Unravelling interior evolution of terrestrial planets using Machine Learning

Siddhant Agarwal, ESO AIA2019

PhD Supervisors

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Dr. Pan Kessel
Dr. Grégoire Montavon
Prof. Dr. Klaus-Robert Müller

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Berlin Research School in Data Science

Agenda

- **Introduction** to mantle convection and the inverse problem
- **Data** used for inversion
- **Results** using Mixture Density Networks
- **Next steps** using this approach
- Acknowledgements
- References

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Introduction

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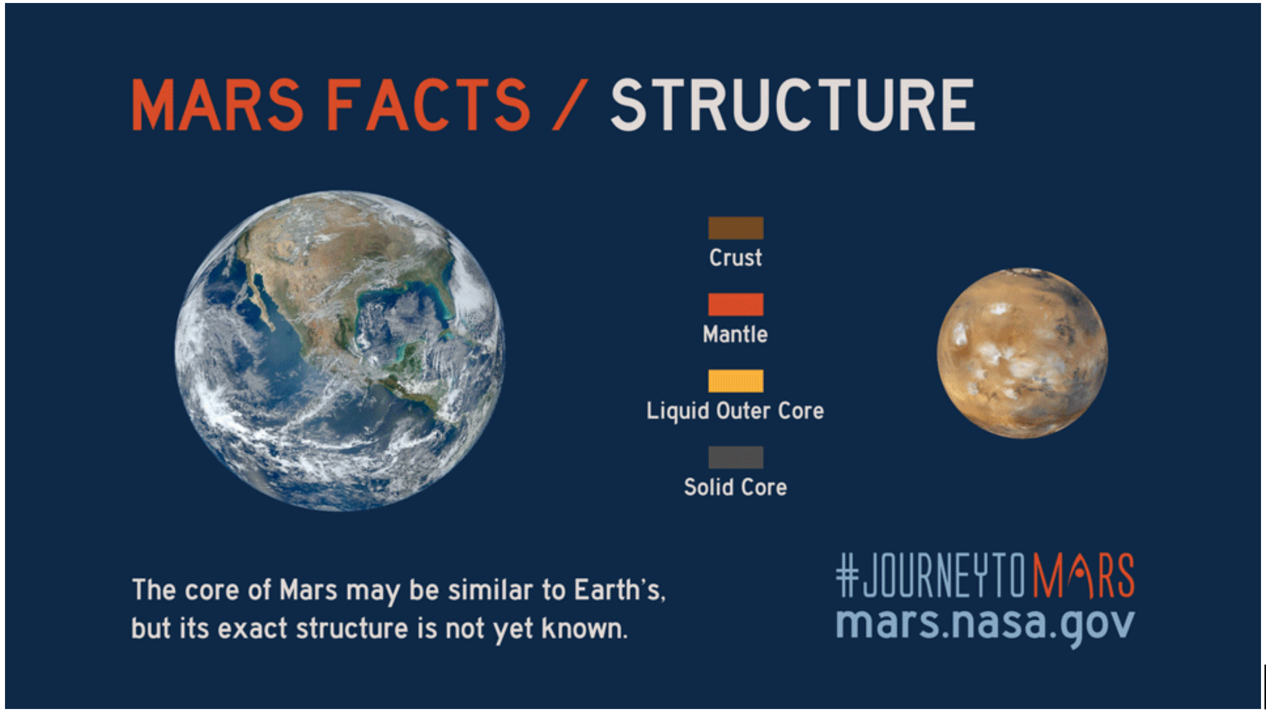
Introduction

We are interested in understanding thermal evolution of terrestrial planets like Mars and Earth.

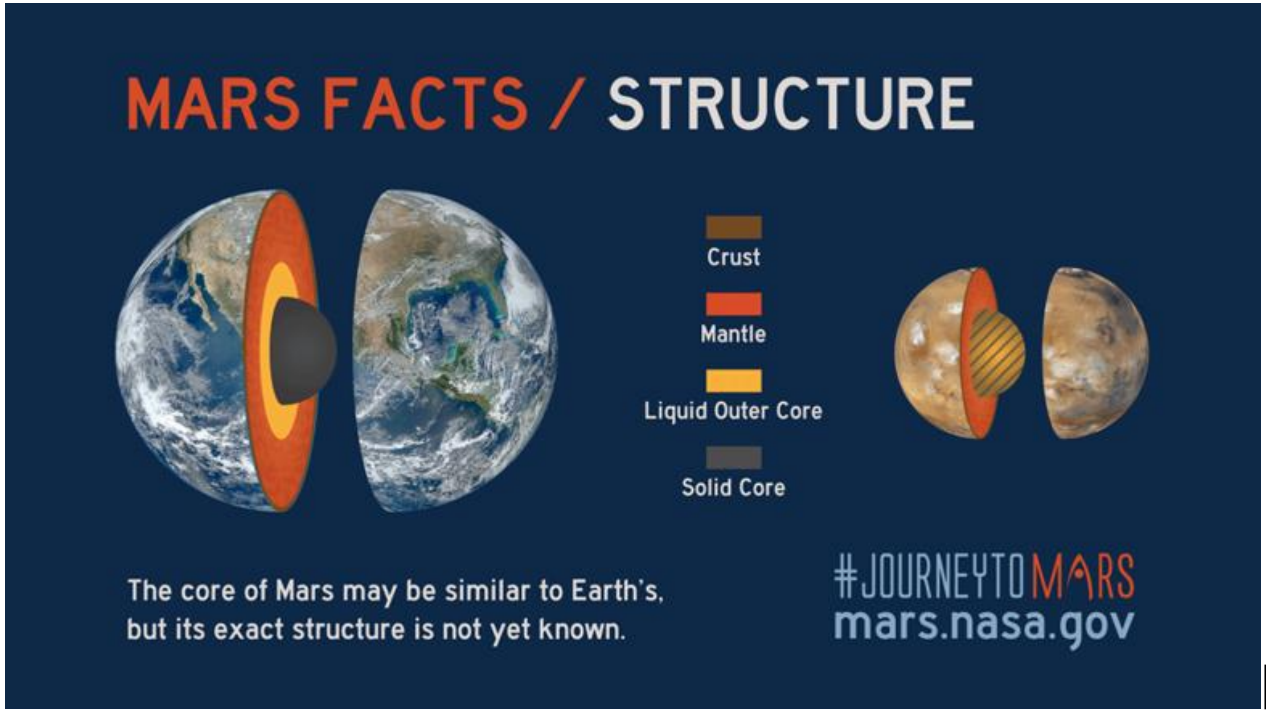


[1]

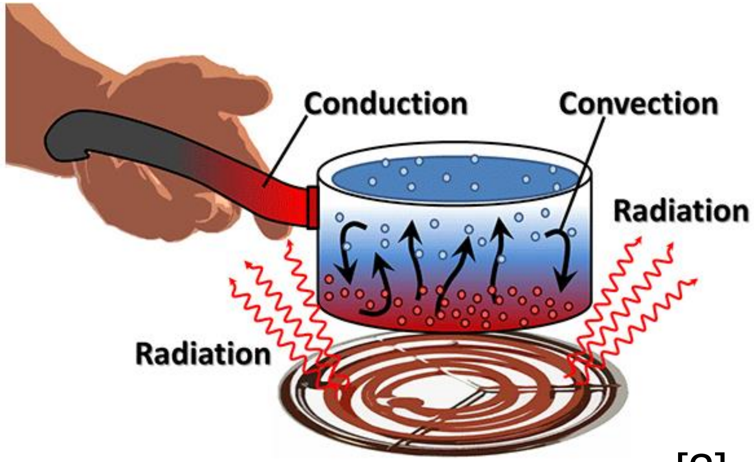
Introduction

We are interested in understanding thermal evolution of terrestrial planets like Mars and Earth.

Mantle convection is an important driver of it.



[1]



[2]

Introduction

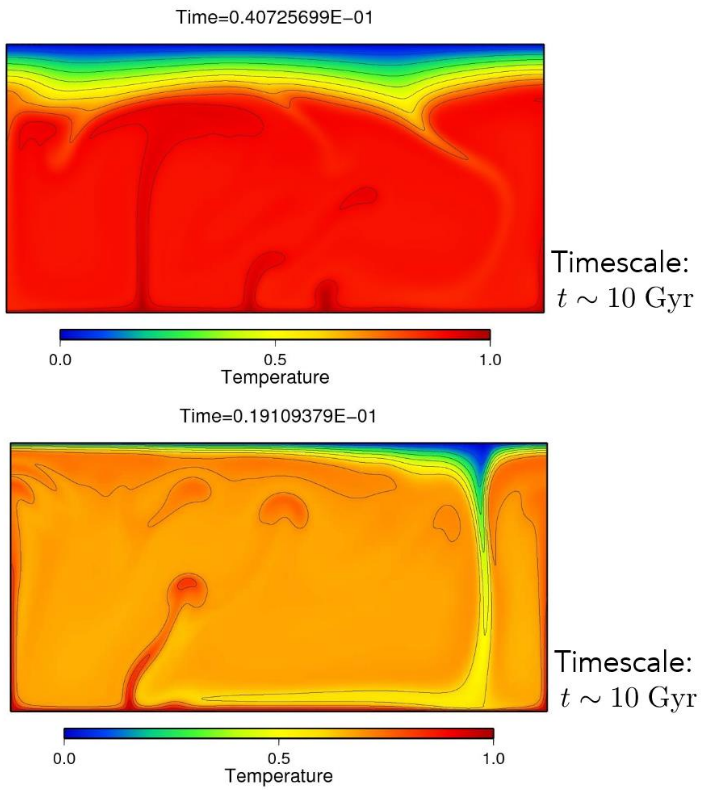
Over geological time scales, rocks behave likes fluids.

[7]

Introduction

Over geological time scales, rocks behave likes fluids.

Hence we use fluid dynamics simulations to study mantle convection.



[7]

Introduction

Inputs

Viscosity

Initial temperature

Radiogenic elements

⋮

In-house C++ code

Conservation of mass:

$$\frac{\partial \rho}{\partial t} + \nabla . (\rho \vec{u}) = 0$$

Conservation of momentum:

$$\frac{D\rho\vec{u}}{Dt} = -\nabla P + \nabla . \tau + \rho\vec{g}$$

Conservation of energy:

$$\rho c_p \frac{DT}{Dt} - \alpha T \frac{DP}{Dt} = \nabla . (k \nabla T) + \rho H + \phi$$

Outputs

Surface heat flux

Radial contraction

Crustal thickness

⋮

- Mantle convection is governed by several poorly constrained parameters and initial conditions

Introduction

- Mantle convection is governed by several poorly constrained parameters and initial conditions
- In planetary science, the outputs are observable (…sometimes)

Introduction

Inputs

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⋮

[3]

Outputs

Surface heat flux

Radial contraction

Crustal thickness

⋮

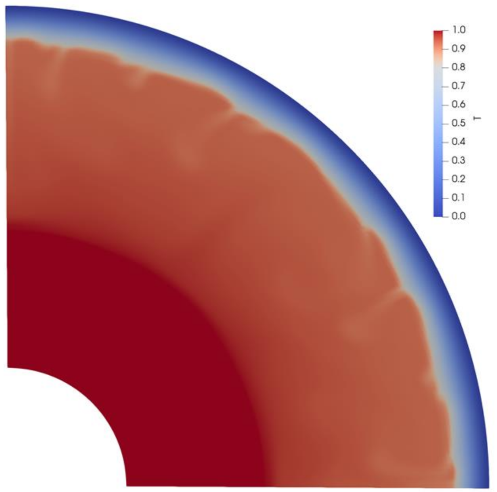
- Mantle convection is governed by several poorly constrained parameters and initial conditions
- In planetary science, the outputs are observable (...sometimes)
- Need Machine Learning for rapid inversion in high-dimensional spaces; Monte Carlo methods are computationally unfeasible

Dataset

Helmholtz Einstein International Berlin Research School in Data Science

Dataset

- Generated some 3200 2D, quarter-cylinder **evolution** simulations for Mars, with:
  - Compressible convection (Extended-Bousinessq Approximation)
  - Heat production from core and radiogenic elements
  - Temperature and pressure dependent viscosity (Arrhenius)
  - Temperature and pressure dependent thermal conductivity and thermal expansion
  - Solid phase transitions



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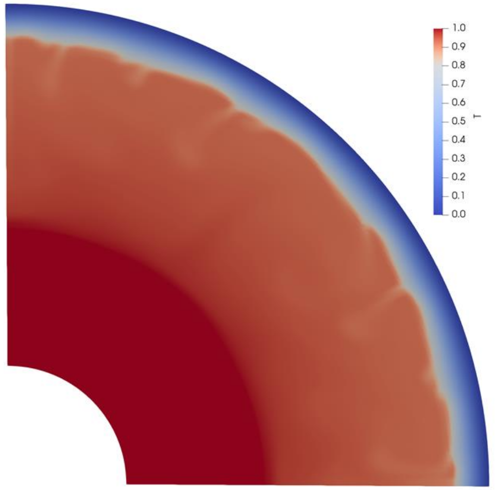
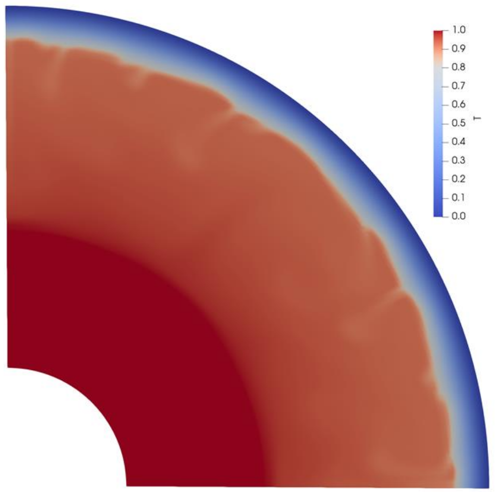


- ~800 GB of data generated using 60,000 CPU hours; ~800 MB used for ML

Dataset



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Parameters

Ra (η_{ref} ϵ $[10^{19}, 10^{22}$ $Pa\ s])$

RaQ (Λ ϵ $[1, 50]$, η_{ref})

$\mathbf{T_{initial}}$ ϵ [1600, 1800 K]

E ϵ [10^5, 5x10^5 J mol^{-1}]

V ϵ [4x10^{-6}, 10x10^{-6} m^3 mol^{-1}]

←

“Observables”

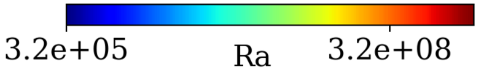
Temperature profile

Radial contraction

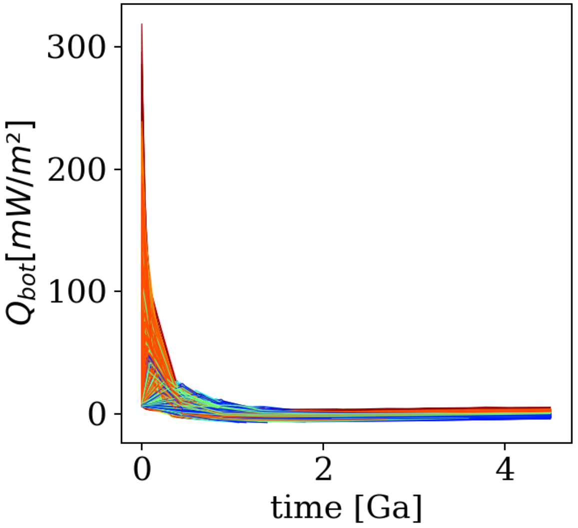
Elastic lithospheric thickness

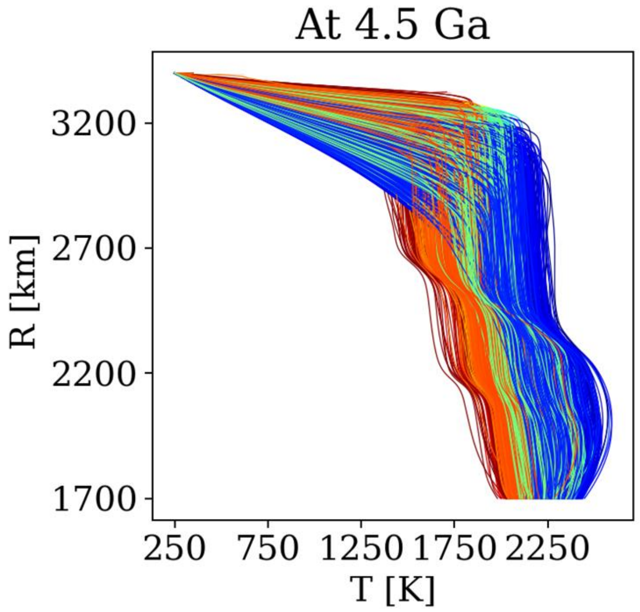
Core heat flux

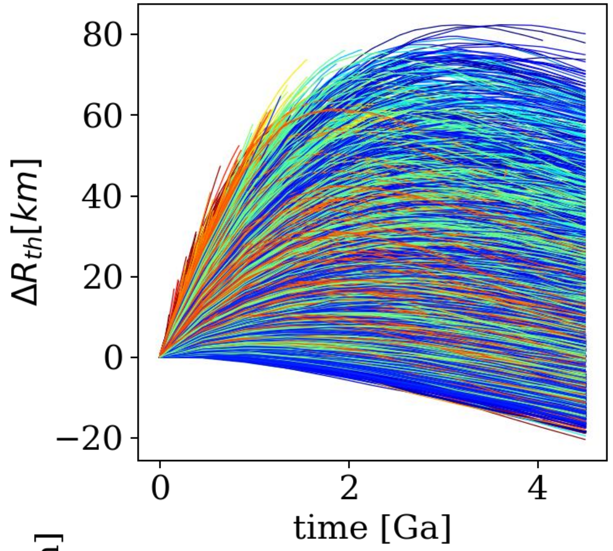
Surface heat flux

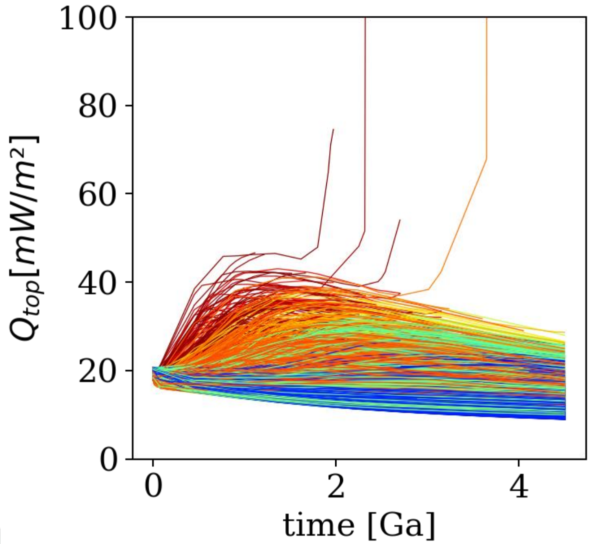


Dataset









"Observables"

Temperature profile

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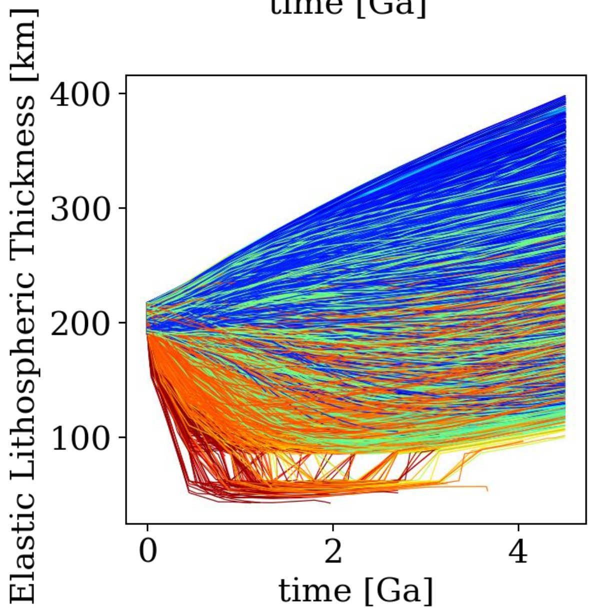

Results

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Results

- Mixture Density Network (MDN) is promising for inverse problems.

Contents lists available at ScienceDirect
Physics of the Earth and Planetary Interiors
journal homepage: www.elsevier.com/locate/pepi

Using pattern recognition to infer parameters governing mantle convection

Suzanne Atkins [a,*], Andrew P. Valentine [a], Paul J. Tackley [b], Jeannot Trampert [a]
[a] Department of Earth Sciences, Utrecht University, P.O. Box 80.115, 3508 TC Utrecht, The Netherlands
[b] Institute of Geophysics, ETH Zurich, Sonneggstrasse 5, 8092 Zurich, Switzerland

[4]

Geophysical Journal International
Geophys. J. Int. (2013) **195,** 408–422 doi: 10.1093/gji/ggt220
Advance Access publication 2013 June 26

Bayesian inference of Earth's radial seismic structure from body-wave traveltimes using neural networks

Ralph W. L. de Wit, Andrew P. Valentine and Jeannot Trampert
Department of Earth Sciences, Utrecht University, Budapestlaan 4, 3584 CD, Utrecht, the Netherlands. E-mail: r.w.l.dewit@uu.nl

[5]

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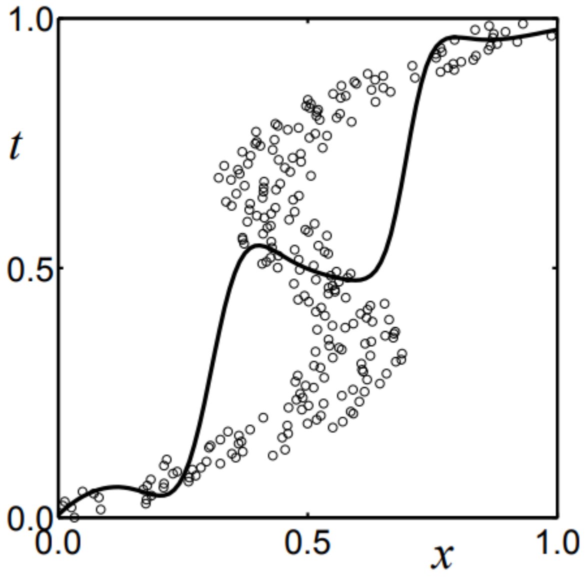
Results

- Mixture Density Network (MDN) is promising for inverse problems.
- Based on the algorithm by Bishop [6]



$$E^S = \frac{1}{2}\sum_{q=1}^{n}\sum_{k=1}^{c}\left[f_k(x^q; w) - t_k^q\right]^2$$

Results

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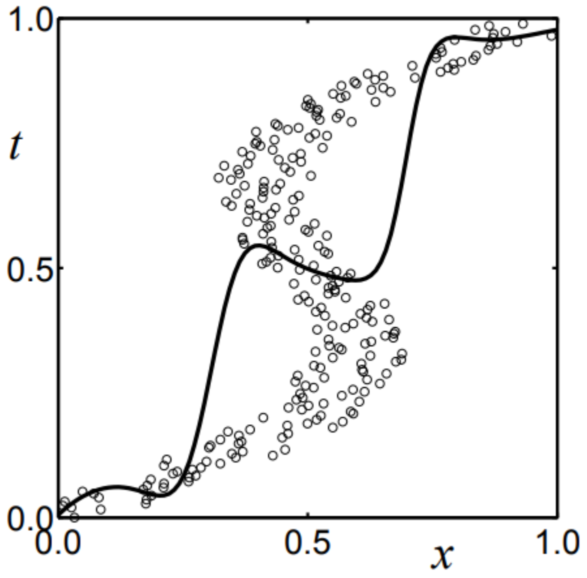

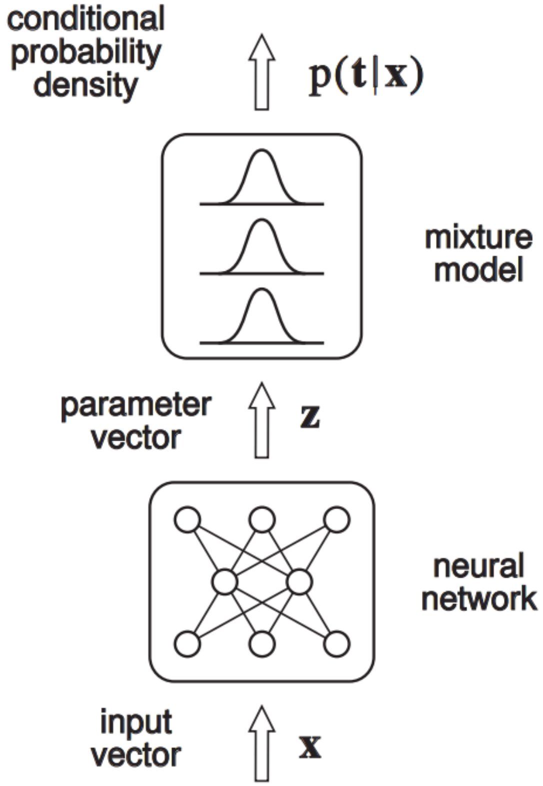

$$E^S = \frac{1}{2}\sum_{q=1}^{n}\sum_{k=1}^{c}\left[f_k(x^q;w) - t_k^q\right]^2$$

$$E^S = -\ln\left\{\sum_{i=1}^{m}\alpha_i(x^q)\emptyset_i(t^q|x^q)\right\}$$

Results

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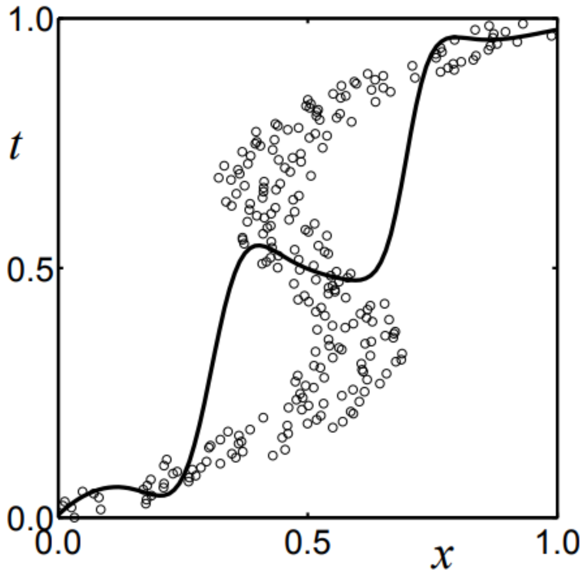

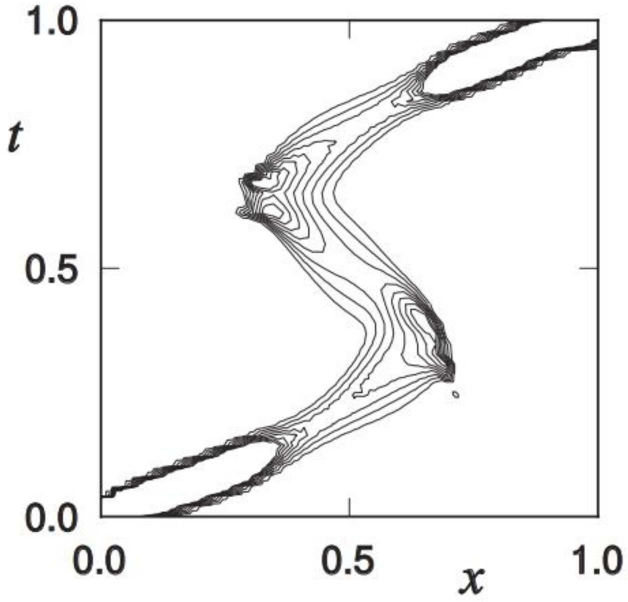

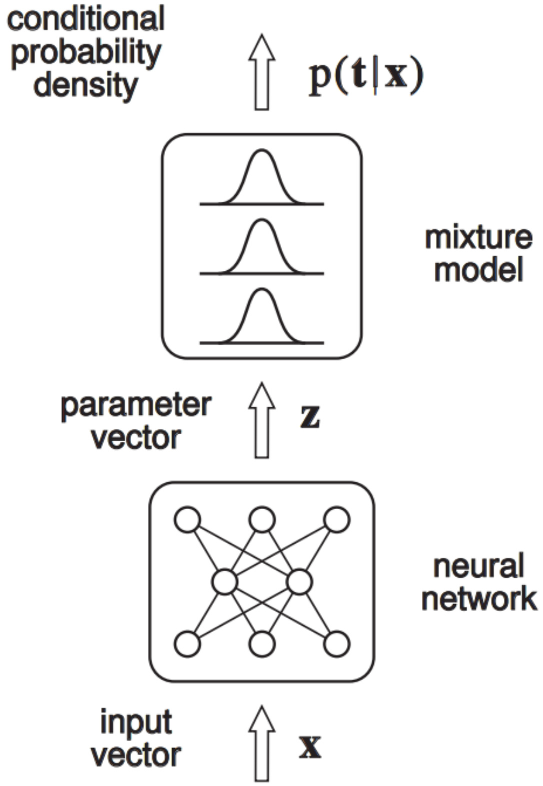

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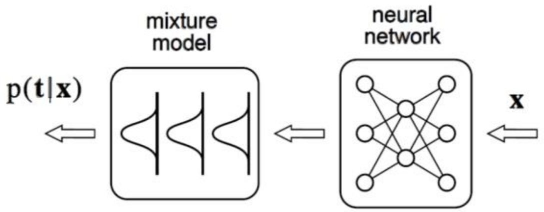
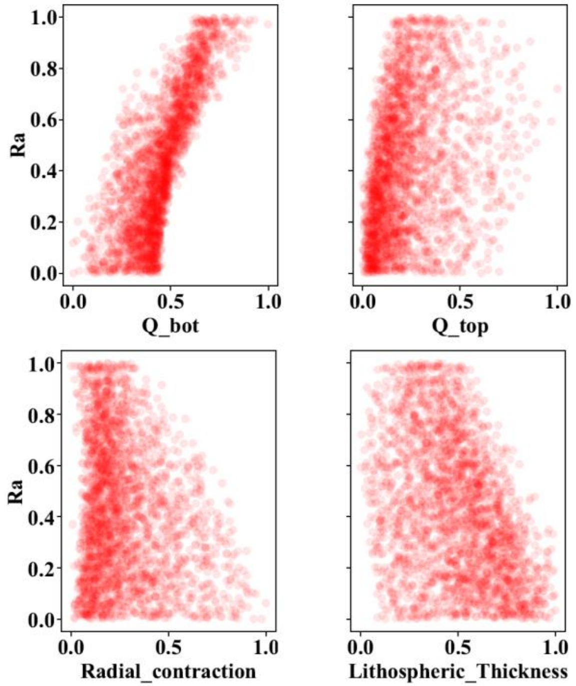
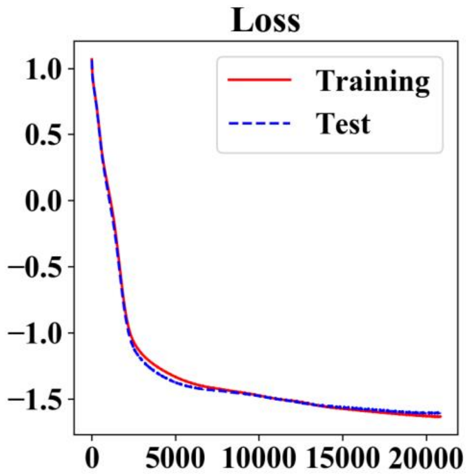
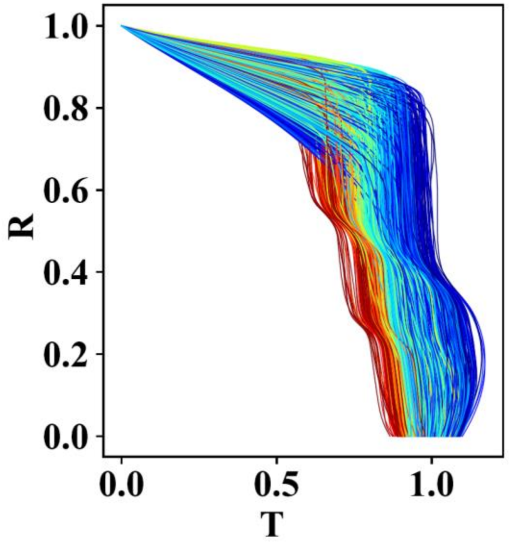
Results

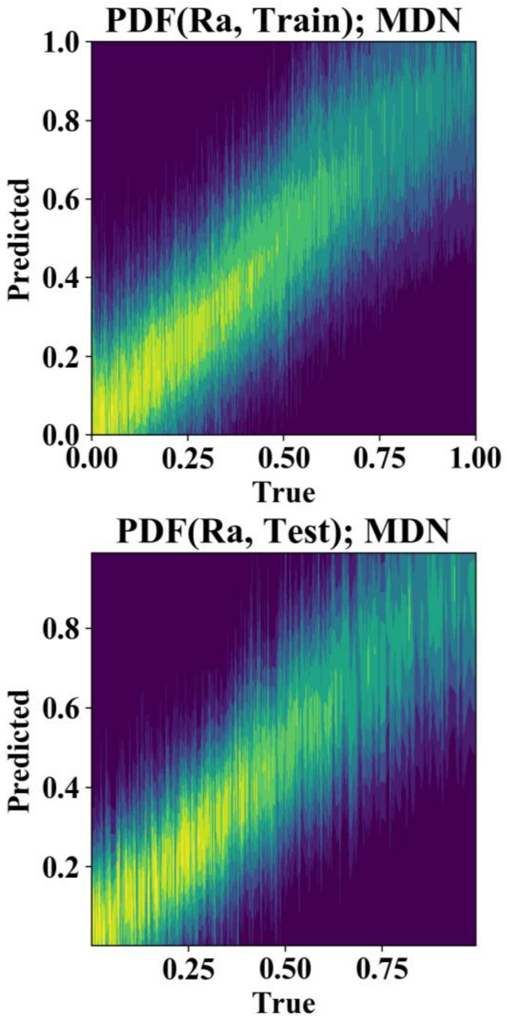

mixture model
neural network
p(t|x)
x

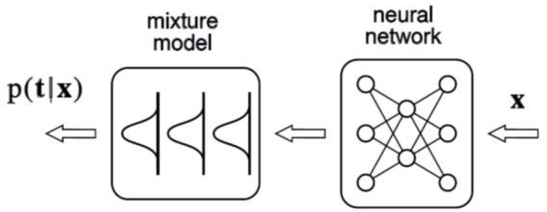

Ra
Q_bot
Q_top
Radial_contraction
Lithospheric_Thickness
0.0
0.5
1.0

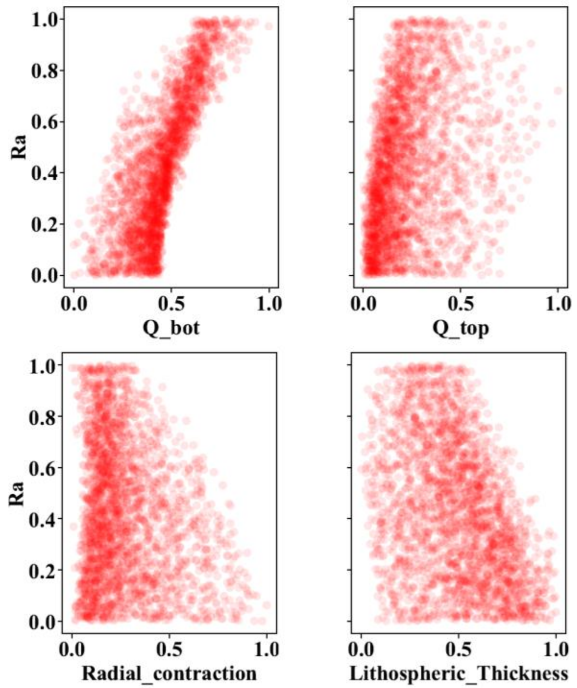

Loss
Training
Test
1.0
0.5
0.0
−0.5
−1.0
−1.5
0
5000
10000
15000
20000

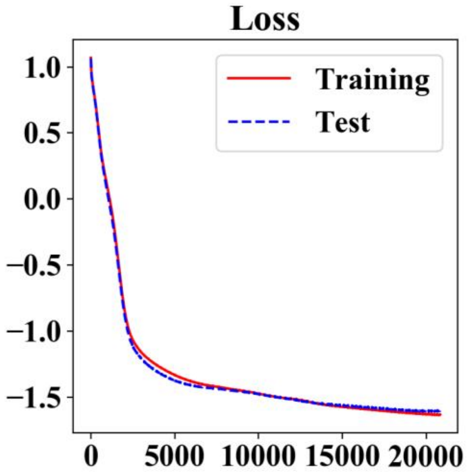

R
T
0.0
0.2
0.4
0.6
0.8
1.0
0.5

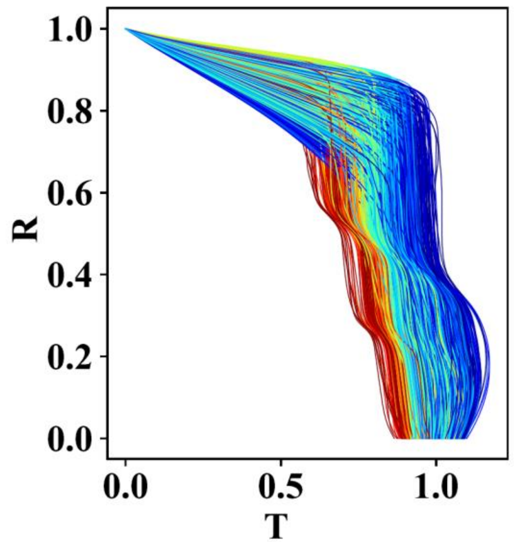
Results


PDF(Ra, Train); MDN
Predicted
True
PDF(Ra, Test); MDN
Predicted
True

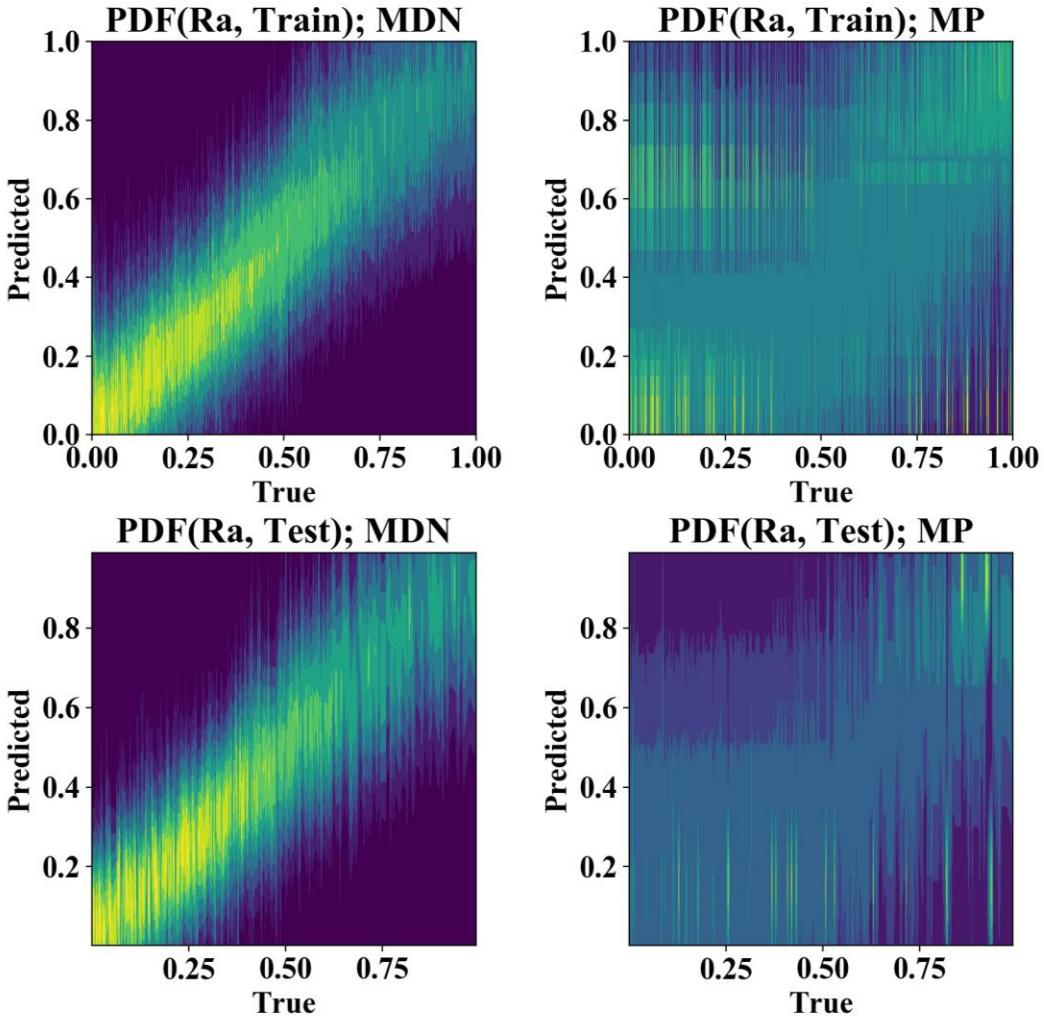

p(t|x)
mixture model
neural network
x

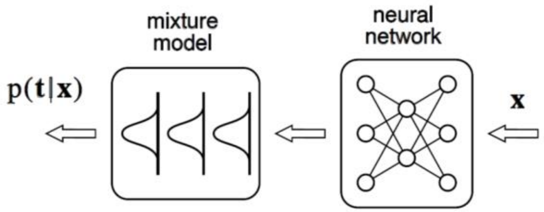

Ra
Q_bot
Q_top
Radial_contraction
Lithospheric_Thickness

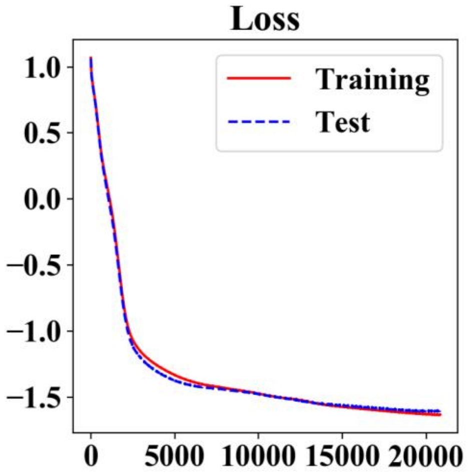

Loss
Training
Test

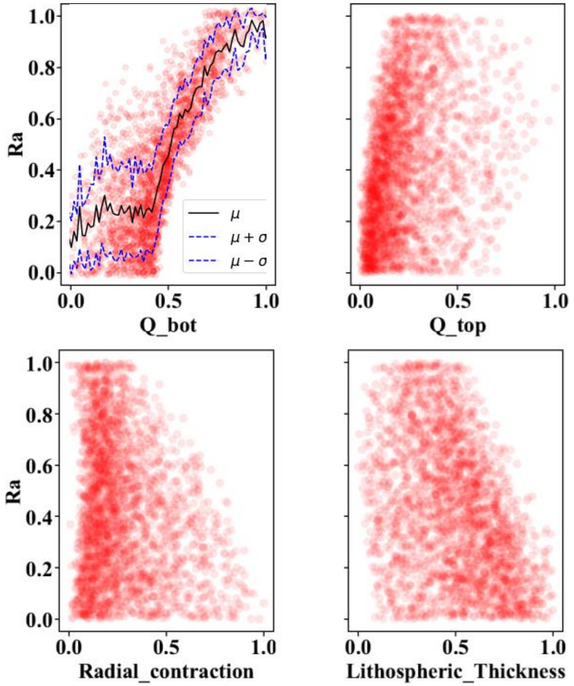

R
T

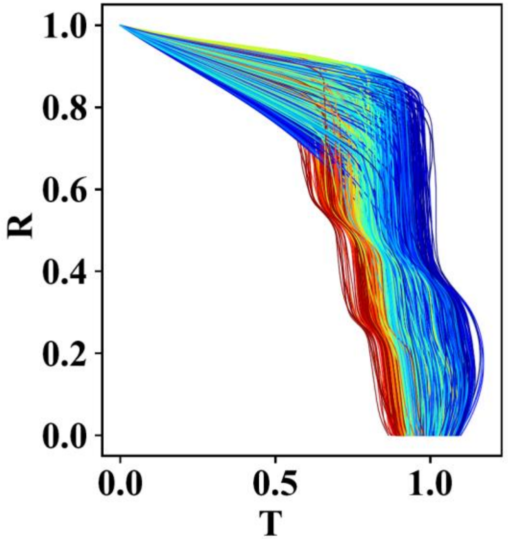
Results


PDF(Ra, Train); MDN
PDF(Ra, Train); MP
PDF(Ra, Test); MDN
PDF(Ra, Test); MP
Predicted
True
0.00 0.25 0.50 0.75 1.00
0.0 0.2 0.4 0.6 0.8 1.0

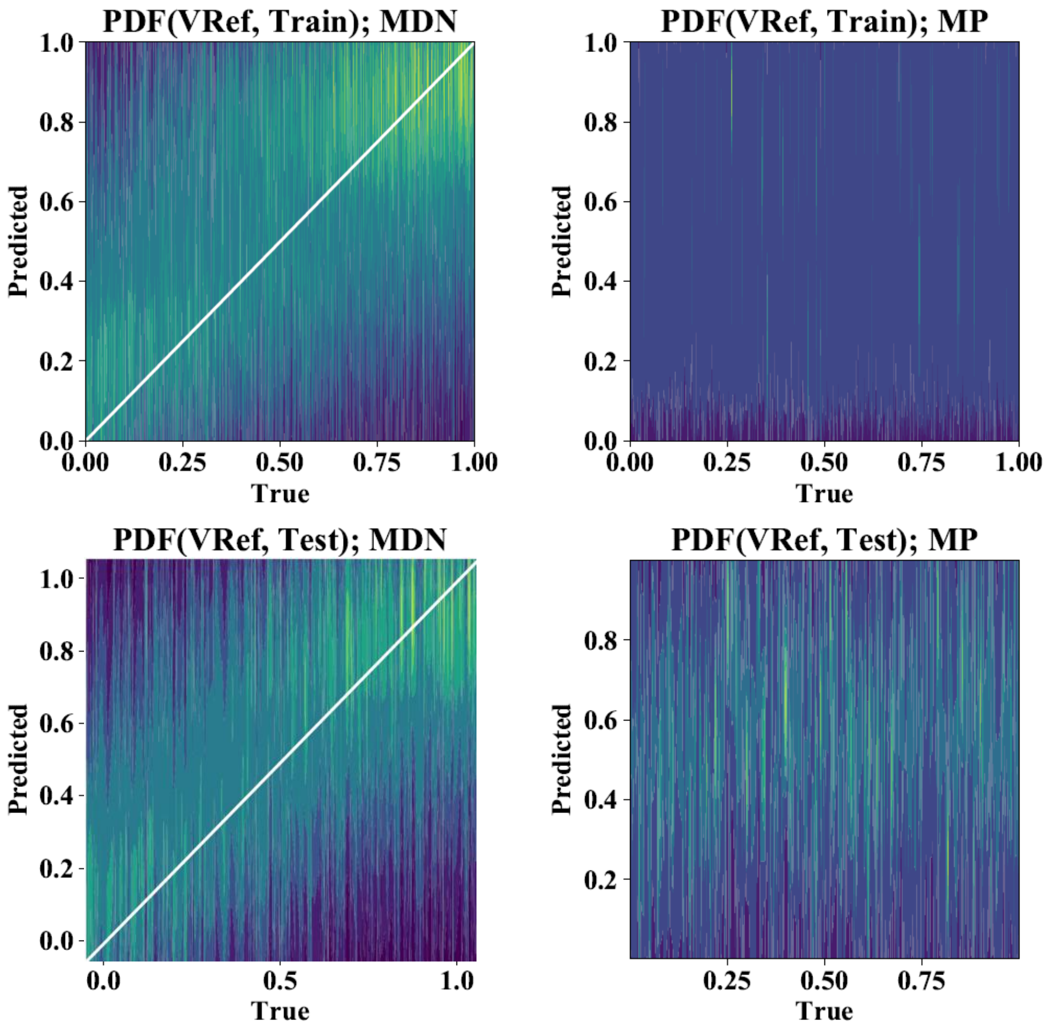

p(t|x)
mixture model
neural network
x

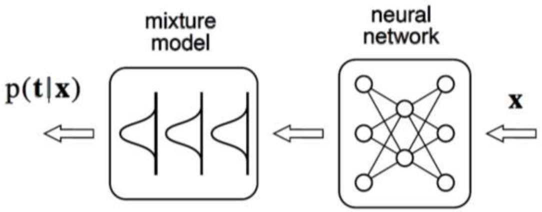

Loss
Training
Test
1.0 0.5 0.0 −0.5 −1.0 −1.5
0 5000 10000 15000 20000

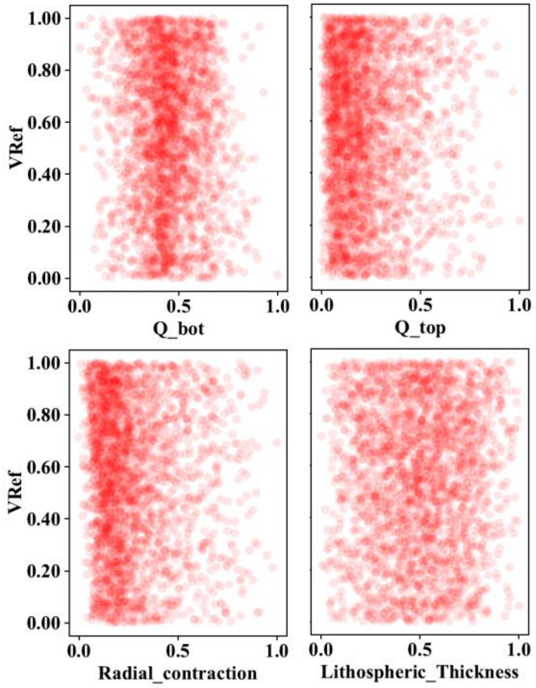

Ra
Q_bot
Q_top
Radial_contraction
Lithospheric_Thickness
μ
$\mu+\sigma$
$\mu-\sigma$
0.0 0.5 1.0

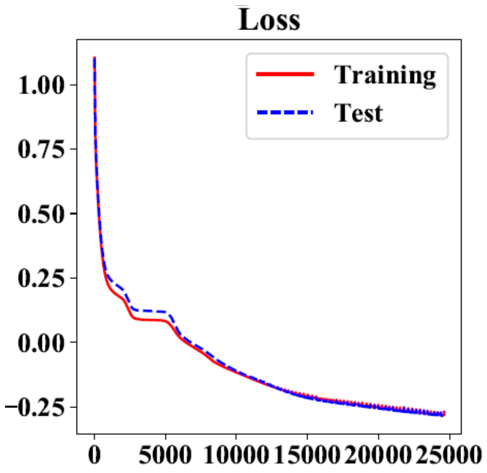

R
T
0.0 0.2 0.4 0.6 0.8 1.0
0.0 0.5 1.0

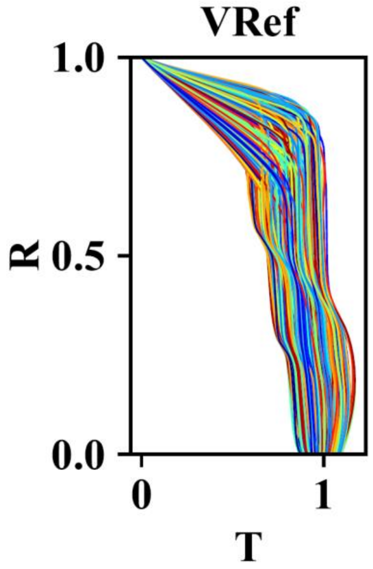
Results


PDF(VRef, Train); MDN
PDF(VRef, Train); MP
PDF(VRef, Test); MDN
PDF(VRef, Test); MP
Predicted
True
0.0
0.2
0.4
0.6
0.8
1.0
0.00
0.25
0.50
0.75
1.00
0.5


p(t|x)
mixture model
neural network
x

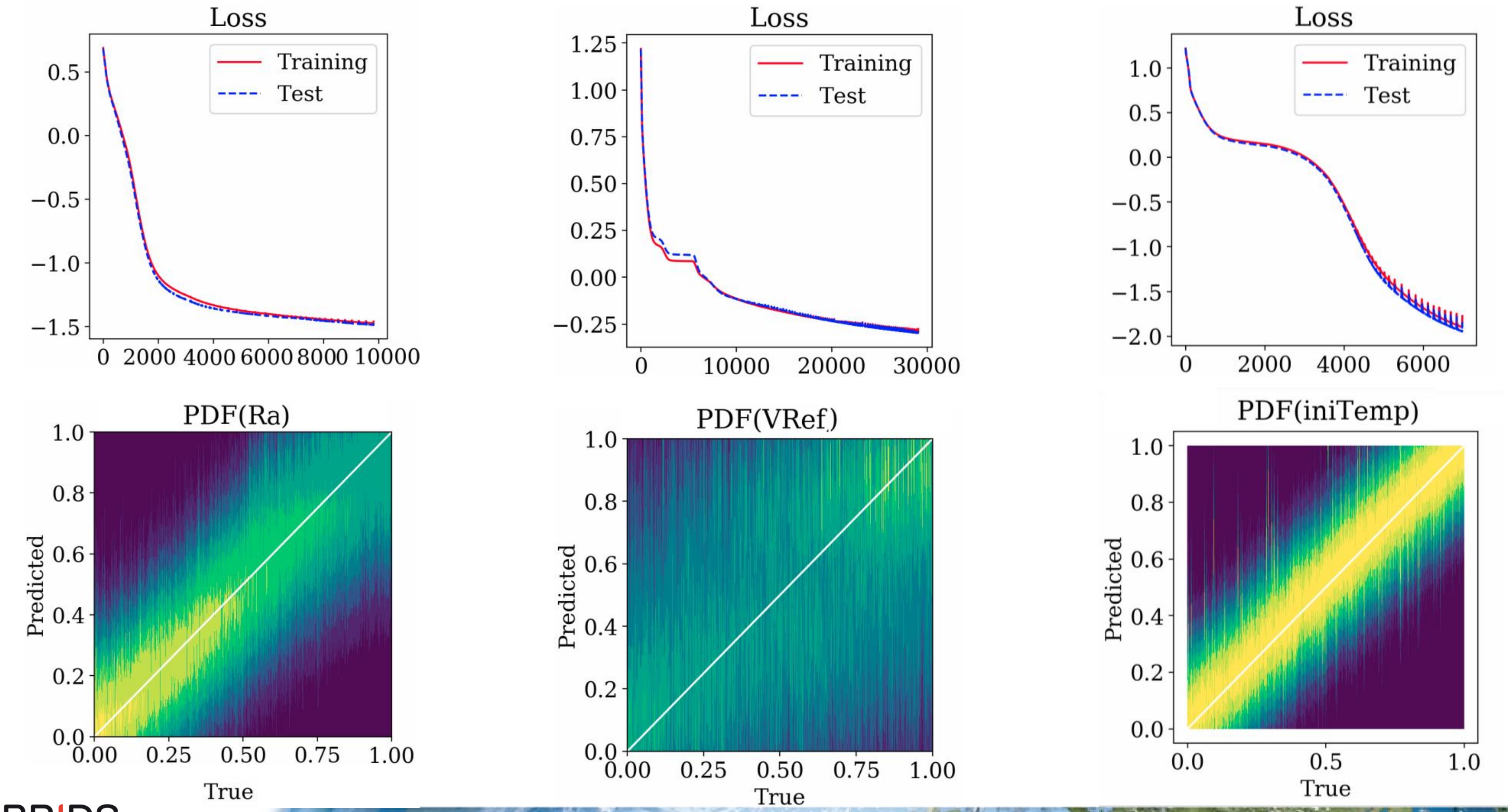

VRef
Q_bot
Q_top
Radial_contraction
Lithospheric_Thickness
0.00
0.20
0.40
0.60
0.80
1.00
0.0
0.5
1.0


Loss
Training
Test
1.00
0.75
0.50
0.25
0.00
−0.25
0
5000
10000
15000
20000
25000


VRef
R
T
1.0
0.5
0.0
0
1

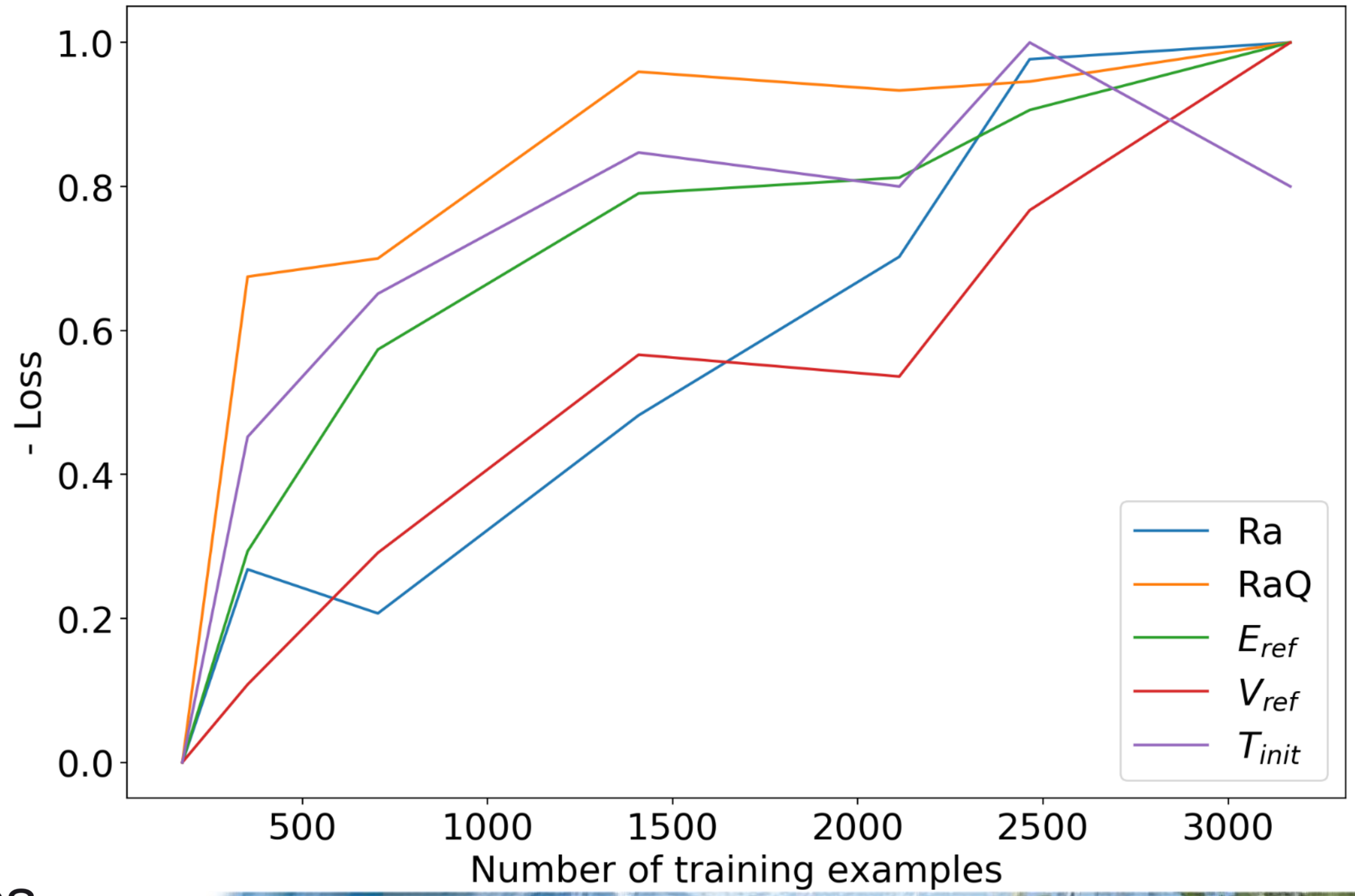
Results

Using loss as a measure of ‘constrainability’

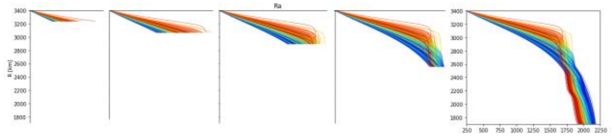


Results

Asymptotic behavior of loss shows number of simulations is sufficient for this set of parameters and observables



Results



Parameters / Observables (colour scale: -(Mean Loss), 0.0–1.5)

Parameters	Q_{bot}	Q_{top}	$R_{contract}$	L_{thick}	$T_{prof;\,90,\,10}$	$T_{prof;\,80,\,20}$	$T_{prof;\,70,\,30}$	$T_{prof;\,60,\,40}$	$T_{prof;\,50,\,50}$	$T_{prof;\,0,\,100}$
Ra	0.66	0.14	0.06	0.16	0.49	0.99	1.21	1.31	1.35	1.43
RaQ	0.61	0.33	0.14	0.34	0.57	1.01	1.30	1.36	1.39	1.44
ERef	0.01	0.09	0.01	0.09	0.14	0.22	0.36	0.36	0.38	0.63
VRef	-0.07	-0.07	-0.11	-0.09	-0.11	-0.07	-0.03	-0.02	-0.02	0.08
T_{init}	-0.06	-0.05	-0.02	-0.02	-0.03	-0.02	-0.00	0.01	0.06	0.07

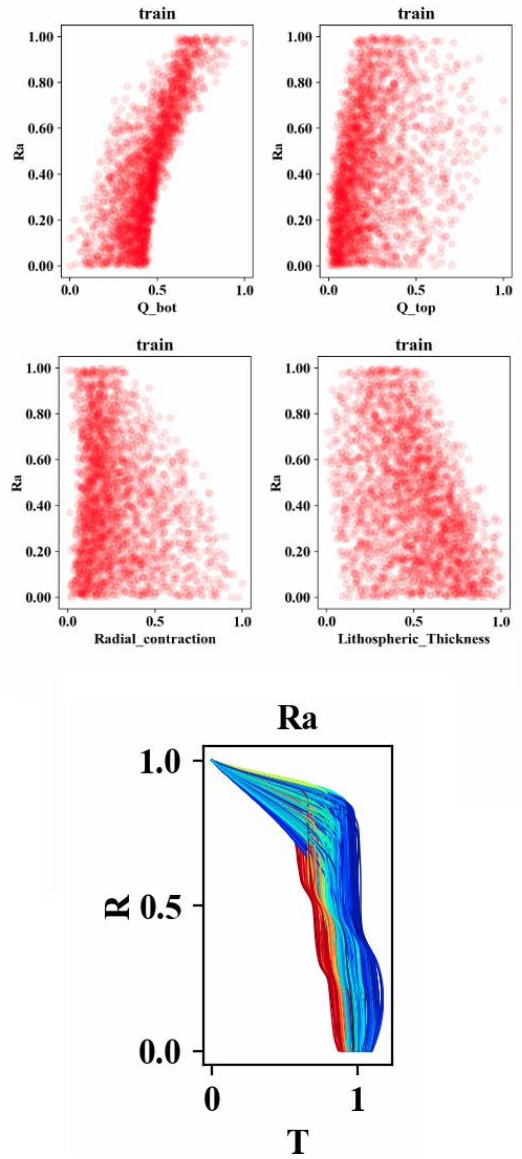
Parameters	Q_{bot}, Q_{top}	$Q_{bot}, R_{contract}$	Q_{bot}, L_{thick}	$Q_{top}, R_{contract}$	Q_{top}, L_{thick}	$R_{contract}, L_{thick}$	$Q_{bot}, Q_{top}, R_{contract}$	$Q_{bot}, Q_{top}, L_{thick}$	$Q_{top}, R_{contract}, L_{thick}$	$Q_{bot}, Q_{top}, R_{contract}, L_{thick}$	$Q_{bot}, Q_{top}, R_{contract}, L_{thick}, T_{prof;\,0,\,100}$
Ra	1.11	1.02	1.12	0.59	0.26	0.60	1.15	1.11	0.65	1.21	1.59
RaQ	1.19	1.05	1.19	0.71	0.44	0.73	1.25	1.21	0.79	1.33	1.60
ERef	0.18	0.11	0.18	0.15	0.09	0.16	0.24	0.35	0.15	0.39	0.69
VRef	-0.06	-0.08	-0.07	-0.07	-0.10	-0.07	-0.07	-0.09	-0.09	-0.07	0.29
T_{init}	-0.04	-0.03	-0.01	0.34	-0.02	0.27	0.94	-0.02	0.42	0.95	1.92

Observables

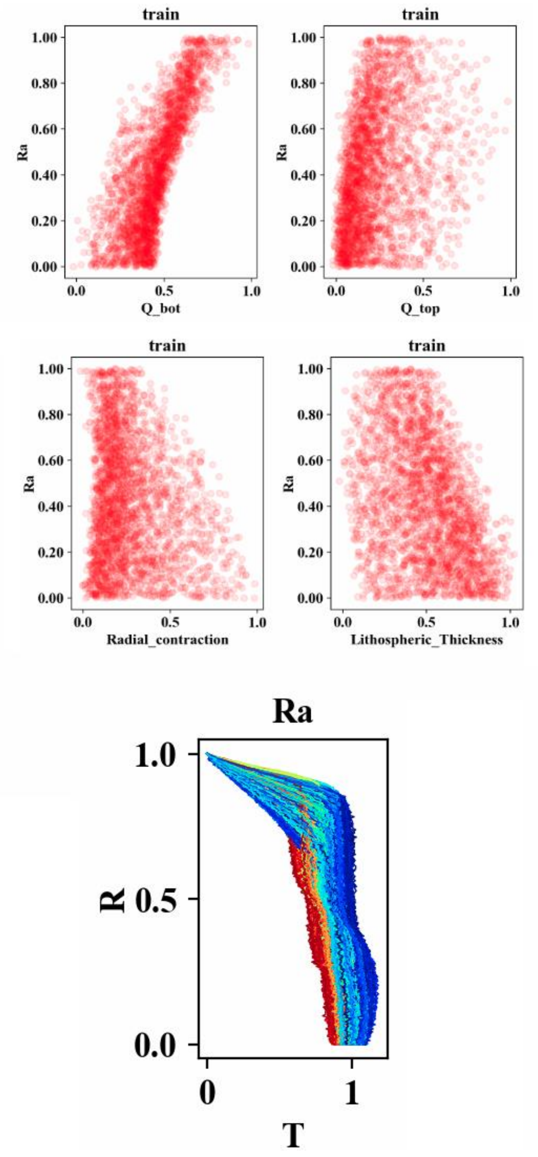
-(Mean Loss)

Results

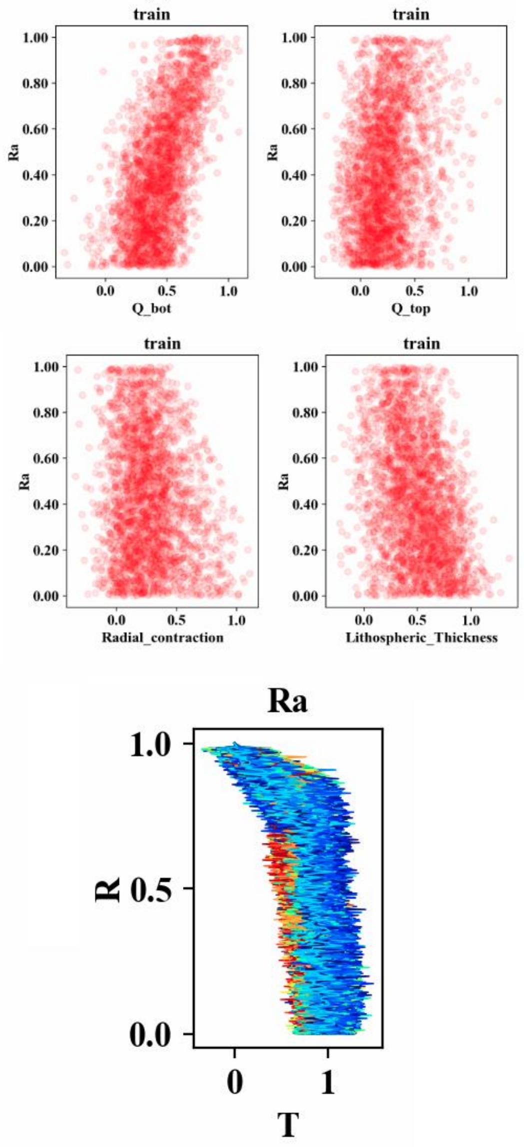
σ = 0% noise



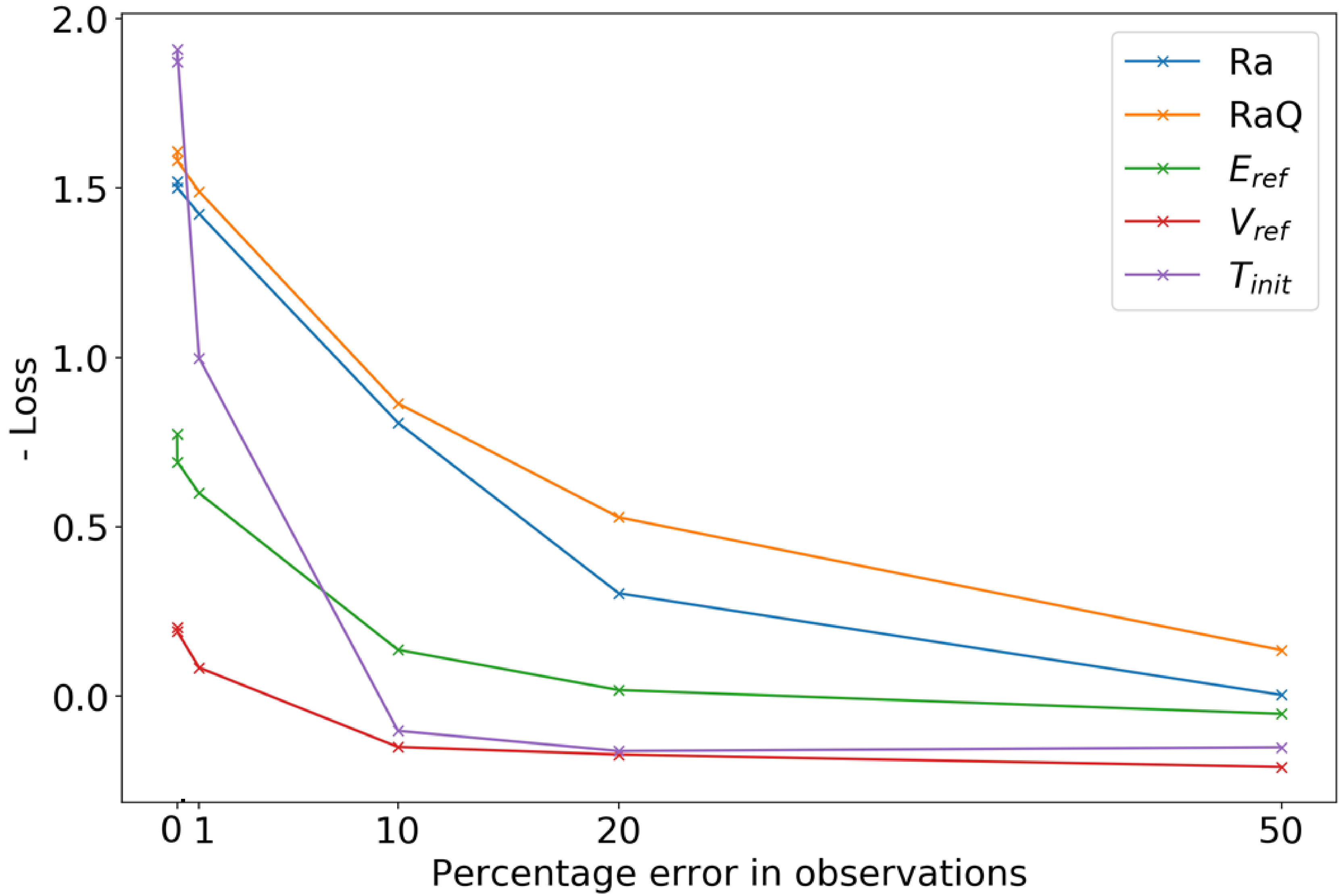
σ = 1% noise



σ = 10% noise



Results



2.0
1.5
1.0
0.5
0.0
- Loss
0 1
10
20
50
Percentage error in observations
Ra
RaQ
E_{ref}
V_{ref}
T_{init}

Future steps

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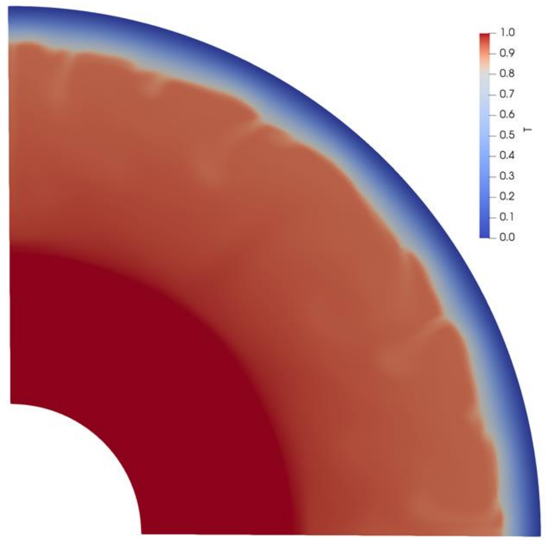
Future steps

- Generate a new dataset with more parameters and observables
    - Increased degeneracy and uncertainty expected

Parameters		Observables
Ra (η_{ref} $\in [10^{19}, 10^{22}$ Pa s])	←	Temperature profile
RaQ ($\Lambda \in [1, 50], \eta_{ref}$)		Radial contraction
$\mathbf{T_{initial}} \in [1600, 1800$ K]		Elastic lithospheric thickness
$\mathbf{E} \in [10^5, 5\text{x}10^5$ J mol^{-1}]		Core heat flux
$\mathbf{V} \in [4\text{x}10^{-6}, 10\text{x}10^{-6}$ m^3 mol^{-1}]		Surface heat flux
$\mathbf{\Delta\ T_{cmb}} \in [0, 300$ K]		Crustal thickness
$\mathbf{K_{regolith}}, \mathbf{D_{regolith}} \in$ [[const], [0, 5km]]		Duration of volcanism

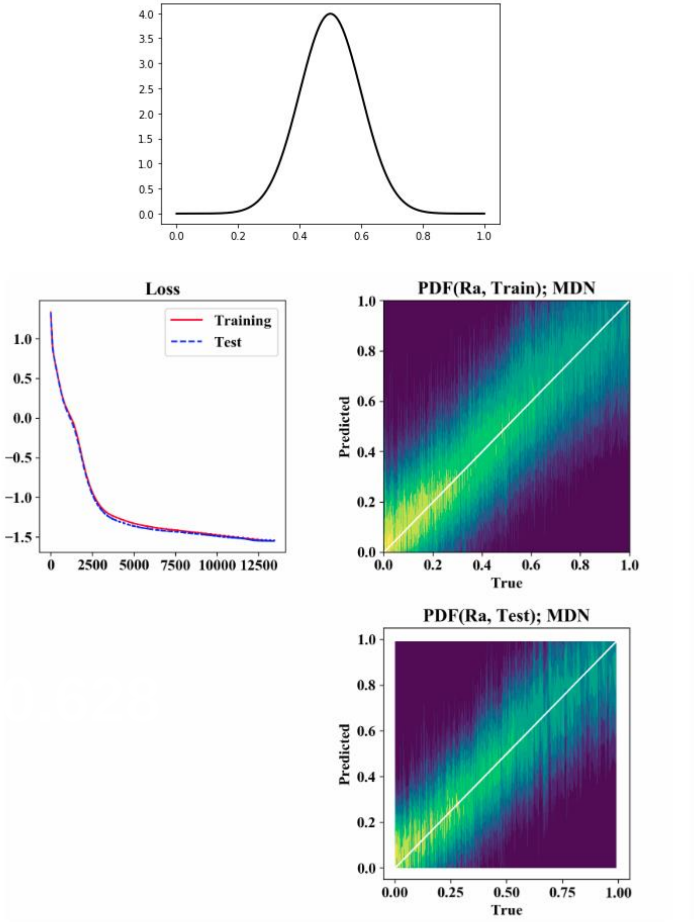
Future steps

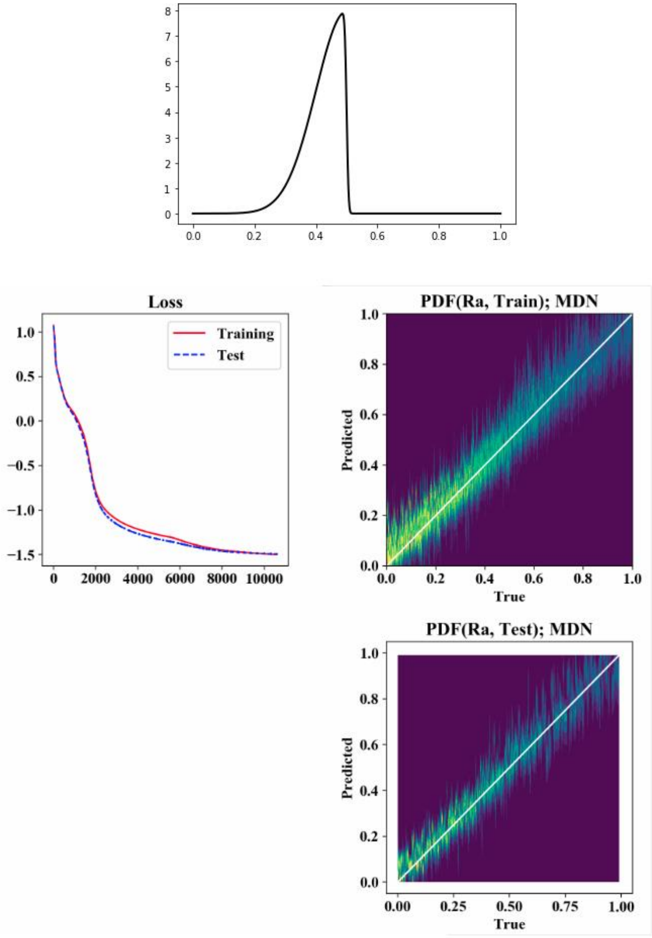
- Generate a new dataset with more parameters and observables
- Investigate higher-dimensional observables



Future steps

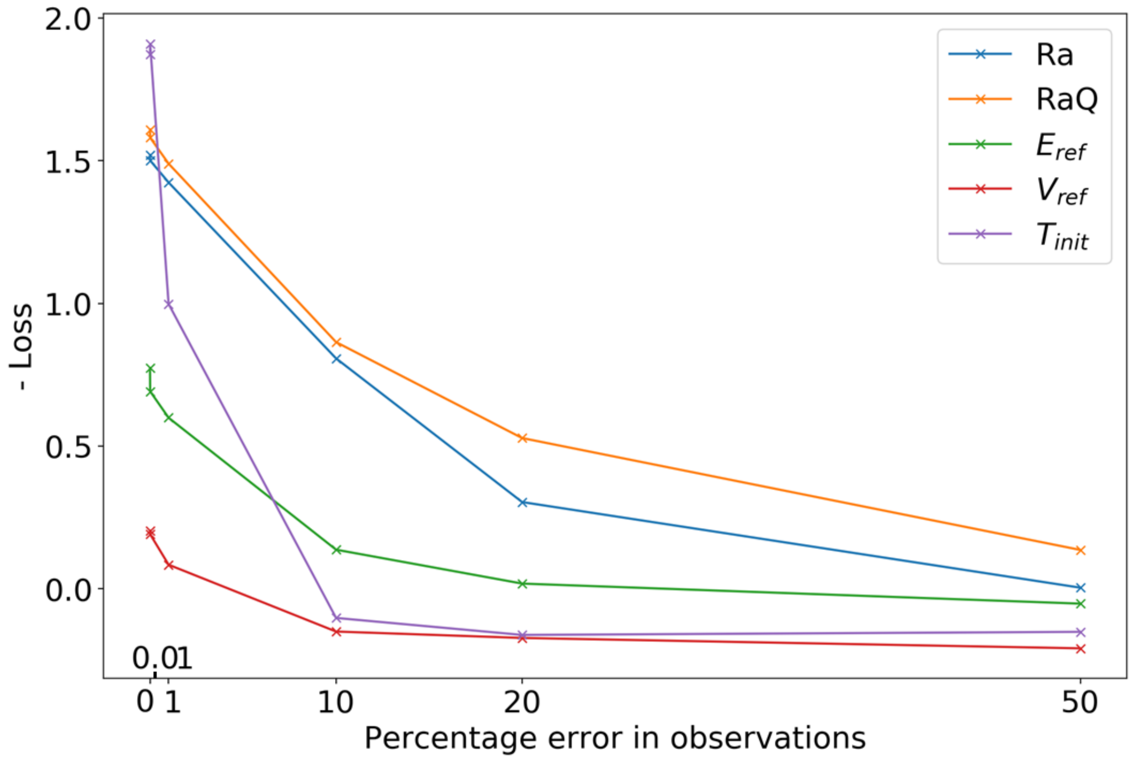
- Generate a new dataset with more parameters and observables
- Investigate higher-dimensional observables
- Explore some algorithmic modifications





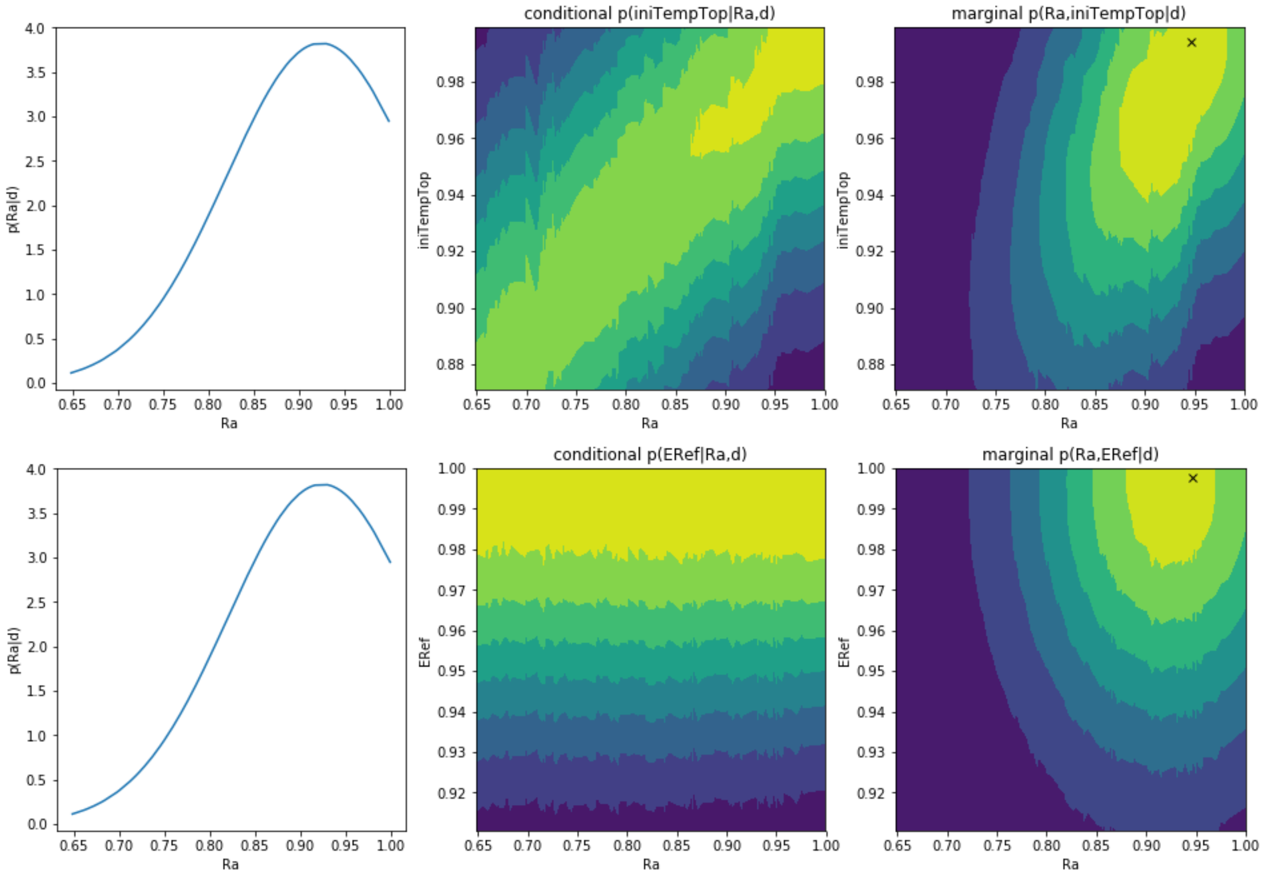
Future steps

- Generate a new dataset with more parameters and observables
- Investigate higher-dimensional observables
- Explore some algorithmic modifications
- Quantify precision requirements for each observable



Future steps

- Generate a new dataset with more parameters and observables
- Investigate higher-dimensional observables
- Explore some algorithmic modifications
- Quantify precision requirements for each observable
- Build a parameter-dimensional marginal PDF [4]



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