# Scientific Machine Learning in Astrophysics

## Machine Learning for Physics; Physics for Machine Learning

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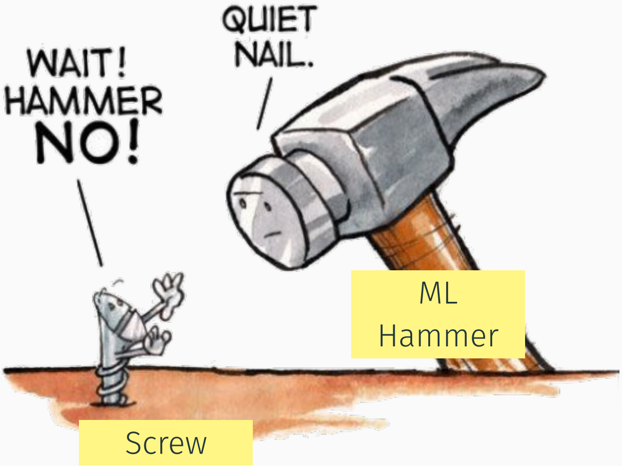
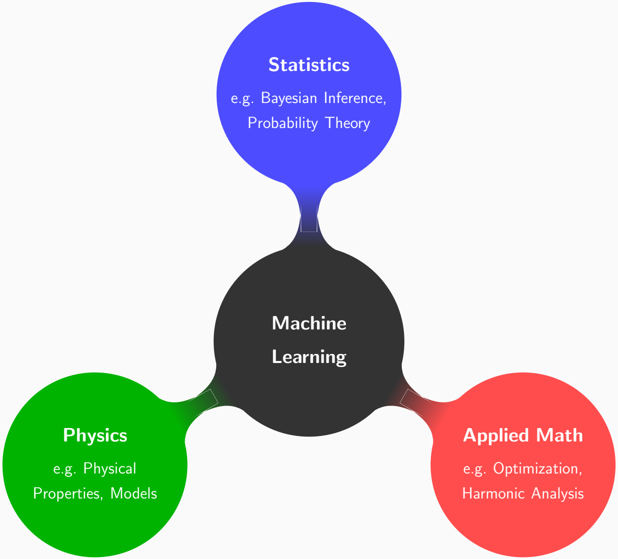
# The machine learning hammer



# The machine learning cog

# Merging paradigms



# Outline

**Physical Machine Learning**

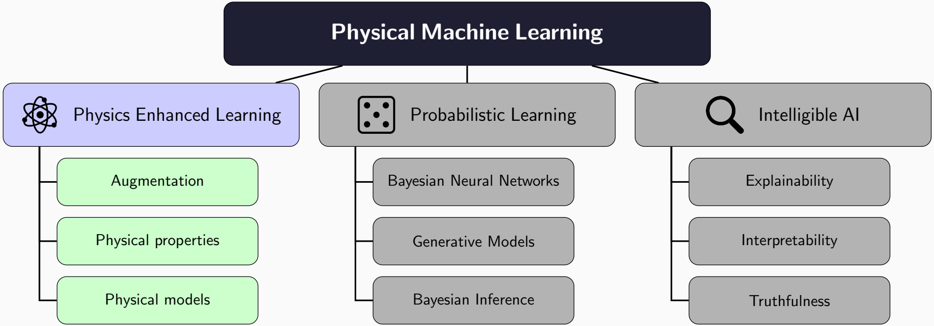
- Physics Enhanced Learning
  - Augmentation
  - Physical properties
  - Physical models
- Probabilistic Learning
  - Bayesian Neural Networks
  - Generative Models
  - Bayesian Inference
- Intelligible AI
  - Explainability
  - Interpretability
  - Truthfulness

# Physics Enhanced Learning

# Physics Enhanced Learning

Embed physical understanding of the world into machine learning models.

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



# Augmentation

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

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

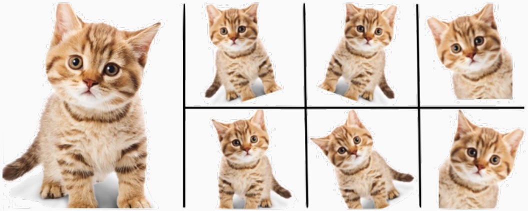
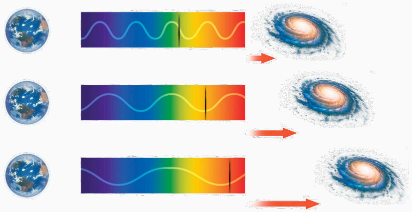


Image augmentation

# 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

# 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.

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

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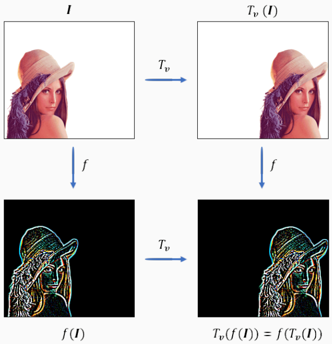
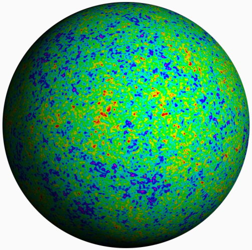
- Key factor CNNs so successful is due to encoding translational equivariance.



# 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** | $\mathrm{O}(d) = \{Q \in \mathbb{R}^{d\times d} : Q^\top Q = Q\,Q^\top = I_d\}$, |
| **Rotation** | $\mathrm{SO}(d) = \{Q \in \mathbb{R}^{d\times d} : Q^\top Q = Q\,Q^\top = I_d,\ \det(Q) = 1\}$ |
| **Translation** | $\mathrm{T}(d) = \{w \in \mathbb{R}^d\}$ |
| **Euclidean** | $\mathrm{E}(d) = \mathrm{T}(d) \rtimes \mathrm{O}(d)$ |
| **Lorentz** | $\mathrm{O}(1,d) = \{Q \in \mathbb{R}^{(d+1)\times(d+1)} : Q^\top \Lambda\, Q = \Lambda,\ \Lambda = \mathrm{diag}([1,-1,\ldots,-1])\}$ |
| **Poincaré** | $\mathrm{IO}(1,d) = \mathrm{T}(d+1) \rtimes \mathrm{O}(1,d)$ |
| **Permutation** | $\mathrm{S}_n = \{\sigma : [n] \to [n] \text{ bijective function}\}$ |

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?

- 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.

$\rightsquigarrow$ **Physics learned in training and embedded in model.**

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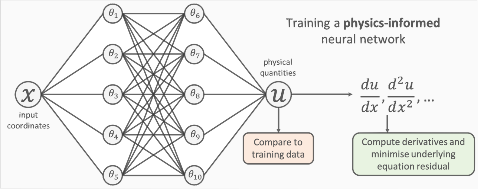
- Physics informed neural networks (PINNs) encode differentiable equations (e.g. boundary conditions) in loss.




PINNs

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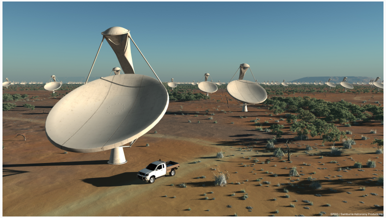
$\rightsquigarrow$ **Physics learned in training and embedded in model.**

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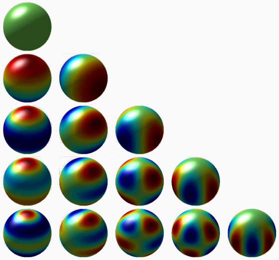
- Differentiable mathematical methods
  - Fourier transforms
  - Spherical harmonic transforms (`s2fft`; Price & McEwen, in prep.)
  - Spherical wavelet transforms (`s2wav`; Price *et al.* in prep.)
  - Spherical scattering transforms (Mousset, Price, Allys, McEwen, in prep.)



Spherical harmonics

# Physical models: PINNS and differentiable physics

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$\rightsquigarrow$ Physics learned in training and embedded in model.

- PINNs only capture limited dynamics via loss.
- Full physical models requires differentiable programming frameworks.

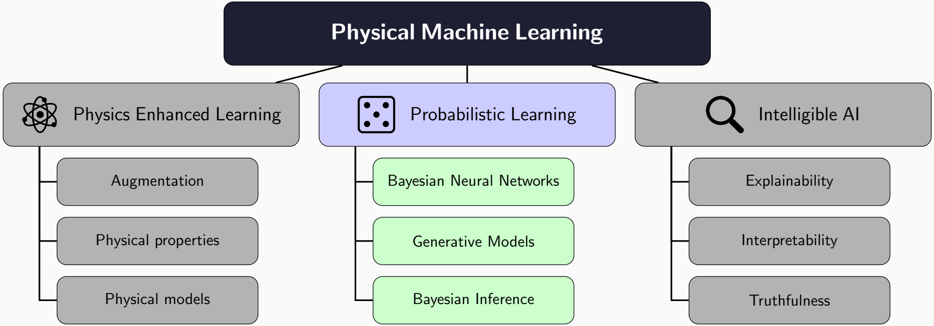
- Capture full physics with differentiable models!
- Emulators also provide differentiability (e.g. `CosmoPower`; Spurio Mancini et al. 2021).
- Write new differentiable codes (e.g. `s2fft`; Price & McEwen, in prep.).

# Probabilistic Learning

# Probabilistic Learning

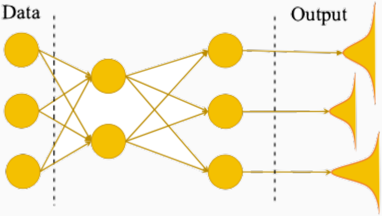
Embed a probabilistic representation of data, models and/or outputs.

(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

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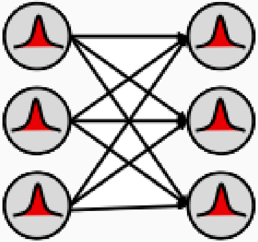
- MC Dropout (Gal & Ghahramani 2016): drop nodes probabilistically to sample an ensemble of networks.



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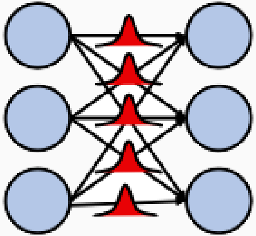
- Bayes by Backprop (Blundel *et al.* 2015): model distribution of weights (by variational inference).



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

# Bayesian neural networks for uncertainty quantification

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

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

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

# Generative models

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

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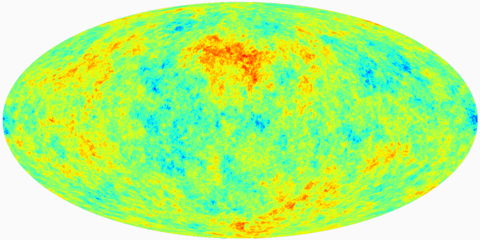
- Emulation: sample from learned prior (Perraudin *et al.* 2020, Allys *et al.* 2020, Price *et al.* 2023, Price *et al.* in prep., Mousset, Price, Allys, McEwen, in prep.)



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

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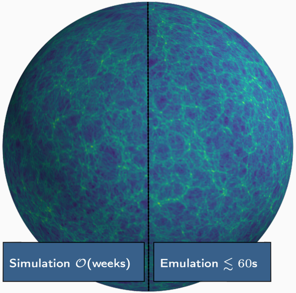
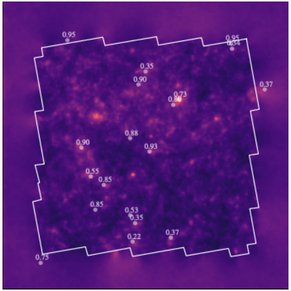



Emulated LSS
(Mousset, Price, Allys, McEwen in prep.)

# 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.

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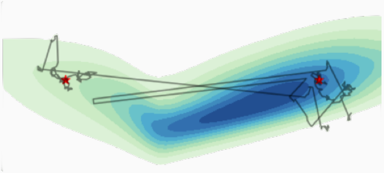
- Enhanced MCMC for parameter estimation (Grabrie *et al.* 2022, Karamanis *et al.* 2022).

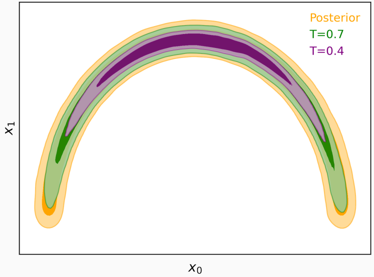


Learned proposal distributions

# Bayesian inference

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

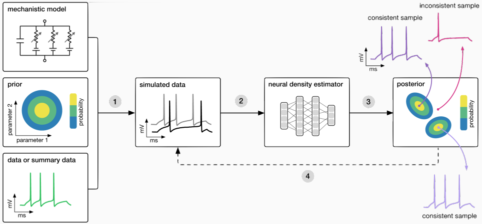
- Enhanced Bayesian model selection (**`harmonic`**; McEwen *et al.* 2021, Polanska *et al.* 2023).
  - Only requires posterior samples (evidence almost for free).
  - Agnostic to sampling technique:
    - Leverage efficient samplers.
    - Variational inference.
  - Scale to high dimensions.




Learned harmonic mean estimator (**`harmonic`**)

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

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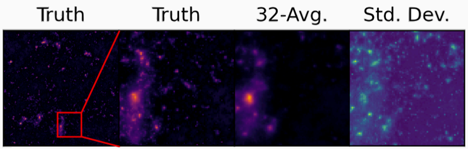
- Variational inference
  (Whitney *et al.* in prep.)




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?

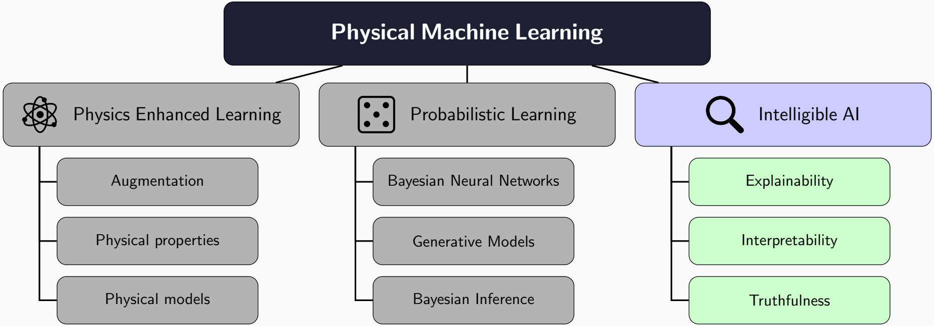
- Public datasets/benchmarks (*e.g.* BASE, IllustrisTNG, CAMELS, Quijote, CosmoGrid).
- Amortized inference (training **not** repeated for new observations).
- Integrate in Bayesian framework to provide statistical guarantees.
- Statistical validation (hold that thought... see upcoming Truthfulness section).

# Intelligible AI

# Intelligible AI

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

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



# Explainability

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

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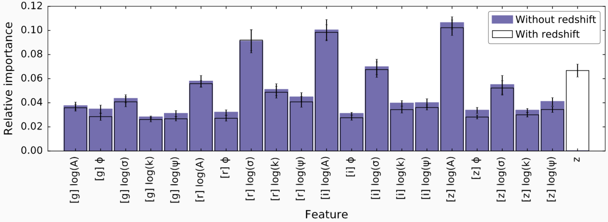
- Feature importances (Lochner *et al.* 2016)

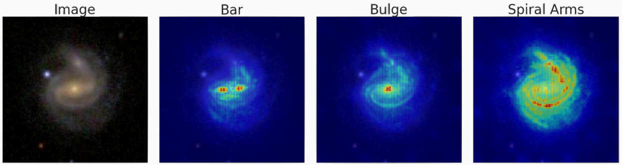



Supernova feature importances

# Explainability

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

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




Galaxy saliency mapping

# Explainability

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

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

# Interpretability

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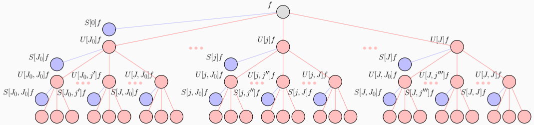
- Designed models such as scattering and wavelet phase harmonic networks (Allys *et al.* 2020, Cheng *et al.* 2020, McEwen *et al.* 2022)



Scattering network (McEwen *et al.* 2022)

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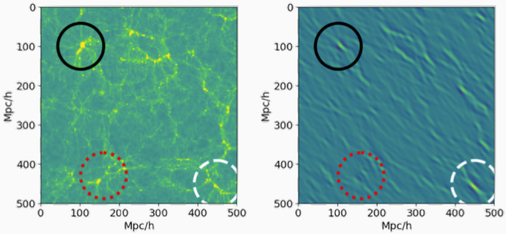


LSS features captured by wavelets
(Allys *et al.* 2020)

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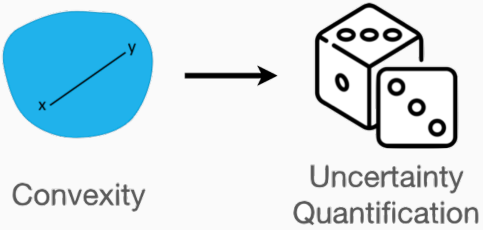
- Interpretable constraints on ML models, *e.g.* convexity
  (Liaudat, McEwen *et al.* in prep.)




Impose convexity on learned model

# Interpretability

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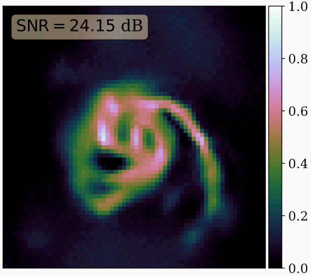
- Deep priors learned from training data (hybrid model-based and data-driven)
  (Remy *et al.* 2022, McEwen *et al.* 2023)




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

# Interpretability

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

- Designed models limit flexibility.
- Availability and representativeness of training data.

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

# Truthfulness

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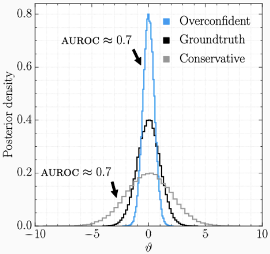
- Validity of statistical distributions
  (Hermans *et al.* 2022, Lemos *et al.* 2023)




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

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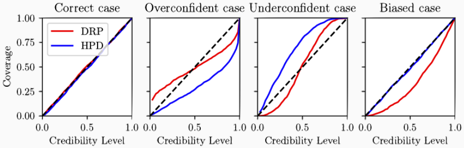


Coverage analysis (Lemos *et al.* 2023)

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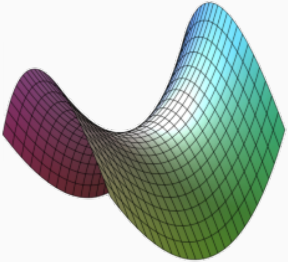
- Diversity (avoiding mode-collapse)
  (Price *et al.* 2023, Whitney *et al.* in prep.)



Recover probability distribution over full underlying manifold

# Truthfulness

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.

- Uncertainties not aways meaningful.
- Diversity of ML model often lacking.

- 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

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ML Cog

## Physical Machine Learning

- **Physics Enhanced Learning**
  - Augmentation
  - Physical properties
  - Physical models
- **Probabilistic Learning**
  - Bayesian Neural Networks
  - Generative Models
  - Bayesian Inference
- **Intelligible AI**
  - Explainability
  - Interpretability
  - Truthfulness

With great power comes great responsibility!