

# Physically Consistent Models

## 3 DESIGN OF DATA SCIENCE MODELS

### 3.1 Theory-guided Specification of Response

choice of model family, link function and probability distribution functions [42]

### 3.2 Theory-guided Design of Model Architecture

modular sub-problems [43]

specifying node connections [44-46]

## 4 LEARNING OF DATA SCIENCE MODELS

### 4.1 Theory-guided Initialization

pretraining strategies [47-49]

### 4.2 Theory-guided Probabilistic Models

graph estimation techniques, graph Lasso [50]

introduce priors in the model space [26,27][51]

### 4.3 Theory-guided Constrained Optimization

linear equality or inequality conditions [25][52-54][57]

partial differential equations (PDE) [55,56][58,59]

### 4.4 Theory-guided Regularization

variants of Lasso, e.g. group Lasso [28][31][60-66]

multitask learning formulations [59][67]

## 5 REFINEMENT OF DATA SCIENCE OUTPUTS

### 5.1 Using Explicit Domain Knowledge

### 5.2 Using Implicit Domain Knowledge

## 6 LEARNING HYBRID MODELS OF THEORY AND DATA SCIENCE

## 7 AUGMENTING THEORY-BASED MODELS USING DATA SCIENCE

### 7.1 Data Assimilation in Theory-based Models

### 7.2 Calibrating Theory-based Models using Data