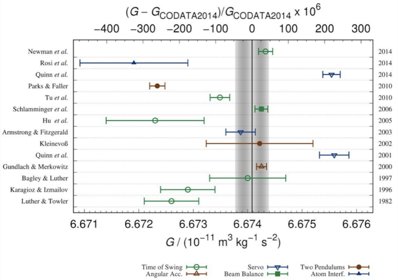
- *Models still have empirical parameters which need to be estimated from data*
- **So what is the difference between physics-based and data-driven modeling?**



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Outlining and classifying some techniques in modeling

- 1) Numerical simulations, 2) regression, 3) classification, 4) equation discovery, 5) generative models, 6) reduced-order models, 7) surrogate models, 8) physics-informed machine learning, 9) data assimilation, 10) constitutive modeling

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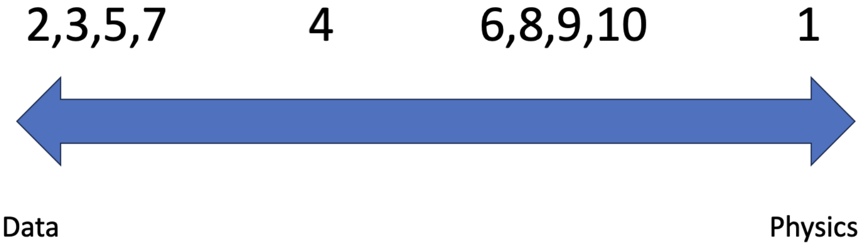

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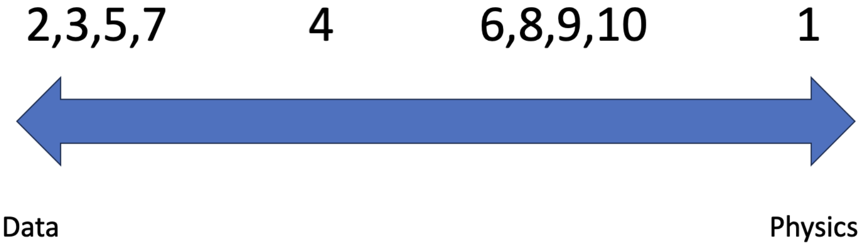
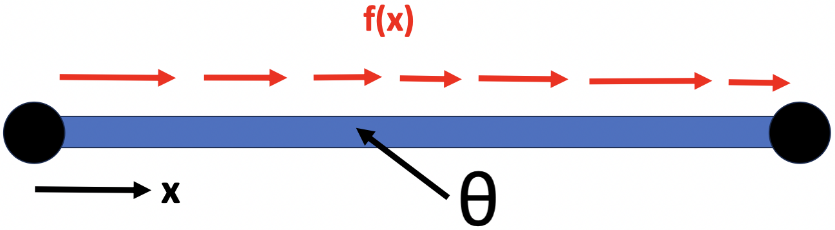


- **Can we make this intuition more precise?**

Canonical mechanics problem



$$\theta \frac{\partial^2 u}{\partial x^2} = f(x), \quad u(0) = u(1) = 0$$

$$u(x) = \int^x \int^y \frac{f(z)}{\theta} dzdy + cx := \mathcal{G}(f(x); \theta)(x)$$

- How do we estimate the material parameter θ if it is unknown?

Constitutive modeling

- Assume that we have data $\hat{u}(x)$ for a given force $f(x)$ at discrete points $x_1, x_2, \ldots, x_N$:

$$\mathcal{L}(\theta) = \frac{1}{2}\sum_{i=1}^{N}\Big(\mathcal{G}(f(x);\theta)(x_i) - \hat{u}(x_i)\Big)^2 \implies \theta = \underset{\theta}{\text{argmin}}\ \mathcal{L}(\theta)$$

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- Something like this has gone on behind the scenes of every physics-based model
- (Experimentalists can correct me if this is the wrong way of thinking about things)

Same problem, different approach

- We have the same data (and boundary conditions) but no knowledge of a governing equation
- Want to fit an input-output relationship–we are going to need more parameters!

$$u(x) = \mathcal{N}(f(x); \theta_1, \theta_2, \dots)(x)$$

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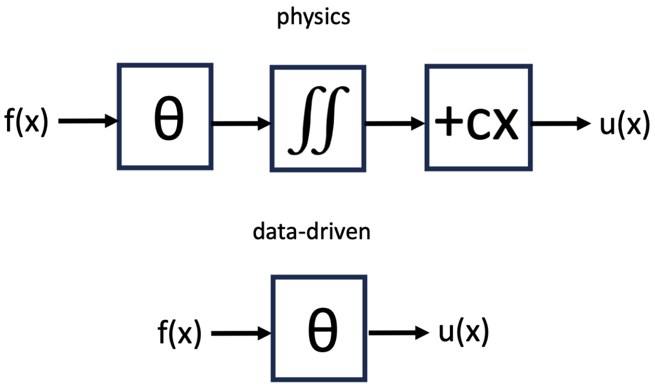
- Choosing the structure of $\mathcal{N}$ is like choosing a regression model (linear, quadratic, neural network, etc.)

What's the difference?



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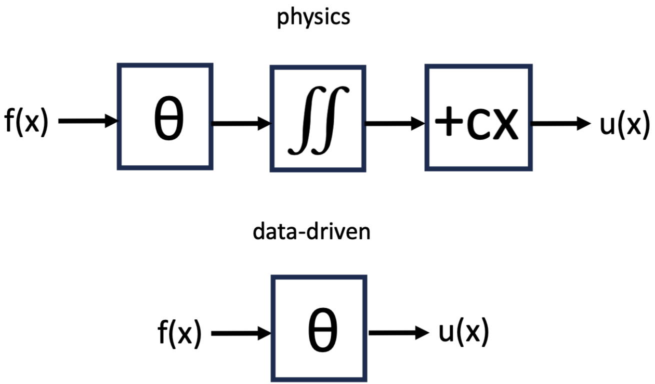

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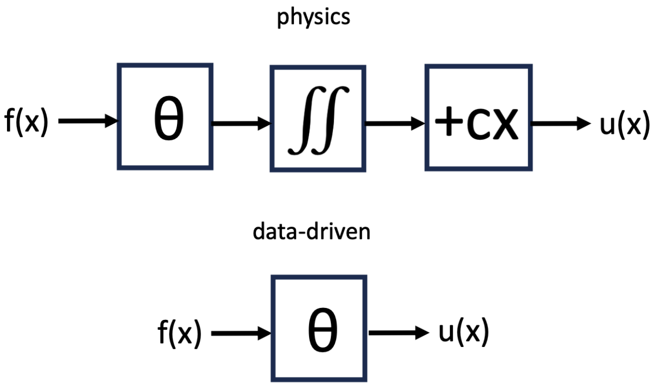

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- Physics model has fewer parameters (?)
- **Why do we expect the physics model to generalize better?**

A complicated story with a simple missing piece

$$\frac{f(x)}{\theta} = \frac{\partial^2 u}{\partial x^2} \implies u(x) = \mathcal{G}(f(x), \theta)(x)$$

- "Applied forces create curvature in the displacement field at a rate controlled by an empirical parameter θ"
- This knowledge is encoded in the operator $\mathcal{G}$, only a small and simple piece of the "story" needs to be filled in
- Small amount of data required

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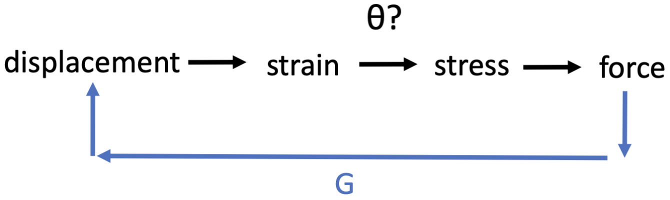
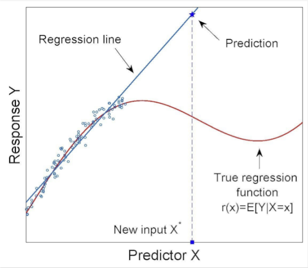
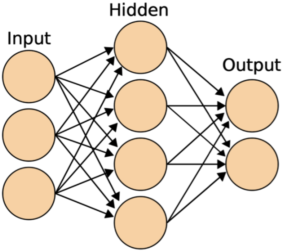


The data-driven model may not learn the story





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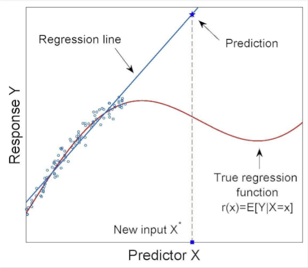

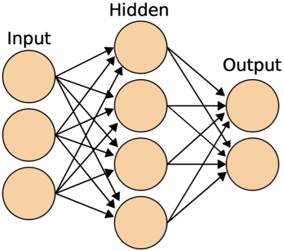

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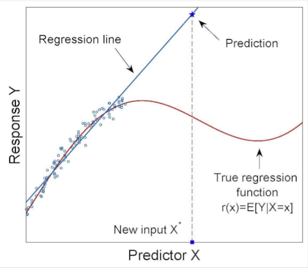

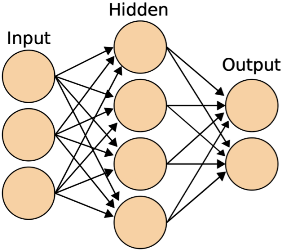

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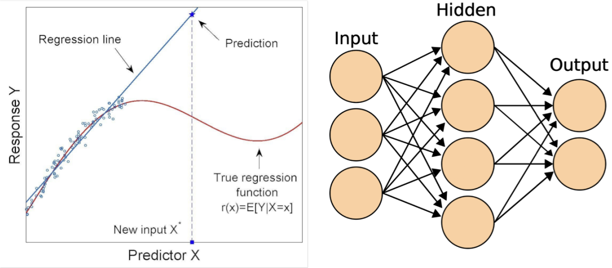

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- The data-driven operator $\mathcal{N}$ is "unstructured" in the sense that it doesn't encode any principles/laws
- Needs a lot of data to even have a chance of being useful

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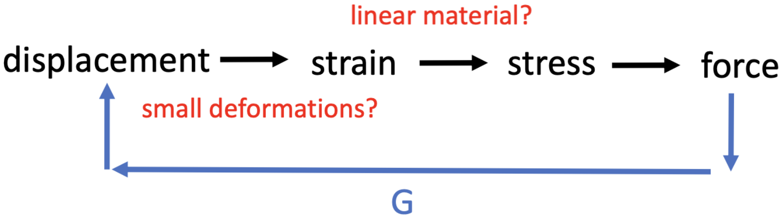
- Maybe this tempers optimism as well? [5]

Another point on generalization



- When an operator is structured, it is built up from a number of steps which have clear assumptions
- Knowing the assumptions helps assess/predict generalization properties of the model

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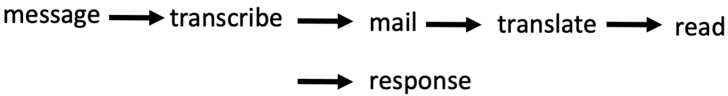
Visualizing the two cases



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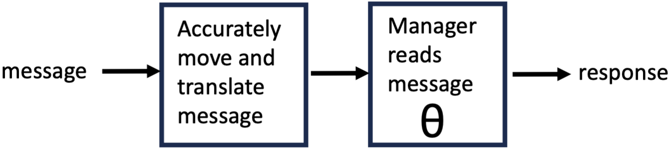
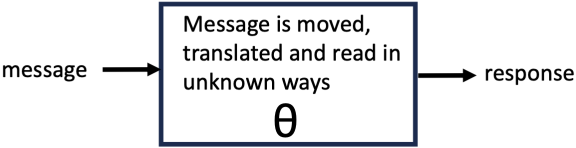


Case 2



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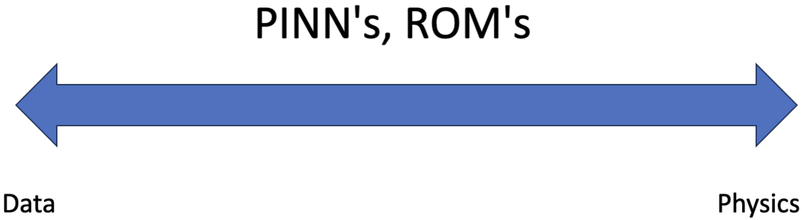
- When we don't know what mediates inputs and outputs, the "black box" is our only hope...

Applying this argument to an example



- Physics-informed neural networks (PINN's) and reduced-order models (ROM's) occupy an intermediate position between data and physics
- Can use the "operator structure" argument to justify this
- We will consider these two examples

PINN's (actually Deep Operator Network)

- Physics-informed Deep Operator Networks [6,7] build physics into a data-driven model in an unusual way
- Using a particular discretization of the solution (neural networks), tune parameters such that data is matched AND governing equations are satisfied:

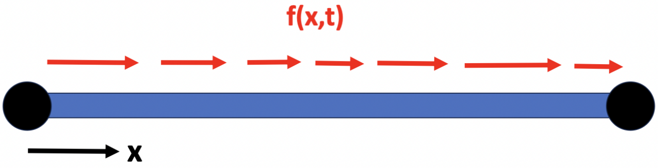
$$u(x) = \sum_i c_i(f(x);\theta)\Psi_i(x;\theta)$$

$$\mathcal{L}^{data}(\theta) = \frac{1}{2}\sum_j \Big(\sum_i c_i(f(x);\theta)\Psi_i(x_j;\theta) - \hat{u}(x_j)\Big)^2$$

$$\mathcal{L}^{physics}(\theta) = \frac{1}{2}\sum_j \Big(\sum_i c_i(f(x);\theta)\frac{\partial^2\Psi_i}{\partial x^2}(x_j;\theta) - f(x_j)\Big)^2$$

$$\theta = \underset{\theta}{\operatorname{argmin}}\ \mathcal{L}^{data}(\theta) + \mathcal{L}^{physics}(\theta)$$

ROM – dynamic bar



$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} - f(x,t), \quad u(x,0) = u(0,t) = u(1,t) = 0$$

$$u(x,t) \approx \sum_{i=1}^{N} a_i(t)\Psi_i(x)$$

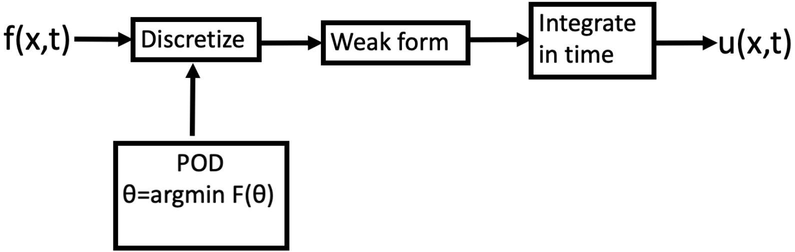
- Cannot write down solution for dynamics of elastic bar, the problem must be solved numerically
- Solution expanded with time varying coefficients $a_i(t)$ scaling given spatial shape functions $\Psi_i(x)$

Proper orthogonal decomposition (POD)

$$\underline{\underline{X}} = \begin{bmatrix} u(x_1, t_1) & u(x_2, t_1) & \dots & u(x_N, t_1) \\ u(x_1, t_2) & u(x_2, t_2) & \dots & u(x_N, t_2) \\ \vdots & \vdots & \dots & \vdots \\ u(x_1, t_T) & u(x_2, t_T) & \dots & u(x_N, t_T) \end{bmatrix}$$

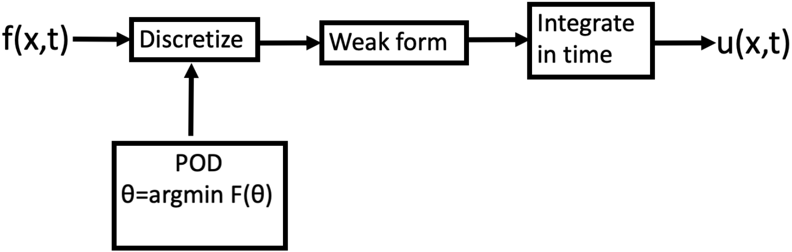
- POD is a common model reduction technique
- Uses data on a dynamical system to find an "optimal" set of spatial shape functions $\Psi_i(x)$ [8]
- Using our same notation, we could say abstractly that $\Psi_i(x) = \Psi_i(x; \theta)$ because they are computed from data

Operator structure with POD



- Data used to compute the spatial shape functions $\Psi_i(x)$

Operator structure with POD



- Data used to compute the spatial shape functions $\Psi_i(x)$
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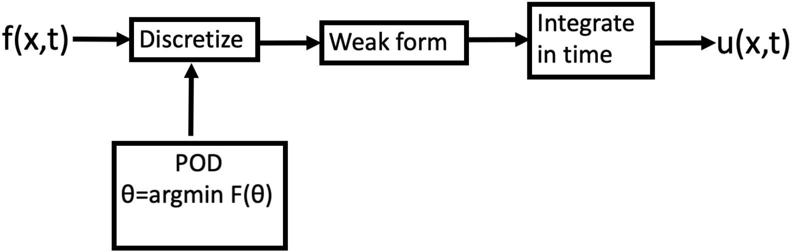

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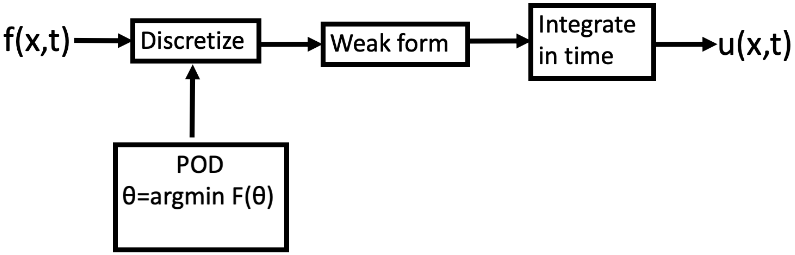
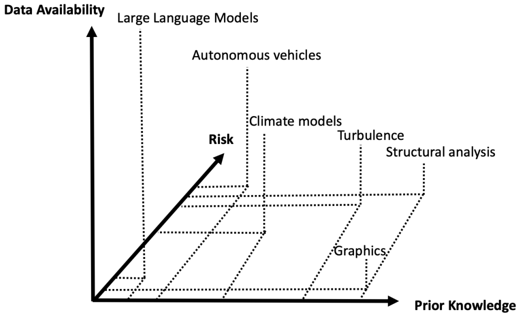


- Data used to compute the spatial shape functions $\Psi_i(x)$
- These inform the "Discretize" step in the operator
- Assumption is that shape functions computed from one forcing will "generalize" to others
- Data plays a more complex role in forming the solution operator than determining a single constitutive parameter, but physics still enforced

Final thought: classifying models along three dimensions



- Talked about data and generalization...are there other things to consider?
- Risk refers to the "cost" associated with model error–this depends on the application and determines the importance of generalization
- More prior knowledge of the problem → more "hard-coded" structure in operator → less data needed → more predictable generalization

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- More structured operators hard-code rules and will tend to generalize better and more predictably
- When deploying a model in the "real world," it is necessary to consider risk
- Data-driven models are best-suited for situations with high data availability, minimal prior knowledge, and low risk

Thanks!

Questions? Comments? Concerns?

References

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[8] Kutz, N., "Optimal basis elements: the POD expansion," YouTube Available: here

Images, in order of appearance

Neural network, available here
Gravitational constant, available here
Plato's academy, available here
Vienna Circle, available here
Crazy plot, available here
Boring presentation, available here
Babylonian tablet, available here
Ptolemiac system, available here
Copernican system, available here
Generalization error, available here