

Machine Learning in Astrophysics

Machine Learning for Physics; Physics for Machine Learning

Jason D. McEwen

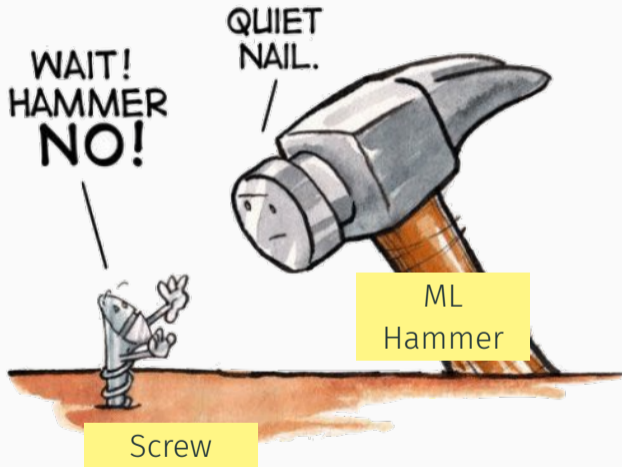
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Mullard Space Science Laboratory (MSSL), University College London (UCL)

Alan Turing Institute, Space Science Interest Group seminar

September 2023

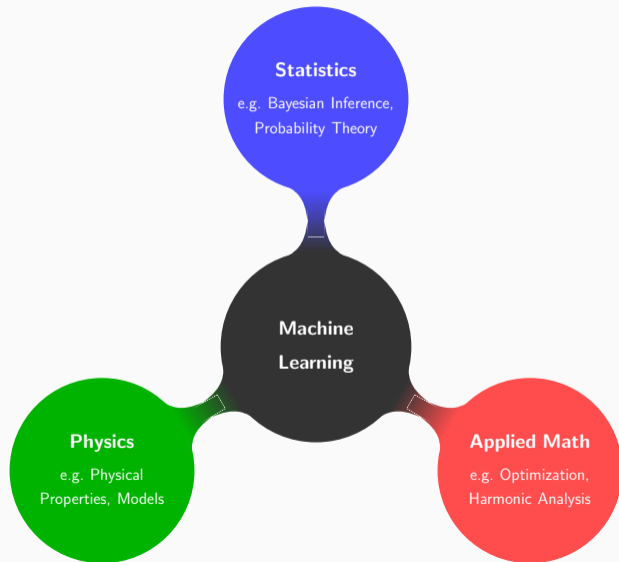
The machine learning hammer

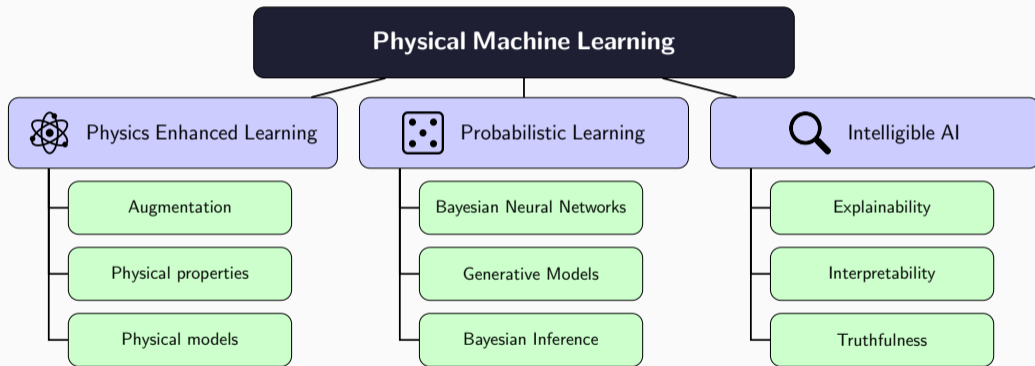


The machine learning cog



Merging paradigms



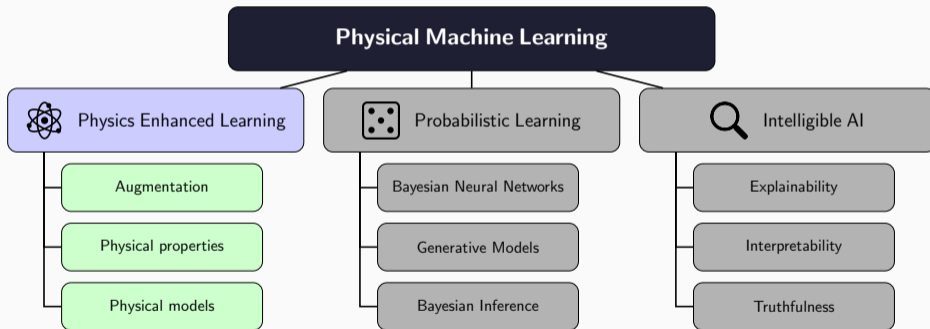


Physics Enhanced Learning

Physics Enhanced Learning

Embed physical understanding of the world into machine learning models.

(See review by Karniadakis *et al.* 2021.)





Apply **physical transformations** that data known to satisfy to augment training data \rightsquigarrow ML model **learns physics through training**.

Augmentation



Apply **physical transformations** that data known to satisfy to augment training data \rightsquigarrow ML model **learns physics through training**.

- ▷ Common to augment image data-set with rotations, flips, shifts, scales, contrast, ...

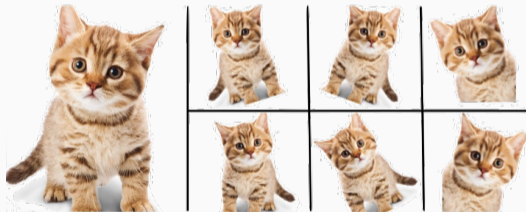
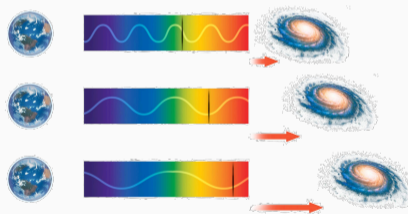


Image augmentation



Apply **physical transformations** that data known to satisfy to augment training data \rightsquigarrow ML model **learns physics through training**.

- ▷ Redshift augmentation of supernovae observations (Boone 2019, Alves *et al.* 2022, 2023)



Redshift augmentation



Apply **physical transformations** that data known to satisfy to augment training data \rightsquigarrow ML model **learns physics through training**.



▷ Data efficiency suffers: data “used” to learn physics, rather than problem.

Physical properties: geometries, symmetries, conservation laws



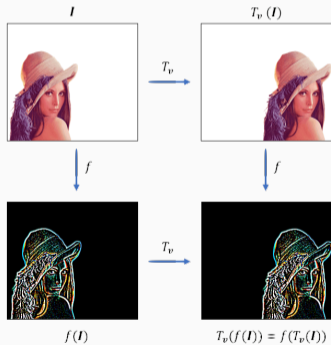
Encode **physical properties** of the world into ML models (e.g. geometry, symmetries, conservation laws) \rightsquigarrow **Physics embedded in architecture** of ML model.

Physical properties: geometries, symmetries, conservation laws



Encode physical properties of the world into ML models (e.g. geometry, symmetries, conservation laws) \rightsquigarrow **Physics embedded in architecture** of ML model.

- ▷ Key factor CNNs so successful is due to encoding translational equivariance.



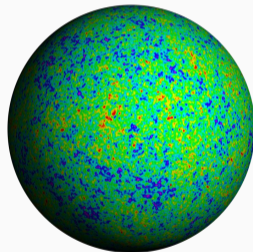
Translational equivariance

Physical properties: geometries, symmetries, conservation laws



Encode physical properties of the world into ML models (e.g. geometry, symmetries, conservation laws) \rightsquigarrow **Physics embedded in architecture** of ML model.

- ▷ Geometric deep learning on the sphere
(Cobb et al. 2021; McEwen et al. 2022;
Ocampo, Price & McEwen 2023)



CMB observed on the
celestial sphere

Physical properties: geometries, symmetries, conservation laws



Encode physical properties of the world into ML models (e.g. geometry, symmetries, conservation laws) \rightsquigarrow **Physics embedded in architecture** of ML model.

- ▷ Equivariant machine learning, structured like classical physics (Villar *et al.* 2021)

Orthogonal	$O(d) = \{Q \in \mathbb{R}^{d \times d} : Q^T Q = Q Q^T = I_d\}$,
Rotation	$SO(d) = \{Q \in \mathbb{R}^{d \times d} : Q^T Q = Q Q^T = I_d, \det(Q) = 1\}$
Translation	$T(d) = \{w \in \mathbb{R}^d\}$
Euclidean	$E(d) = T(d) \times O(d)$
Lorentz	$O(1, d) = \{Q \in \mathbb{R}^{(d+1) \times (d+1)} : Q^T \Lambda Q = \Lambda, \Lambda = \text{diag}([1, -1, \dots, -1])\}$
Poincaré	$IO(1, d) = T(d+1) \times O(1, d)$
Permutation	$S_n = \{\sigma : [n] \rightarrow [n] \text{ bijective function}\}$

Groups considered

Physical properties: geometries, symmetries, conservation laws



Encode **physical properties** of the world into ML models (e.g. geometry, symmetries, conservation laws) \rightsquigarrow **Physics embedded in architecture** of ML model.



- ▷ Highly computationally demanding.
- ▷ Always required?

Physical properties: geometries, symmetries, conservation laws



Encode **physical properties** of the world into ML models (e.g. geometry, symmetries, conservation laws) \rightsquigarrow **Physics embedded in architecture** of ML model.



- ▷ Highly computationally demanding.
- ▷ Always required?



- ▷ Develop efficient algorithms (e.g. Ocampo, Price & McEwen 2023).
- ▷ Inductive biases not enforced.

Physical models: PINNS and differentiable physics

Encode physical models of world into ML models:



1. Encode dynamics (differential equations) via loss functions (PINNs).
2. Embed full (differentiable) physical models inside ML model.

↪ **Physics learned in training and embedded in model.**

Physical models: PINNs and differentiable physics

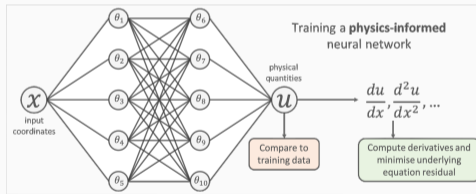
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- ▷ Physics informed neural networks (PINNs) encode differentiable equations (e.g. boundary conditions) in loss.



PINNs

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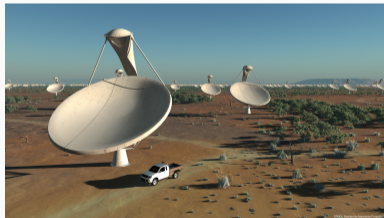


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▷ Differentiable physical models

- ▶ Radio interferometric telescope
(Mars *et al.* 2023, in prep.)
- ▶ Optical PSF
(Liaudat *et al.* 2023)
- ▶ JAX-Cosmo
(Campagne *et al.* 2023)



SKA (artist impression)

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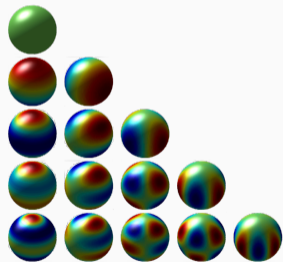


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▷ Differentiable mathematical methods

- ▶ Fourier transforms
- ▶ Spherical harmonic transforms
(`s2fft`; Price & McEwen, in prep.)
- ▶ Spherical wavelet transforms
(`s2wav`; Price *et al.* in prep.)
- ▶ Spherical scattering transforms
(Mousset, Price, Allys, McEwen, in prep.)



Spherical harmonics

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- ▷ Full physical models requires differentiable programming frameworks.

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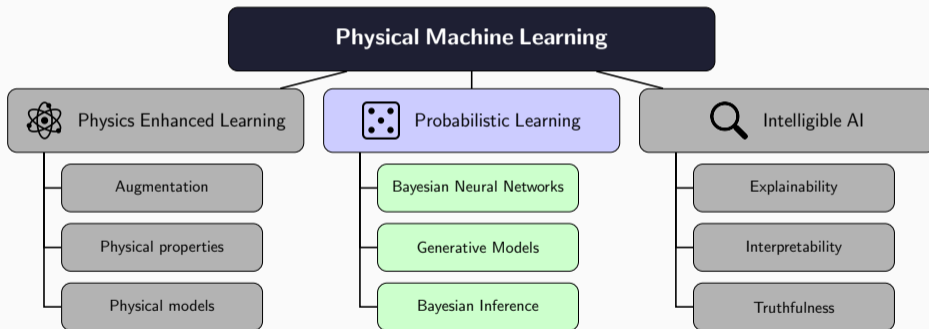
- ▷ Capture full physics with differentiable models!
- ▷ Emulators also provide differentiability (e.g. `CosmoPower`; Spurio Mancini et al. 2021).
- ▷ Write new differentiable codes (e.g. `s2fft`; Price & McEwen, in prep.).

Probabilistic Learning

Probabilistic Learning

Embed a probabilistic representation of data, models and/or outputs.

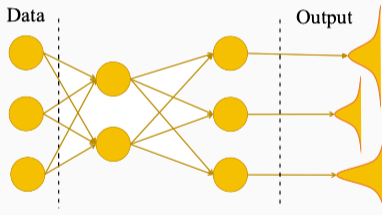
(See Murray 2022.)



Bayesian neural networks for uncertainty quantification



Bayesian neural networks incorporate **probabilistic representation** to quantify **uncertainty of outputs** (idea pioneered by MacKay 1992).

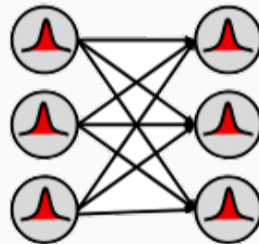


Bayesian neural networks for uncertainty quantification



Bayesian neural networks incorporate **probabilistic representation** to quantify **uncertainty of outputs** (idea pioneered by MacKay 1992).

- ▷ MC Dropout (Gal & Ghahramani 2016): drop nodes probabilistically to sample an ensemble of networks.

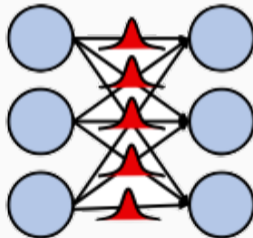


Bayesian neural networks for uncertainty quantification



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- ▷ Bayes by Backprop (Blundel *et al.* 2015): model distribution of weights (by variational inference).



Bayesian neural networks for uncertainty quantification



Bayesian neural networks incorporate **probabilistic representation** to quantify **uncertainty of outputs** (idea pioneered by MacKay 1992).

- ▷ Probabilistic ML frameworks
(e.g. TensorFlow Probability).



Bayesian neural networks for uncertainty quantification



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- ▷ Encode epistemic uncertainty of model.
- ▷ But what does the output distribution represent?
- ▷ Requires careful consideration of training data.

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- ▷ Statistical validation (hold that thought... see upcoming Truthfulness section).



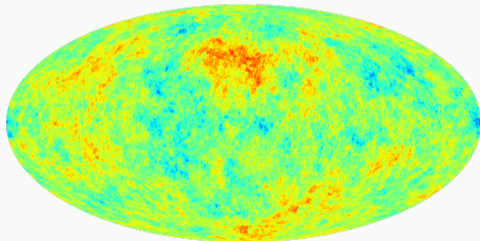
Generative models **learn a prior distribution** from data for sampling and/or evaluating probabilities.

Generative models



Generative models **learn a prior distribution** from data for sampling and/or evaluating probabilities.

- ▷ Emulation: sample from learned prior
(Perraudin *et al.* 2020, Allys *et al.* 2020, Price *et al.* 2023, Price *et al.* in prep.)



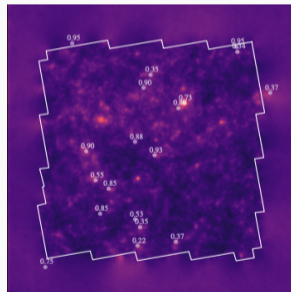
Emulated cosmic string maps
(**stringgen**, Price *et al.* 2023, Price *et al.* in prep.)

Generative models



Generative models **learn a prior distribution** from data for sampling and/or evaluating probabilities.

- ▷ Integrate learned priors into analysis
(Remy *et al.* 2022, McEwen *et al.* 2023)



Learn convergence field prior
(Remy *et al.* 2022)

Generative models



Generative models **learn a prior distribution** from data for sampling and/or evaluating probabilities.



- ▷ Availability and representativeness of training data.
- ▷ Truthfulness, *e.g.* diversity of ML model often lacking.

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- ▷ Public datasets/benchmarks (*e.g.* BASE, IllustrisTNG, CAMELS, Quijote, CosmoGrid).
- ▷ Meta sampling to recover distribution over manifold (*e.g.* Price *et al.* 2023).
- ▷ Truthfulness (hold that thought... see upcoming Truthfulness section).



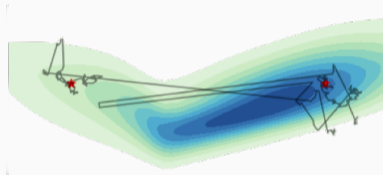
ML techniques can be integrated into Bayesian frameworks to **enhance accuracy and computational efficiency**, making some approaches accessible that were previously intractable.

Bayesian inference



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- ▷ Enhanced MCMC for parameter estimation (Grabrie *et al.* 2022, Karamanis *et al.* 2022).



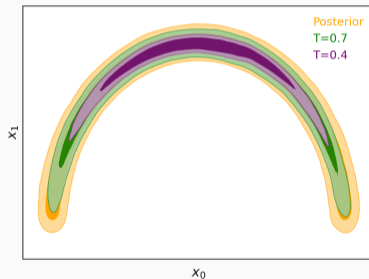
Learned proposal distributions

Bayesian inference



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- ▷ Enhanced Bayesian model selection (**harmonic**; McEwen *et al.* 2021, Polanska *et al.* 2023).



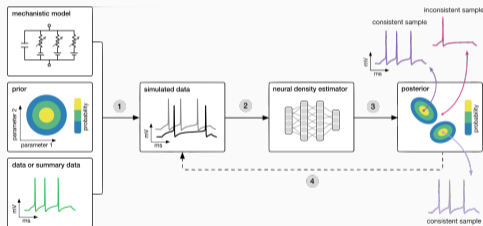
Learned harmonic mean estimator
(**harmonic**)

Bayesian inference



ML techniques can be integrated into Bayesian frameworks to **enhance accuracy and computational efficiency**, making some approaches accessible that were previously intractable.

- ▷ Simulation-based inference (Alsing *et al.* 2018, Cranmer *et al.* 2021).
- ▷ Model selection for simulation-based inference (**harmonic**; Spurio Mancini *et al.* 2022)



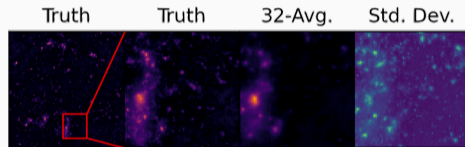
`sbi`

Bayesian inference



ML techniques can be integrated into Bayesian frameworks to **enhance accuracy and computational efficiency**, making some approaches accessible that were previously intractable.

- ▷ Variational inference
(Whitney *et al.* in prep.)



Mass mapping with uncertainties
by variational inference

Bayesian inference



ML techniques can be integrated into Bayesian frameworks to **enhance accuracy and computational efficiency**, making some approaches accessible that were previously intractable.



- ▷ Availability and representativeness of training data.
- ▷ Cost of training.
- ▷ Truthfulness?

Bayesian inference



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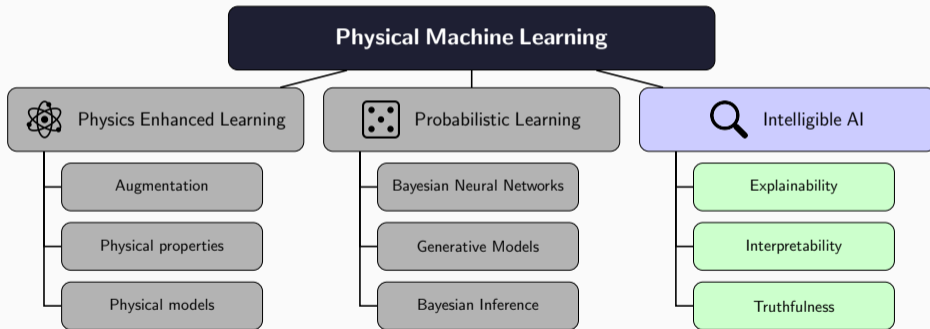
- ▷ Public datasets/benchmarks (*e.g.* BASE, IllustrisTNG, CAMELS, Quijote, CosmoGrid).
- ▷ Amortized inference (training **not** repeated for new observations).
- ▷ Integrate in Bayesian framework to provide statistical guarantees.
- ▷ Statistical validation (hold that thought... see upcoming Truthfulness section).

Intelligible AI

Intelligible AI

Machine learning methods that are able to be understood by humans.

(See Weld & Bansal 2018, Ras *et al.* 2020.)



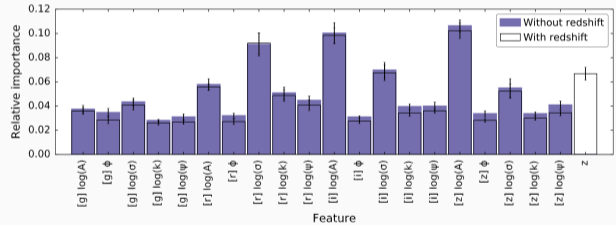


Explainable ML techniques may or may not be interpretable themselves but their outputs can be explained to humans.



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- ▷ Feature importances (Lochner *et al.* 2016)

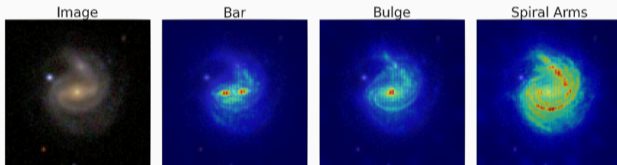


Supernova feature importances



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- ▷ Saliency maps
(Bhambra *et al.* 2022)



Galaxy saliency mapping



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Poking the black box: may provide some explanation of outputs but humans still not able to comprehend underlying process.

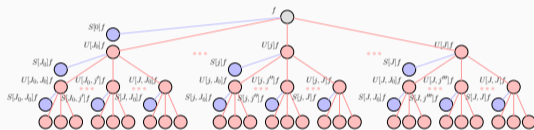


Interpretable ML models are **white boxes** that can be understood by humans.



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- ▶ Designed models such as scattering and wavelet phase harmonic networks (Allys *et al.* 2020, Cheng *et al.* 2020, McEwen *et al.* 2022)

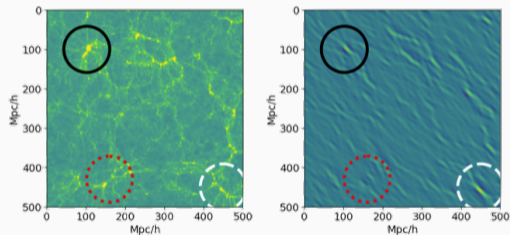


Scattering network (McEwen *et al.* 2022)



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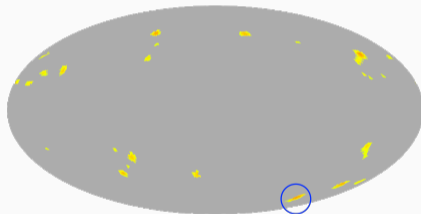


LSS features captured by wavelets
(Allys *et al.* 2020)



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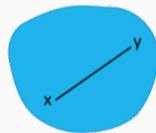
First evidence that CMB cold spot due to supervoid (McEwen *et al.* 2007)

Interpretability



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- ▷ Interpretable constraints on ML models,
e.g. convexity
(Liaudat, McEwen *et al.* in prep.)



Convexity



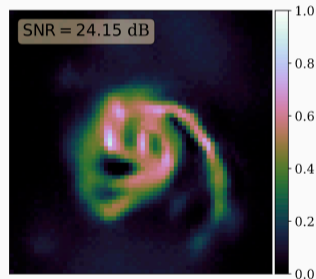
Uncertainty
Quantification

Impose convexity on learned model



Interpretable ML models are **white boxes** that can be understood by humans.

- ▷ Deep priors learned from training data (hybrid model-based and data-driven) (Remy *et al.* 2022, McEwen *et al.* 2023)



Compute Bayesian evidence for model selection
(**proxnest**, McEwen *et al.* 2023)

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- ▷ Availability and representativeness of training data.



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- ▶ Designed models limit flexibility.
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- ▶ Benefits of designed models often outweigh (minimal) reduced flexibility.
- ▶ Public datasets/benchmarks (e.g. IllustrisTNG, CAMELS, Quijote, CosmoGrid).
- ▶ Transfer learning, self-supervised learning.



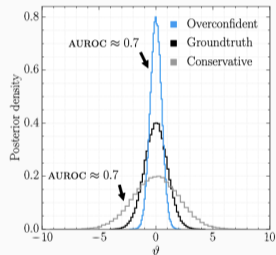
Truthfulness **critical for science** in order for humans to have confidence in results of ML models. Closely coupled with a **meaningful statistical distribution** of outputs.

Truthfulness



Truthfulness **critical for science** in order for humans to have confidence in results of ML models. Closely coupled with a **meaningful statistical distribution** of outputs.

- ▷ Validity of statistical distributions
(Hermans *et al.* 2022, Lemos *et al.* 2023)

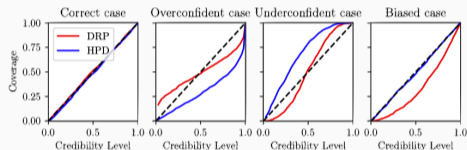


Validity of distribution
(Hermans *et al.* 2022)



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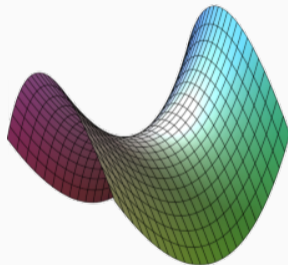
Coverage analysis (Lemos *et al.* 2023)

Truthfulness



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- ▷ Diversity (avoiding mode-collapse)
(Price *et al.* 2023, Whitney *et al.* in prep.)



Recover probability
distribution over full
underlying manifold

Truthfulness



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- ▷ Diversity of ML model often lacking.



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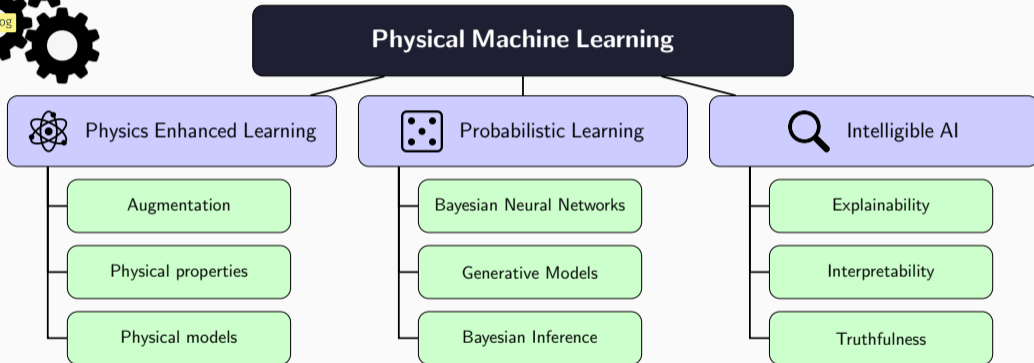
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- ▷ Integrate in statistical framework to inherit theoretical guarantees.
- ▷ Extensive validation tests (*e.g.* Hermans *et al.* 2022, Lemos *et al.* 2023).
- ▷ Meta sampling to recover distribution over manifold (*e.g.* Price *et al.* 2023).
- ▷ Well-posed frameworks (*e.g.* physics enhanced, probabilistic).

Summary

Summary



With great power comes great responsibility!