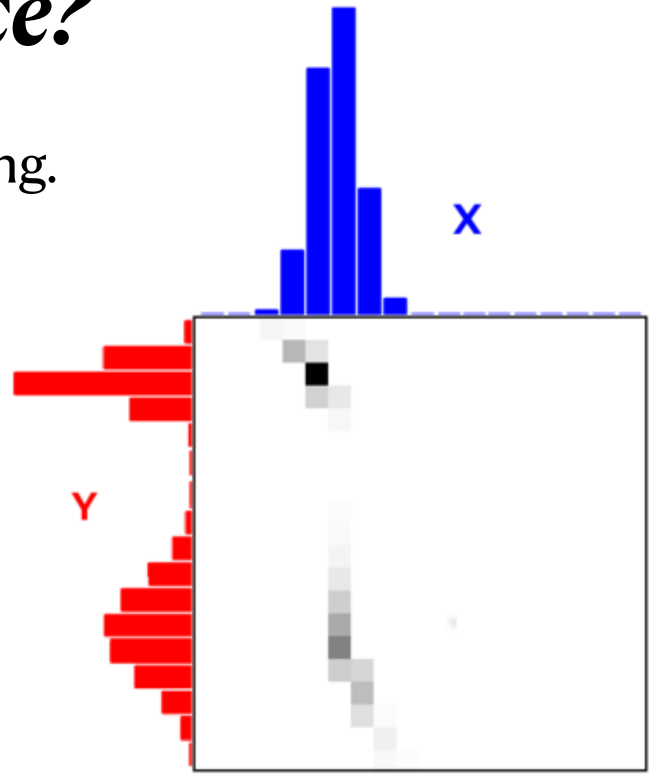
What is… The Wasserstein Distance?

An introduction, with application to climate modelling.

(joint with Mat Chantry, Milan Klöwer & Tim Palmer)



E. Adam Paxton

Predictability group internal seminar 09.11.20

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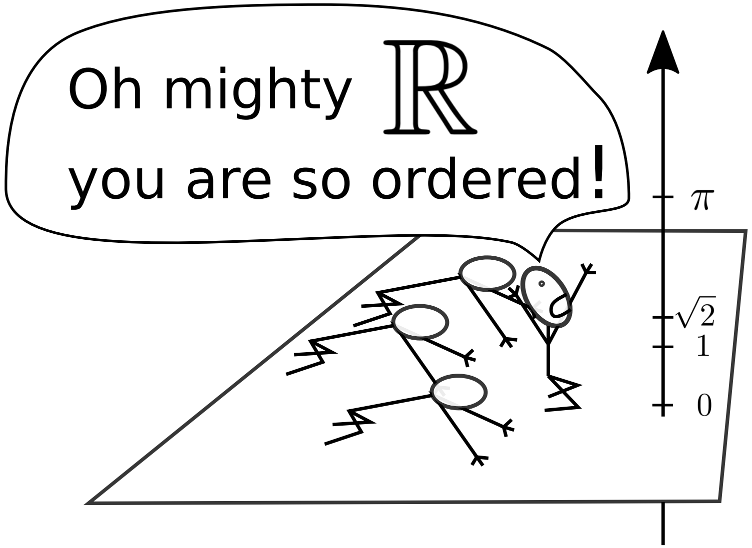
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you are so ordered!
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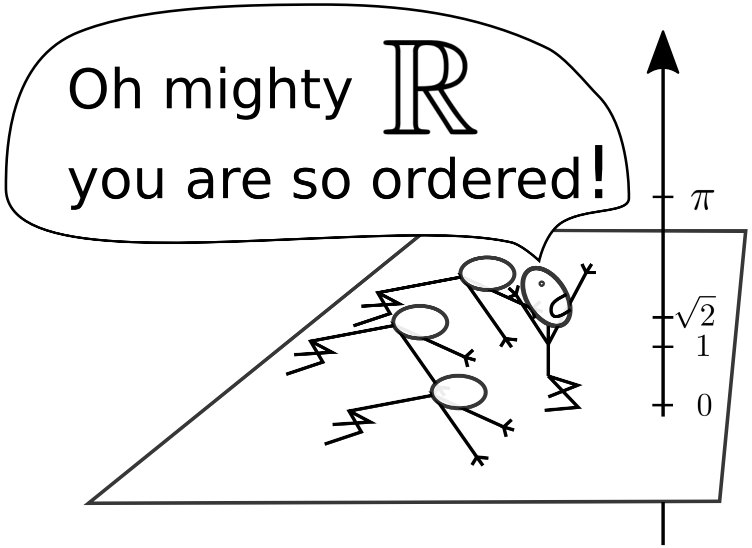
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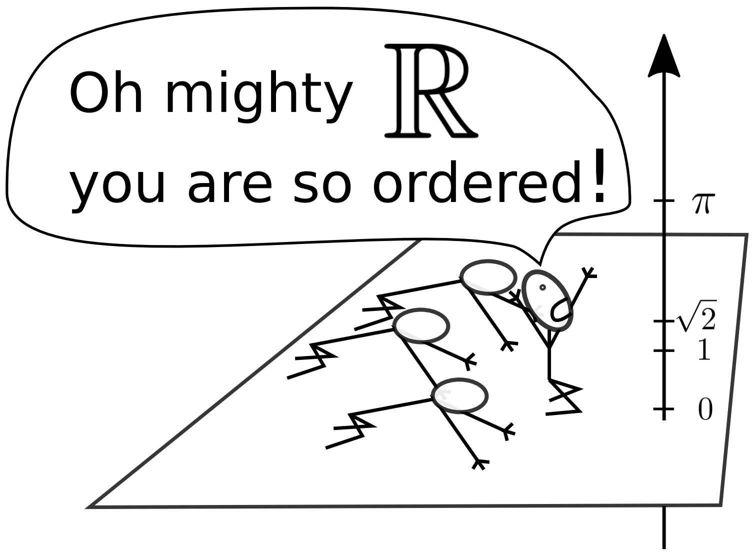
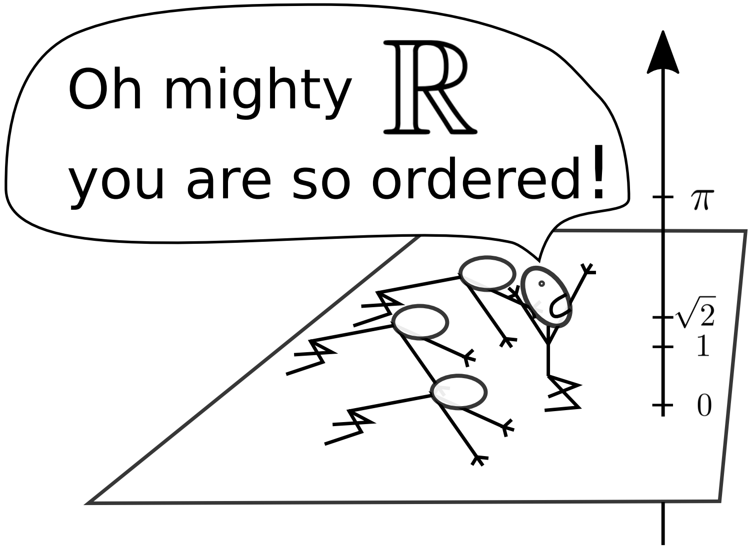
My country is the best! We have the *highest GDP.*
Actually, mine is the best. We have the *longest ski-slope.*
I think my country is best. We have the *most biodiversity.*
???...



- **Real world problems are multi-dimensional.**



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Newsweek

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WORLD

How China Buried the Green GDP

BY MELINDA LIU ON 6/28/08 AT 8:03 AM EDT

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Ask Chinese officials why their nation's environment is so toxic; you'll get a list of scientific-sounding explanations. The population is huge and dense. Arable land per capita is alarmingly sparse. Despite stunning rates of economic growth, many Chinese remain poor and rural, prone to ungreen behaviors such as tossing pollutants and trash into the rivers. But the real question is why China fares poorly in Yale and

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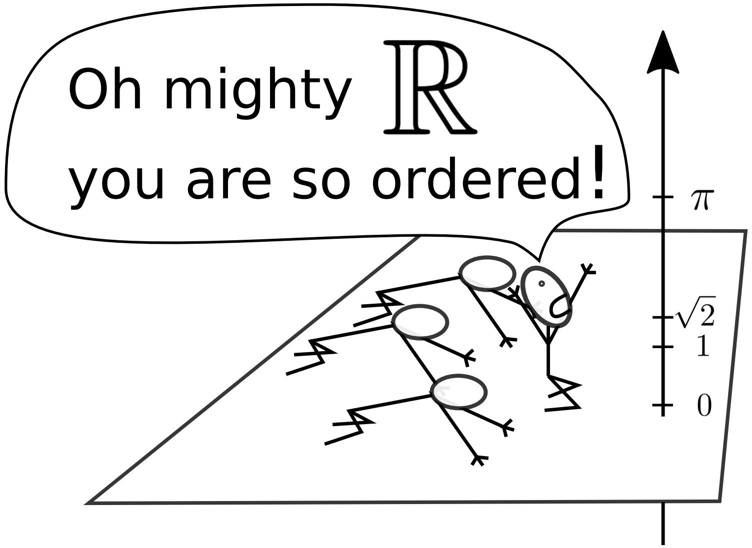

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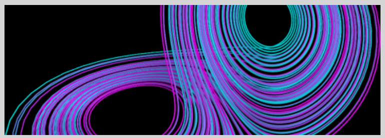
- **Real world problems are multi-dimensional.**
- If anyone says that their metric is the *best*, you should probably be cynical!

I'm now going to tell you that the Wasserstein Metric is the best way to measure distance between probability distributions.



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Plan of talk:

1. What is the Wasserstein distance?
2. What are the advantages of the WD, and how to compute it.
3. An application: exploring model climatology in low-precision.

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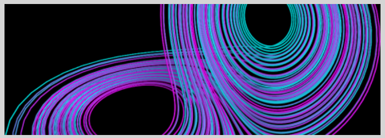

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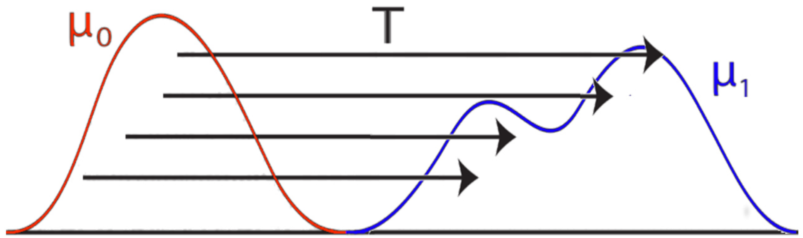

N. Papadakis, Optimal Transport for Image Processing, habilitation à diriger des recherches, Université de Bordeaux, Dec. 2015

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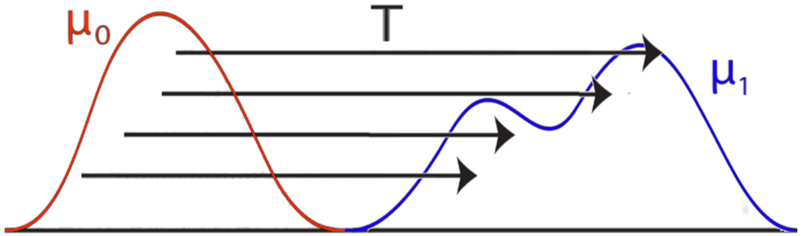

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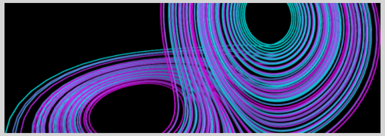

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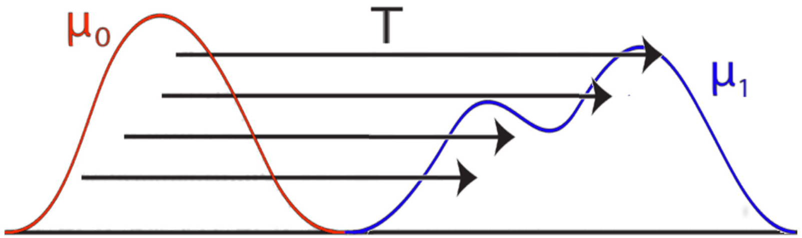

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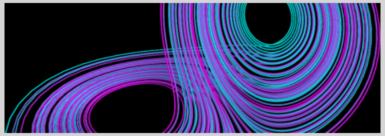

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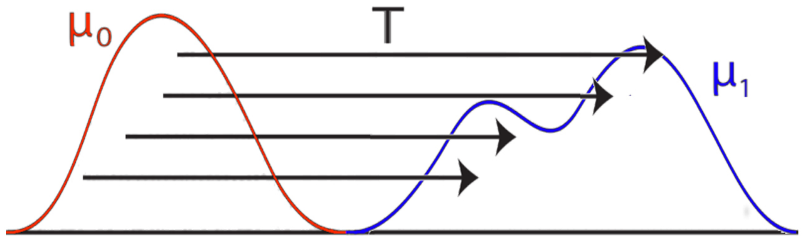
- For the case $c(x, y) = |x - y|^p$ we call the optimal cost the p-Wasserstein Distance (we'll always take $p = 1$)



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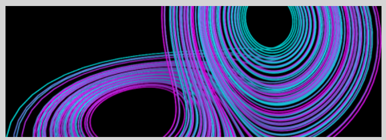

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- A *transport strategy* is a permutation of N objects $\sigma \in S_N$.

The cost of a strategy is $\displaystyle\frac{1}{N}\sum_{i=1}^{N} c(x_i, y_{\sigma(i)})$.

$$\boxed{\mathrm{WD}_1(\mu,\nu) := \min_{\sigma\in S_N} \frac{1}{N}\sum_{i=1}^{N} |x_i - y_{\sigma(i)}|}$$

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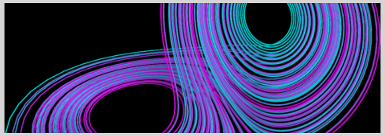

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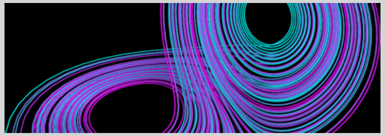
nb. when $M_1 = M_2 = N$ and $p_i = q_i = \frac{1}{N}$ it turns out the two definitions are equivalent.



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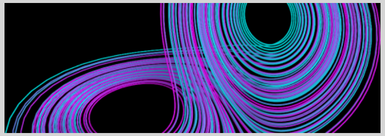
(i) It *metrizes* the space of probability distributions.



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If μ_k is a sequence of probability distributions, then

$$\mathrm{WD}_1(\mu_k, \mu) \to 0 \quad \textit{if \& only if} \quad \mu_k \to \mu \ \textit{(weak}\star\textit{)}$$

where $\mu_k \to \mu$ (weak$\star$) means:

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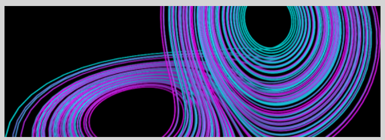

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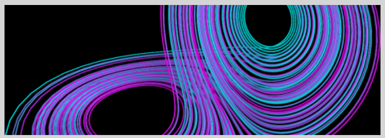
nb. (i) $\Longrightarrow$ It takes into account the whole distribution (i.e. "all moments")



(ii) It is versatile.

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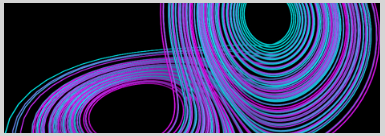
You can compare *any* two probability distributions:

- Continuous distributions.
- Discrete / singular distributions.
- Distributions defined on different spaces.



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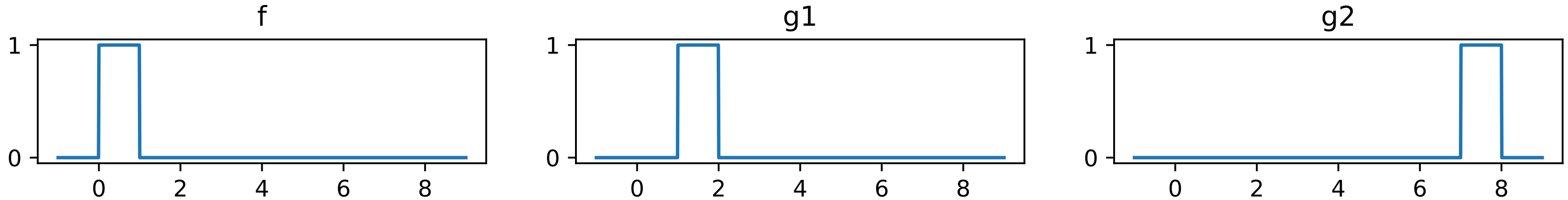

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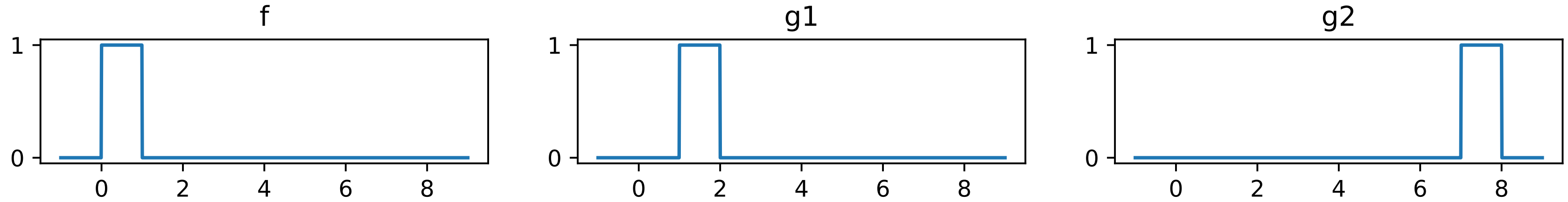

With L^p-distance we have $\|f - g_1\|_{L^p} = \|f - g_2\|_{L^p} = 2$.
But $\mathrm{WD}_1(f, g_1) = 1$, $\mathrm{WD}_1(f, g_2) = 7$.

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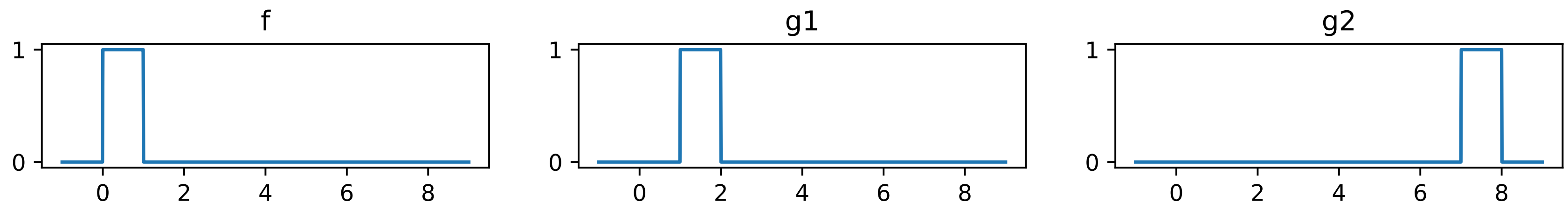

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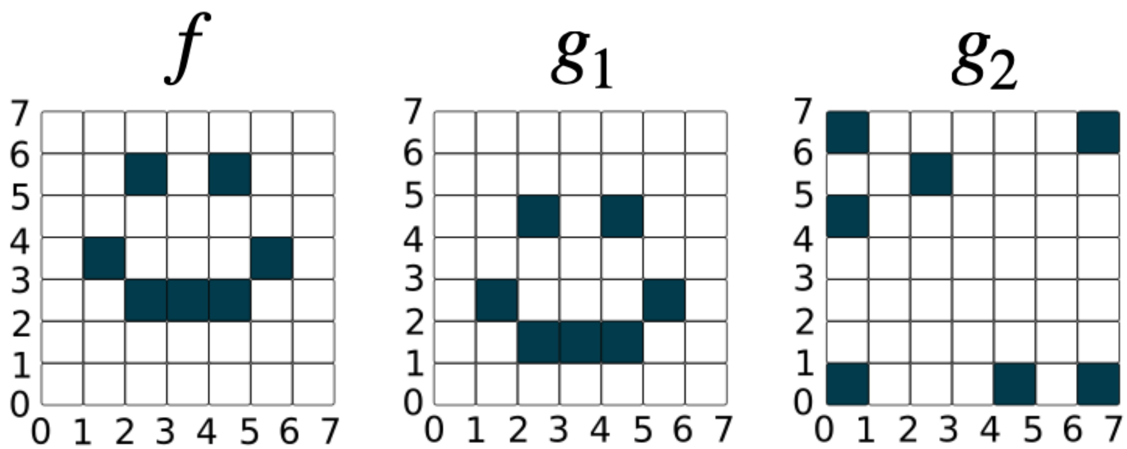

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Nb. This is a shortcoming of many common metrics e.g. K-S test / K-L divergence

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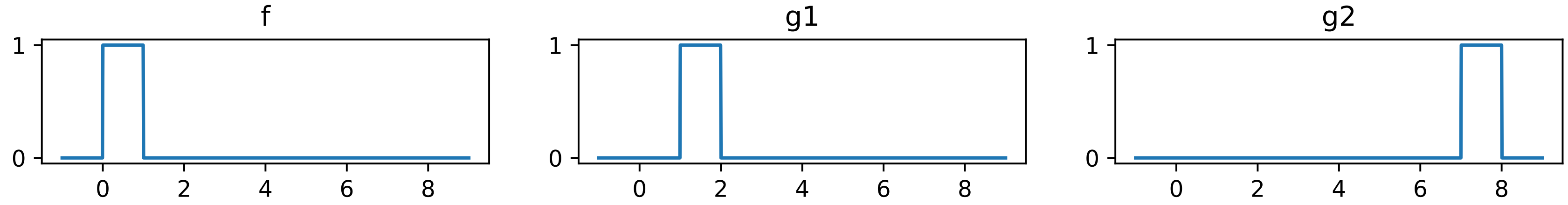

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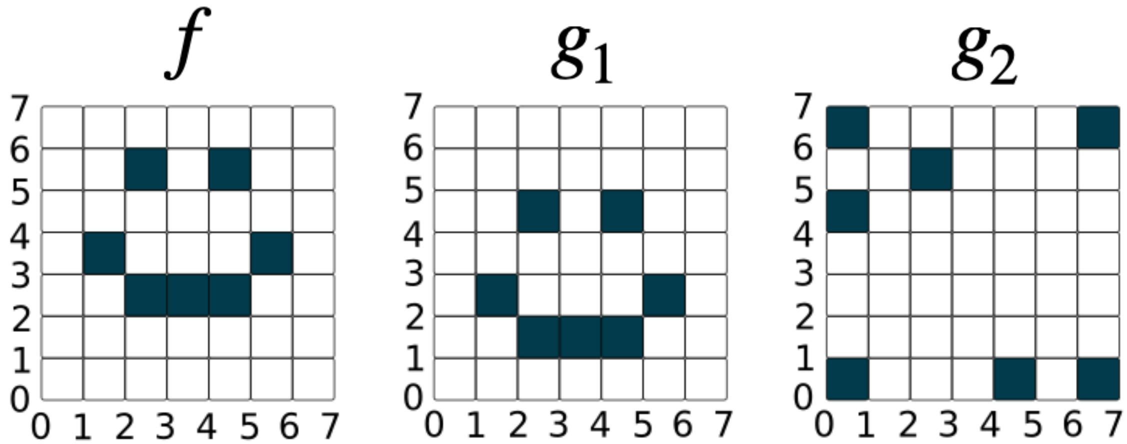

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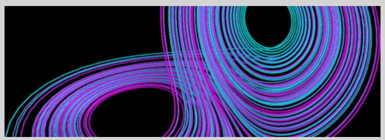

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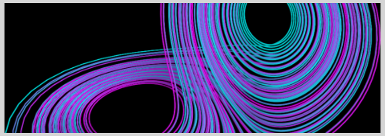

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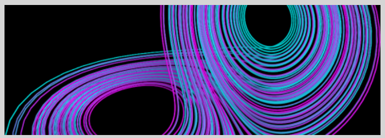

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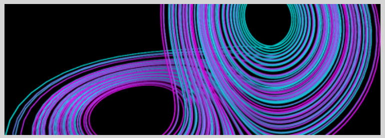
All of these can be found at github.com/eapax/EarthMover.jl



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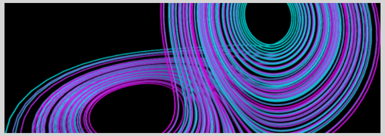

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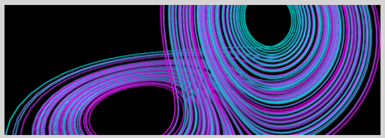
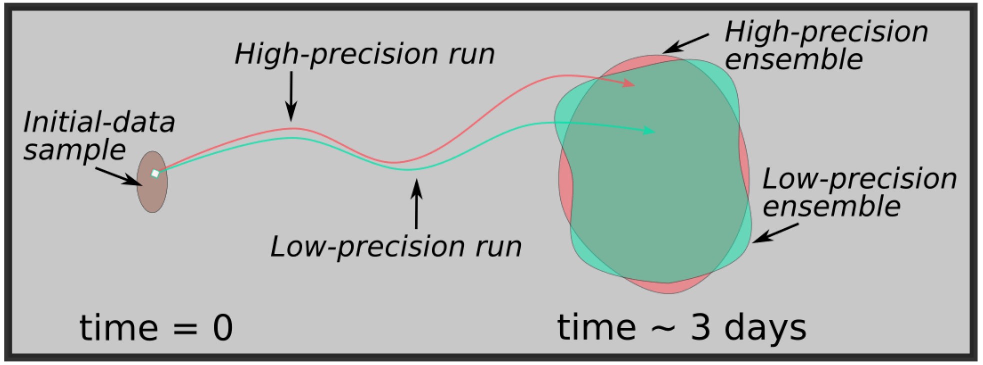
- Recently there has been lots of interest in low (<64bit) precision arithmetic for high-performance computing.
- Operational weather forecasting centres have begun porting models to low-precision.
- As forecast models move to low-precision, it's natural to ask if these models are suitable for climate modelling (some have argued NOT).



Climate modelling & weather forecasting are different methodologies.

Test for low-precision weather forecast	Test for low-precision climate model
Does it produce the same probabilistic ensemble forecast as high-precision?	*?*



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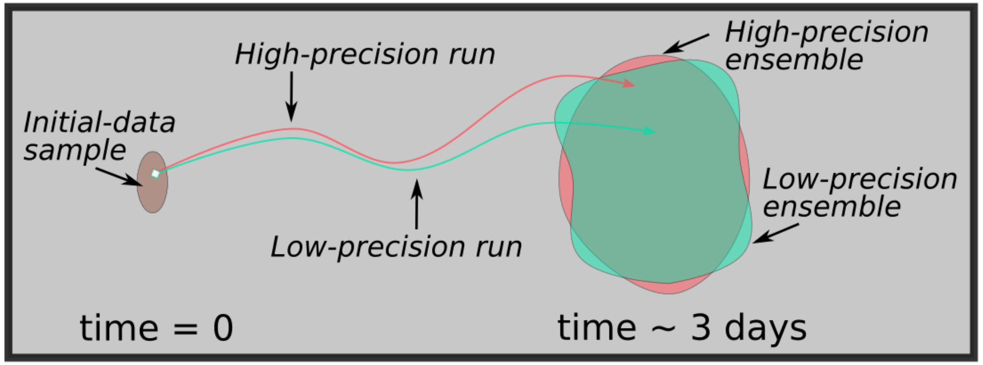

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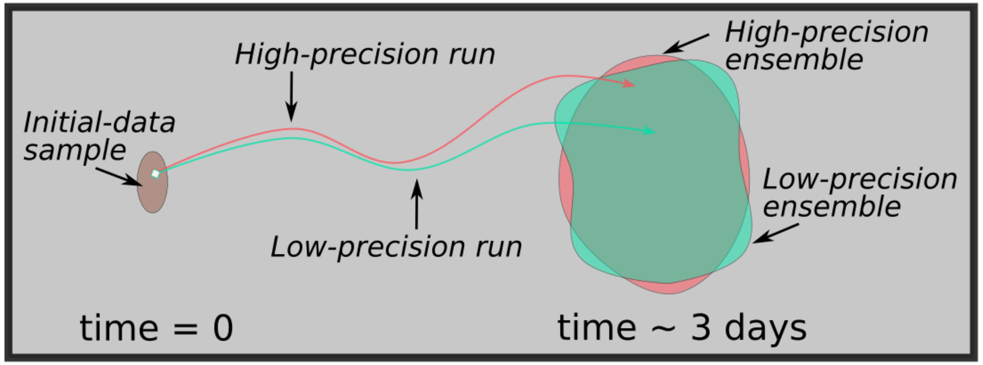
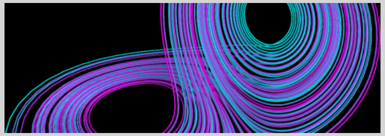
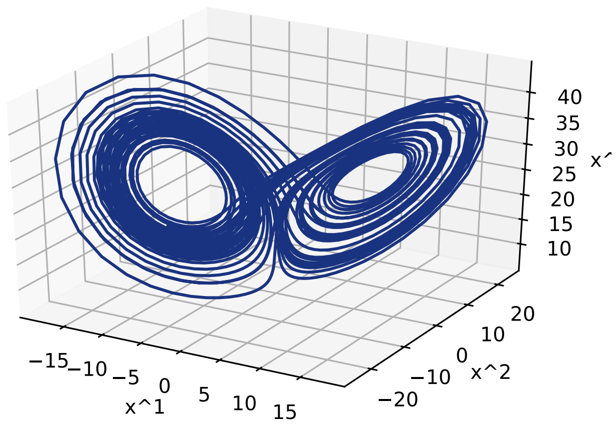


Idea: use the Wasserstein Distance to test this.



Example: L63 (toy model).



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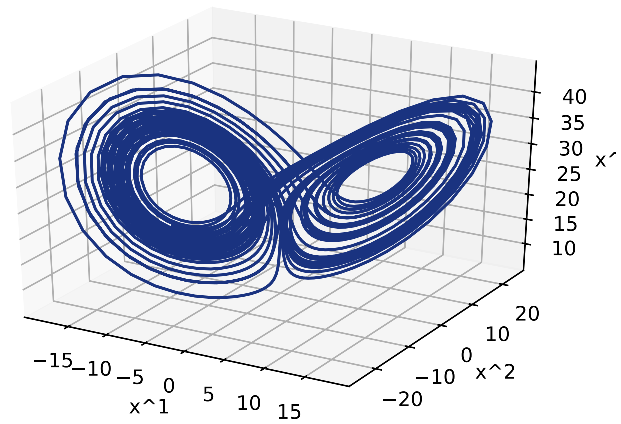

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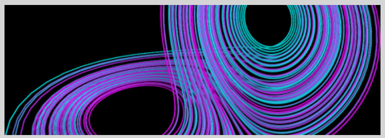

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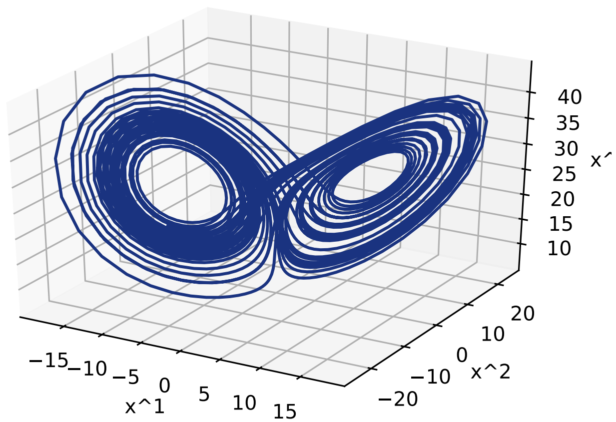

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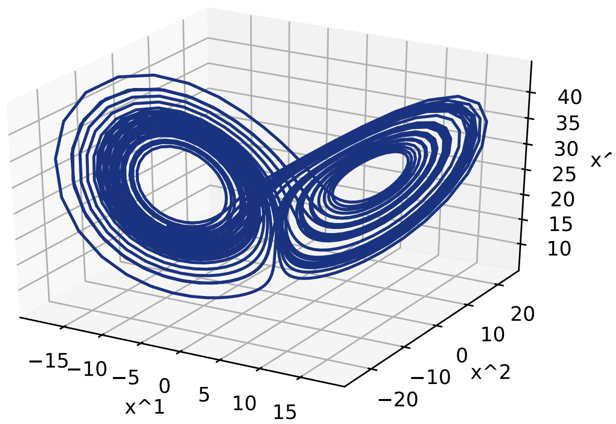

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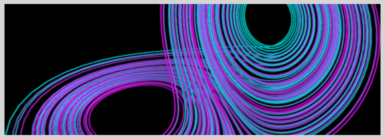

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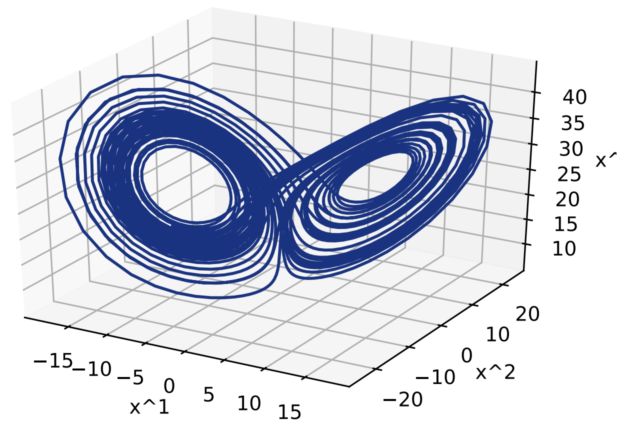

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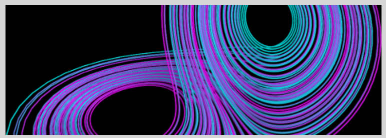

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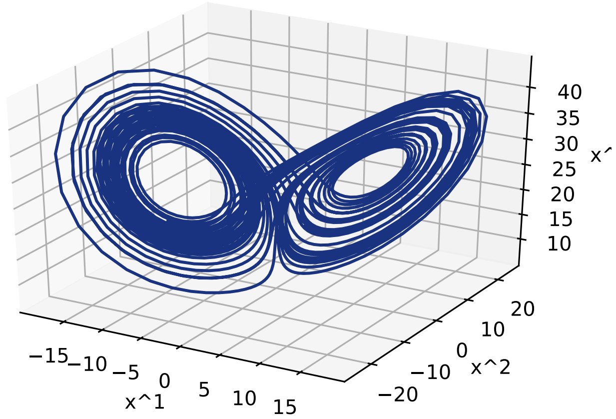

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nb. link to weak★ convergence!

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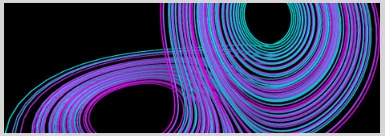

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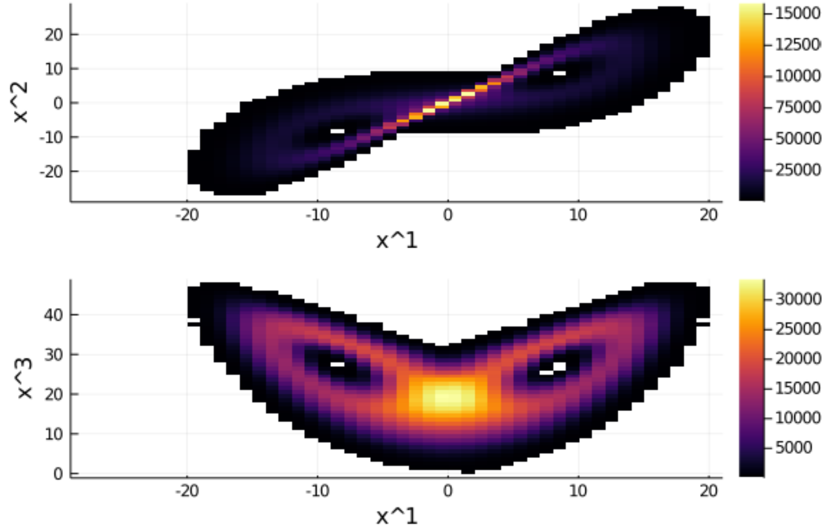

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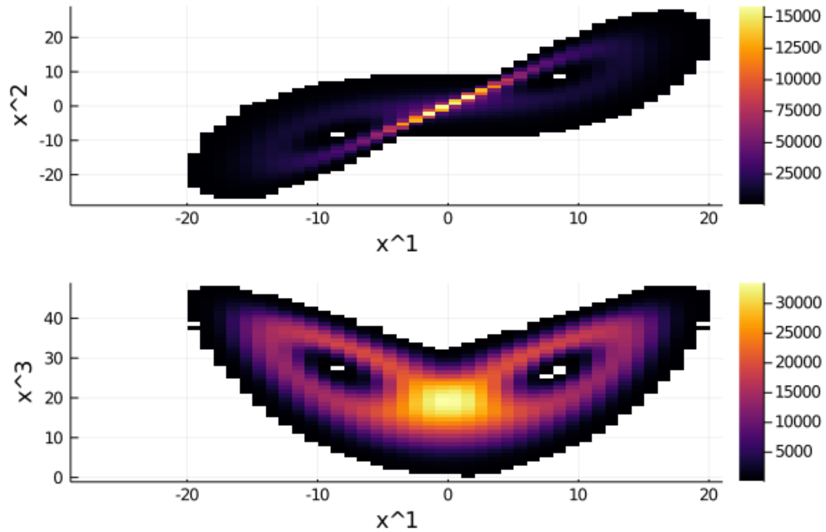
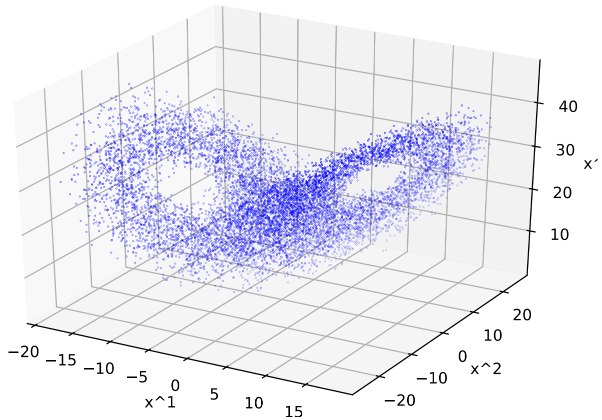
Two methods:

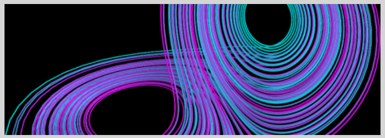
1. Data-binning
   (i.e. approximate μ as a histogram)

2. Scatter-plotting
   (i.e. approximate directly from sampling as $\mu \approx \frac{1}{N}\sum_{i=1}^{N} \delta_{x_i}$)





E. Adam Paxton



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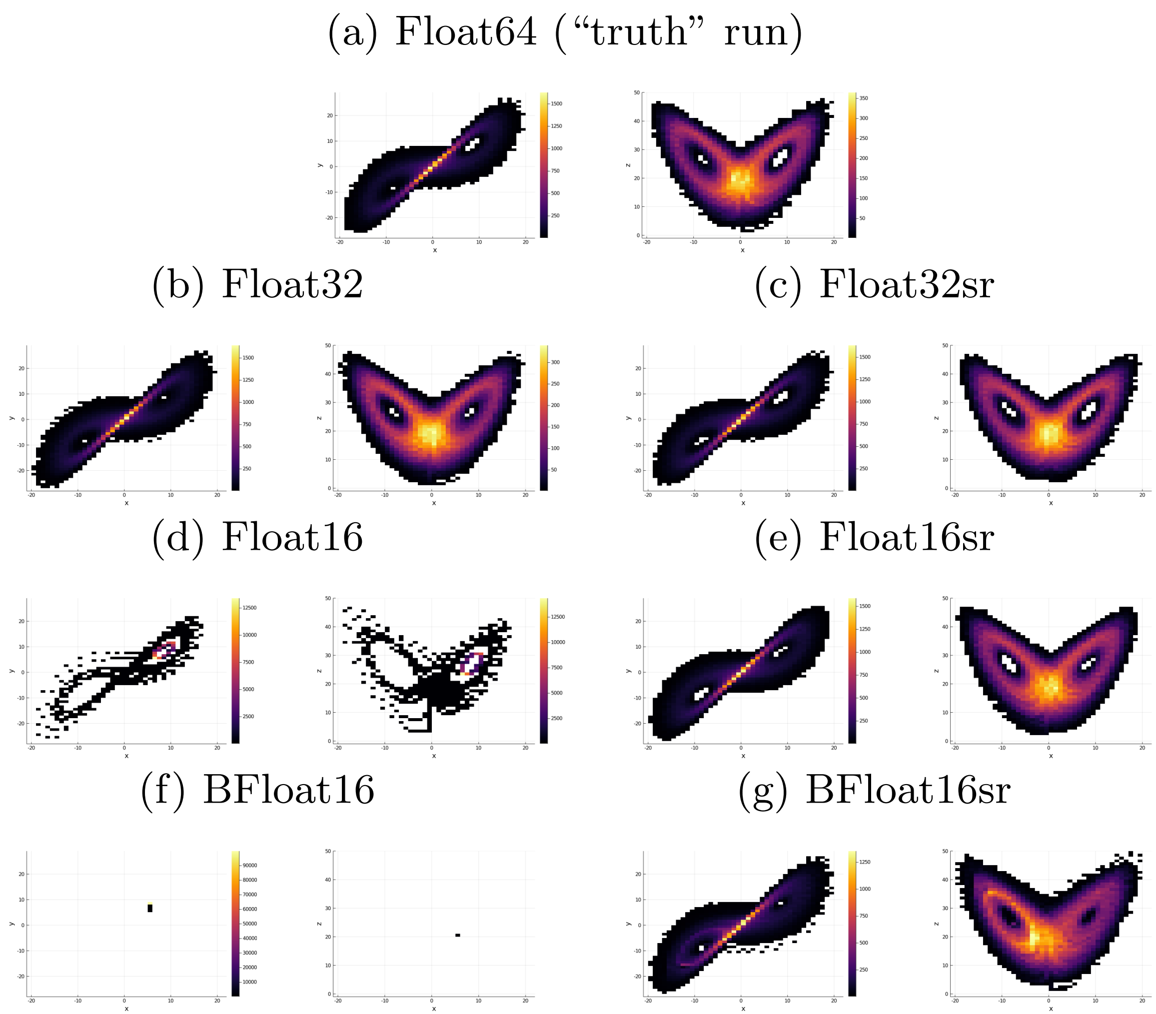

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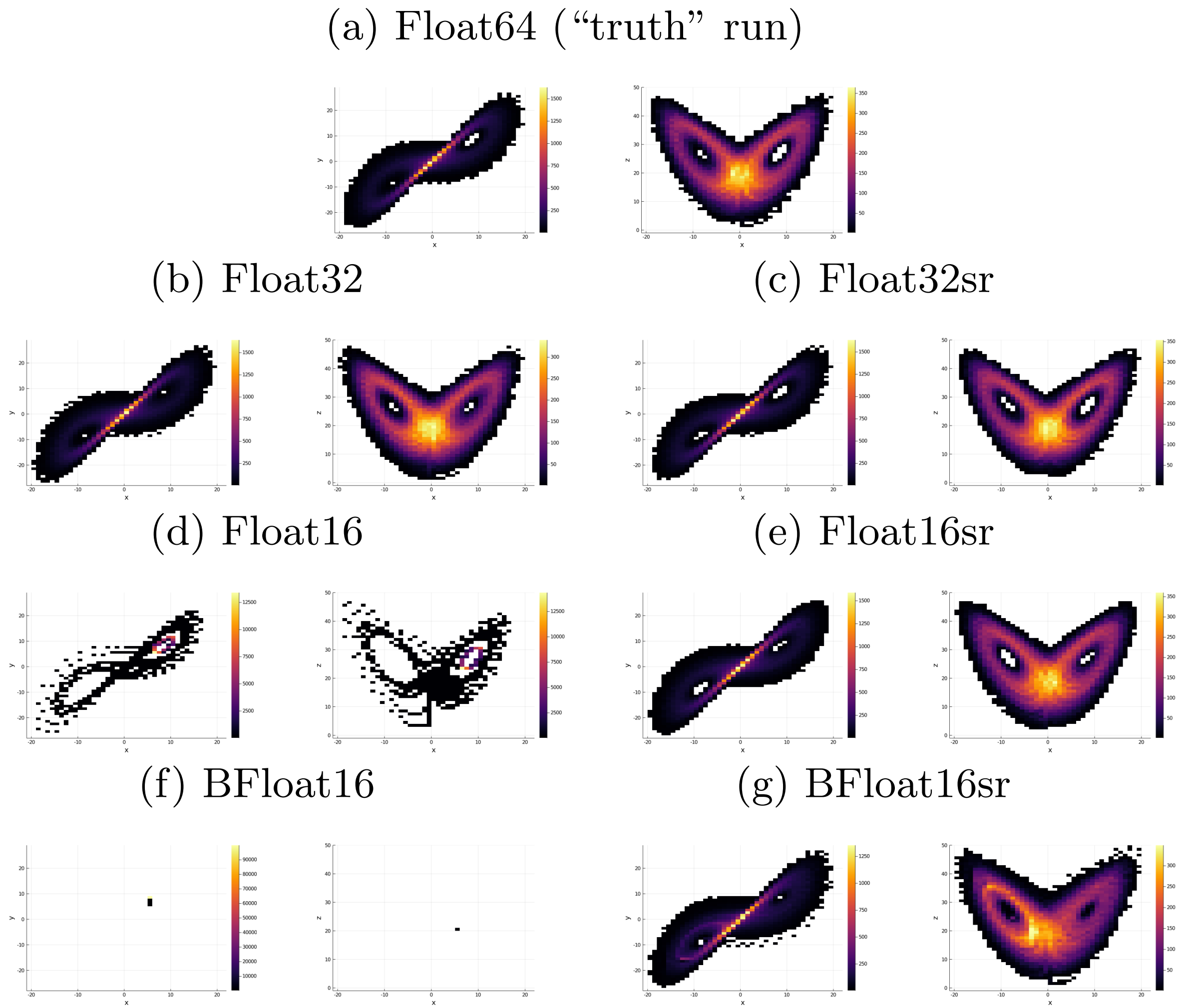

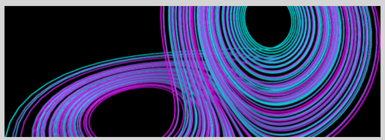

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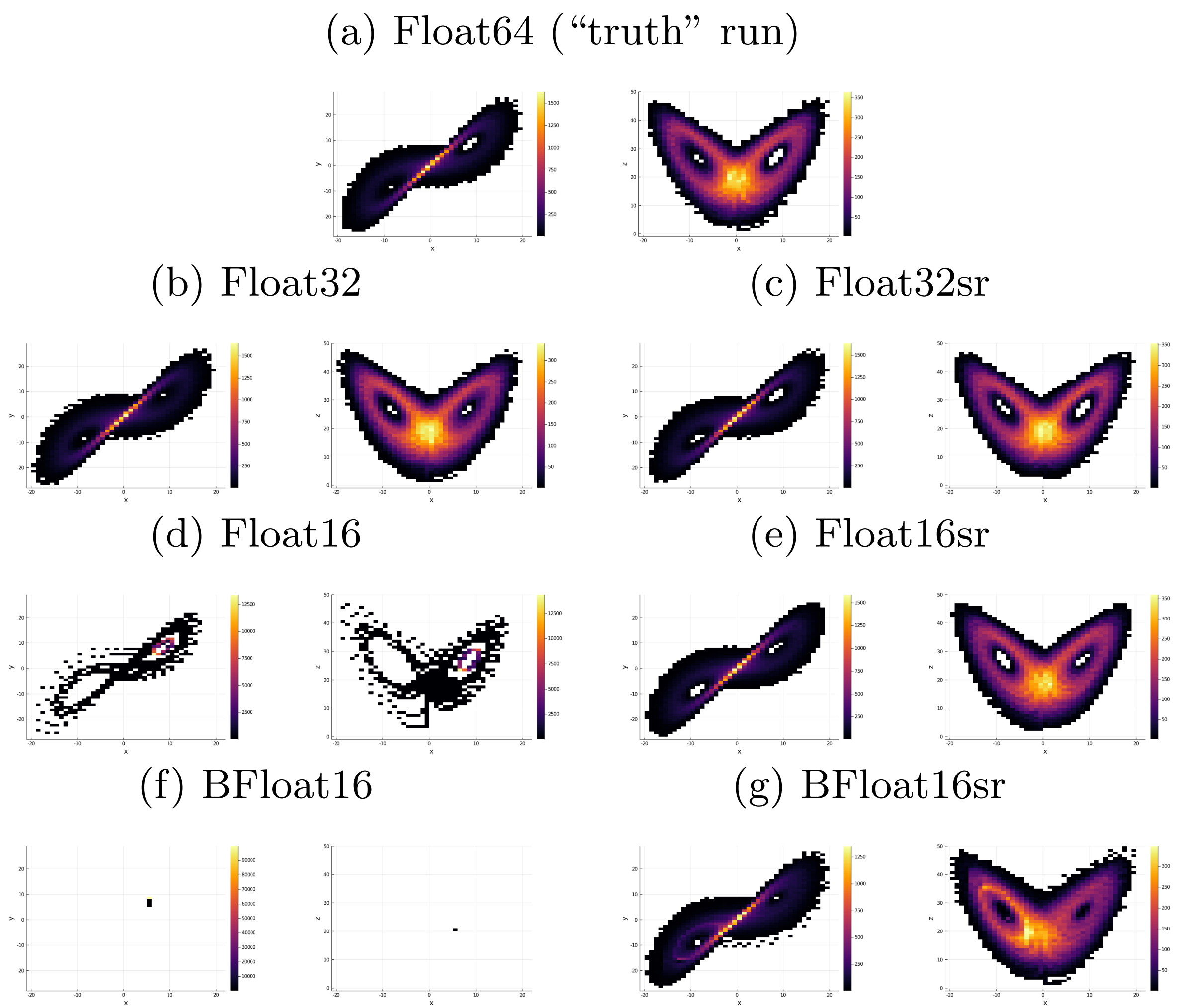

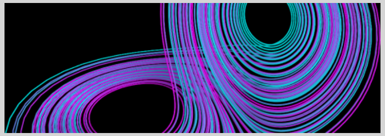

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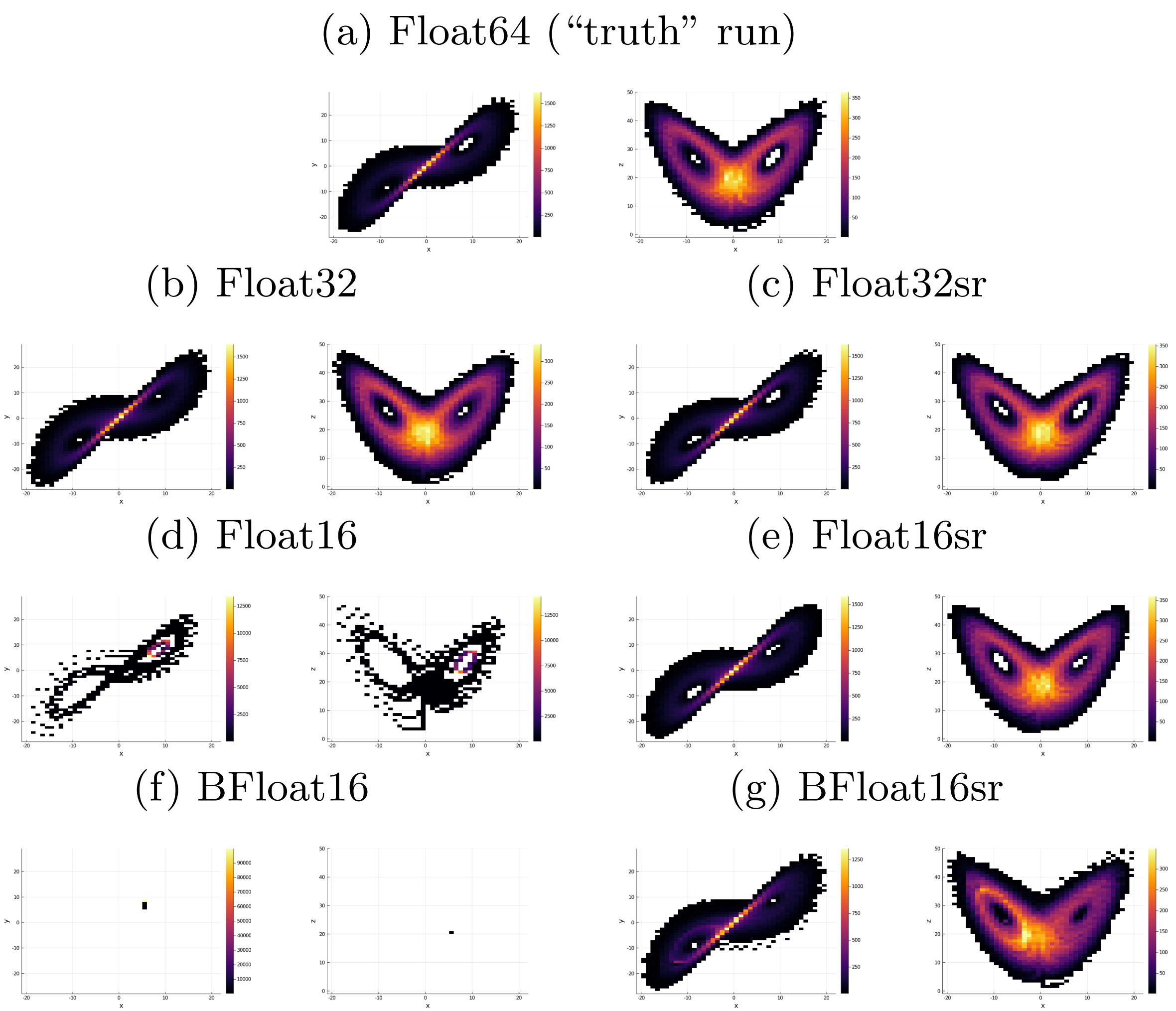
- We want a method for quantitative comparison.
- Let’s compute the Wasserstein Distances!



- Here are the results...

precision	WD(precision, Float64)
Float64	0.0
Float32	0.456
Float32sr	0.353
Float16	14.8
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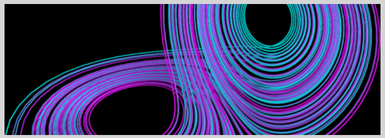

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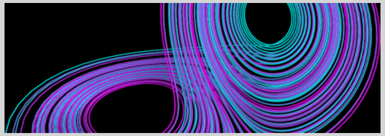

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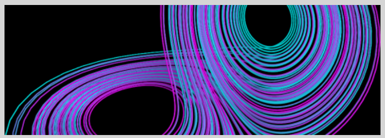

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- Idea: use an *ensemble.*

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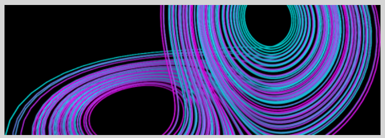

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- Take one 5-member Float64 ensemble (Control)
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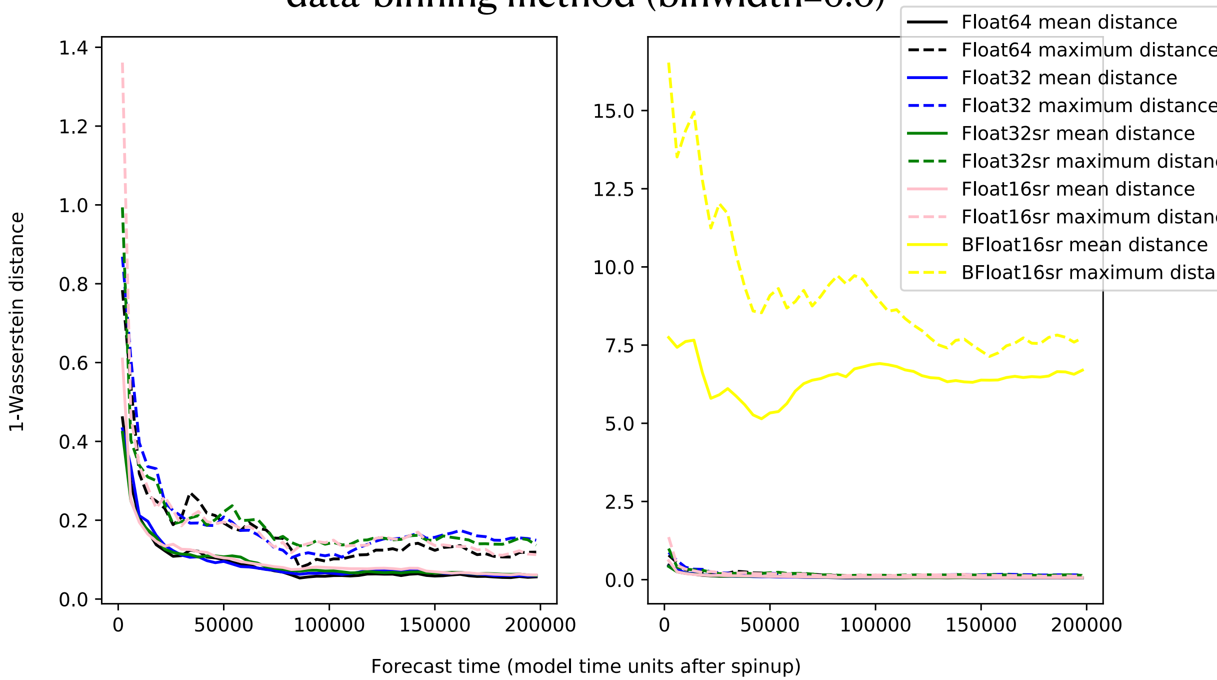

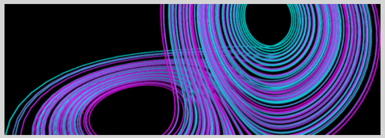

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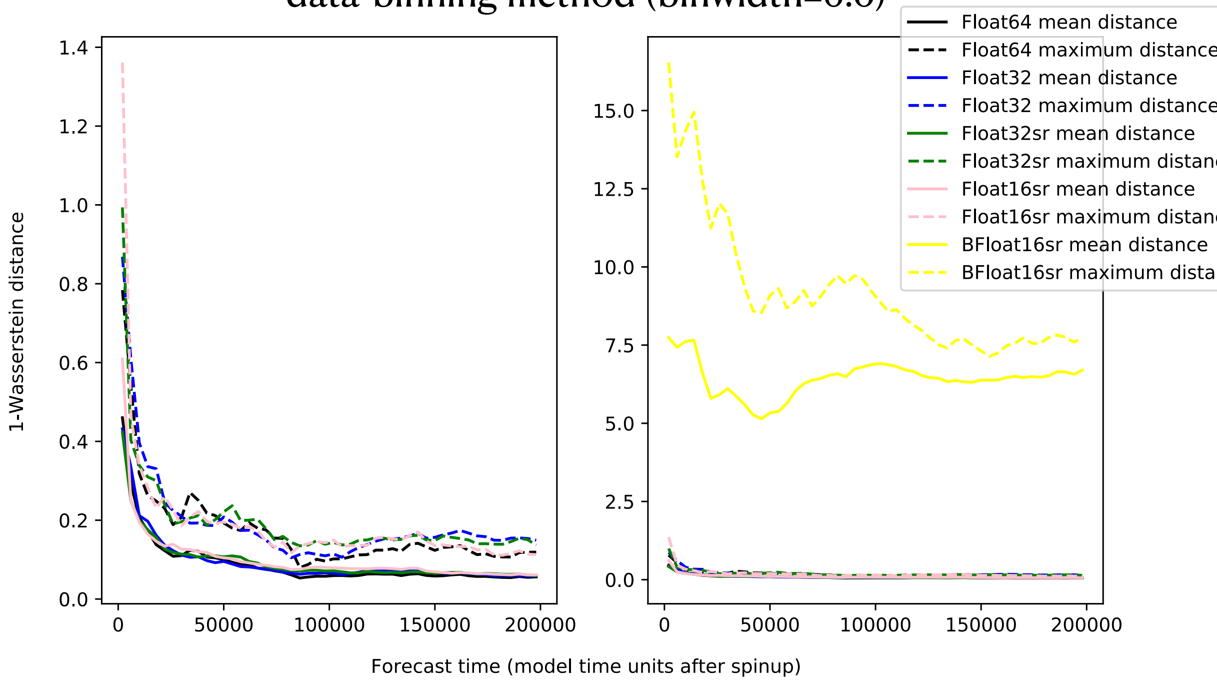
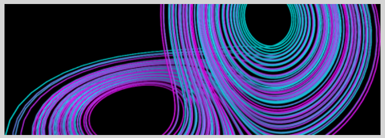


The Float64 vs Control test (black lines) serves 2 purposes:

1. It gives a null hypothesis.

2. It shows that enough time has elapsed to reach statistical equilibrium.



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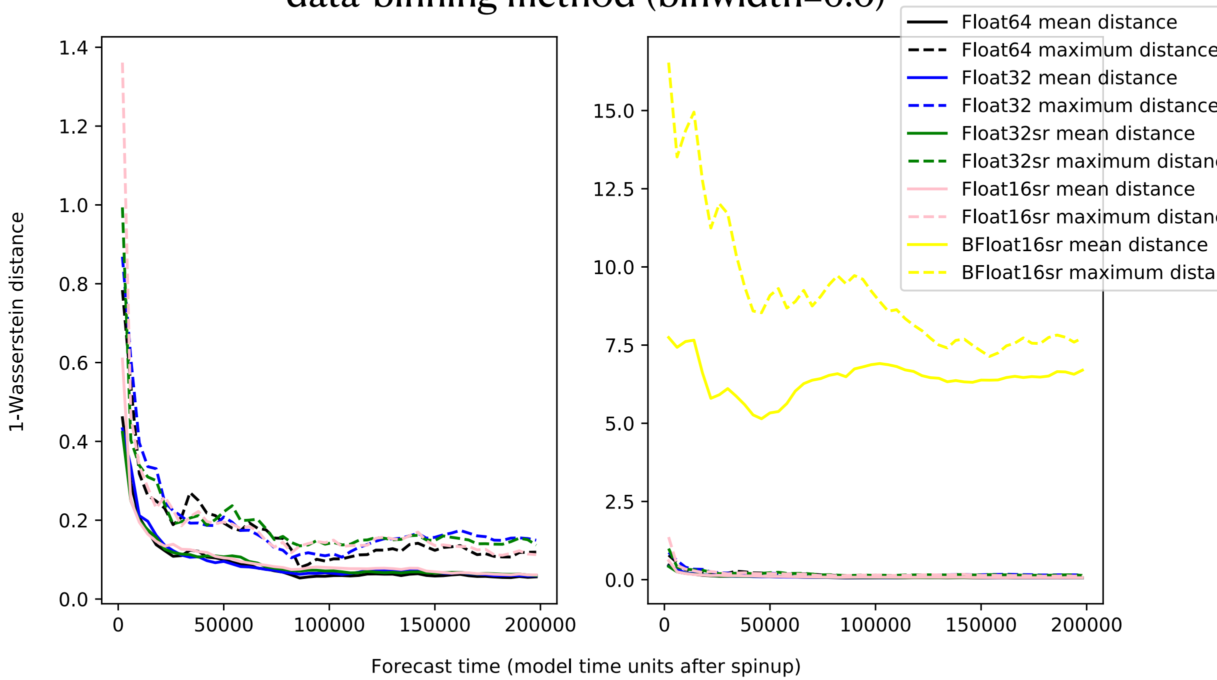
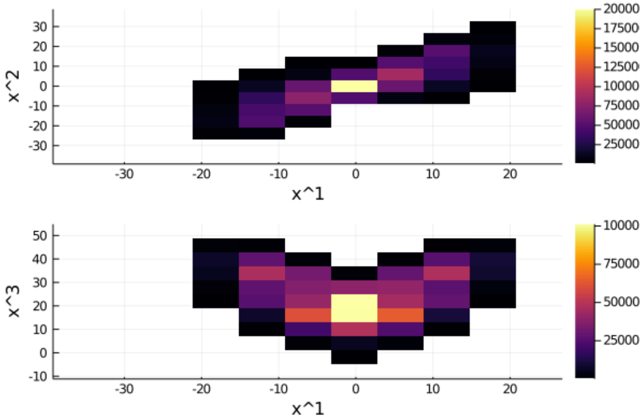
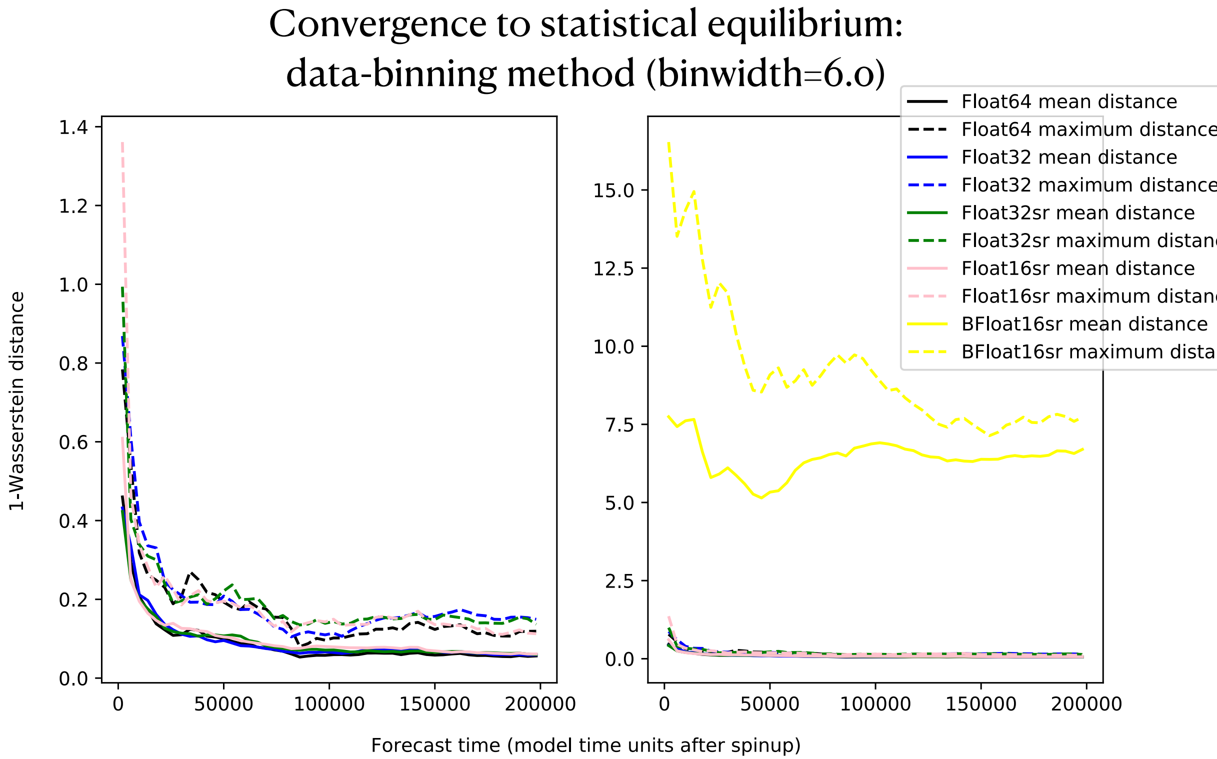


nb. bin-width=6.0 looks like:





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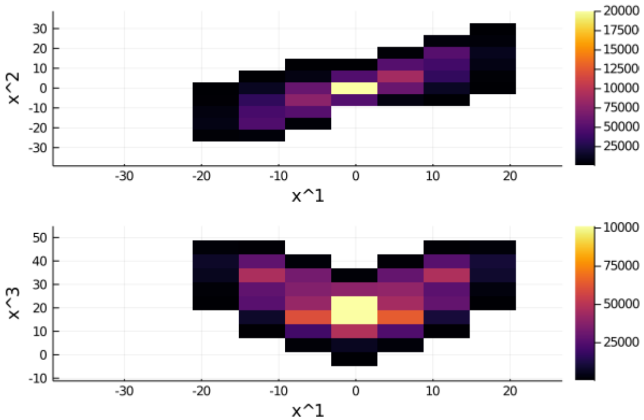

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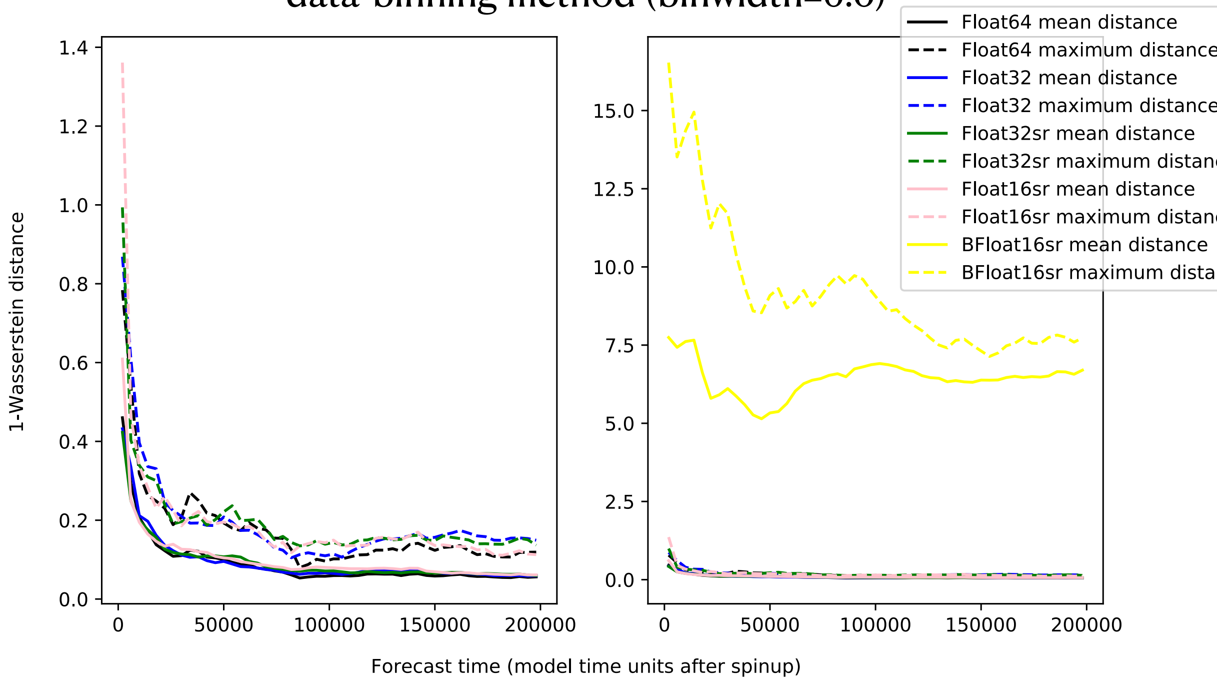
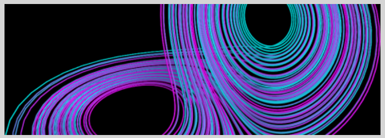


- Results are not sensitive to decreasing bin-width.



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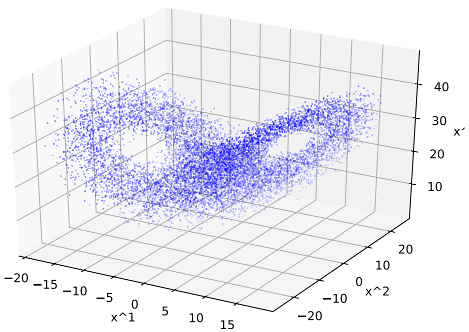

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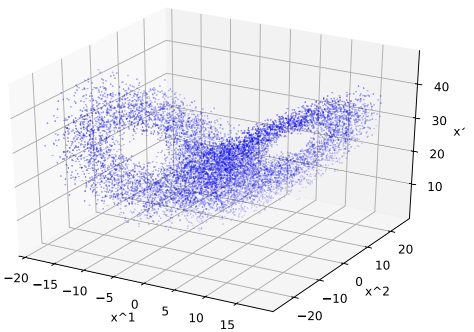
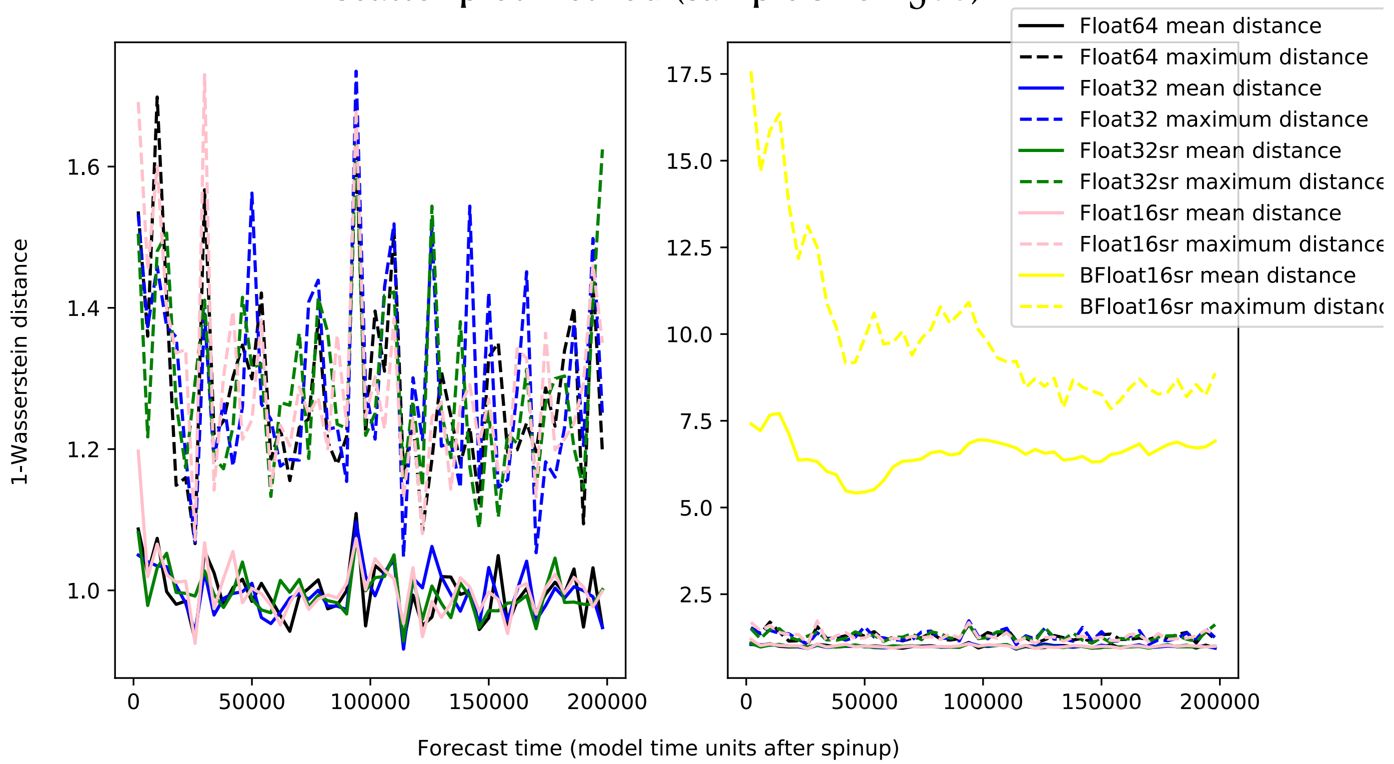


It gives comparable results.

Convergence to statistical equilibrium:
scatter-plot method (sample size=2500)



Shallow Water Model: github.com/milankl/ShallowWaters.jl

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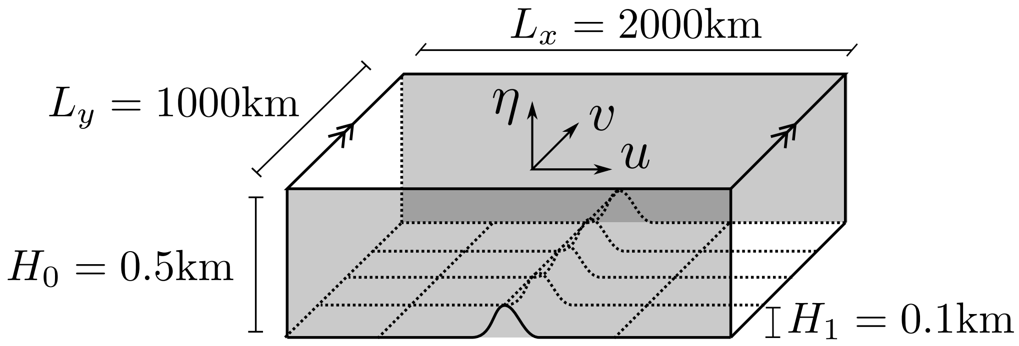


$\mathbf{u}(x, y, t) = (u(x, y, t), v(x, y, t))$ fluid velocity

$h(x, y, t) = H(x) + \eta(x, y, t)$ layer depth

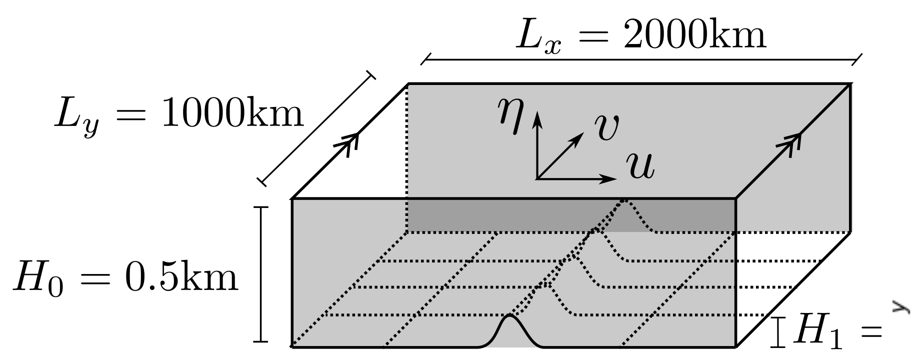
$\mathbf{F}(x, y, t) = (f(y), 0)$ wind forcing

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\,\mathbf{u} + f\mathbf{z} \times \mathbf{u} = -g\nabla\mathbf{u} + \mathbf{D}(\mathbf{u}, \nabla\mathbf{u}) + \mathbf{F}$$

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (h\mathbf{u}) = 0$$

Shallow Water Model:

github.com/milankl/ShallowWaters.jl



$\mathbf{u}(x,y,t) = (u(x,y,t), v(x,y,t))$ fluid velocity

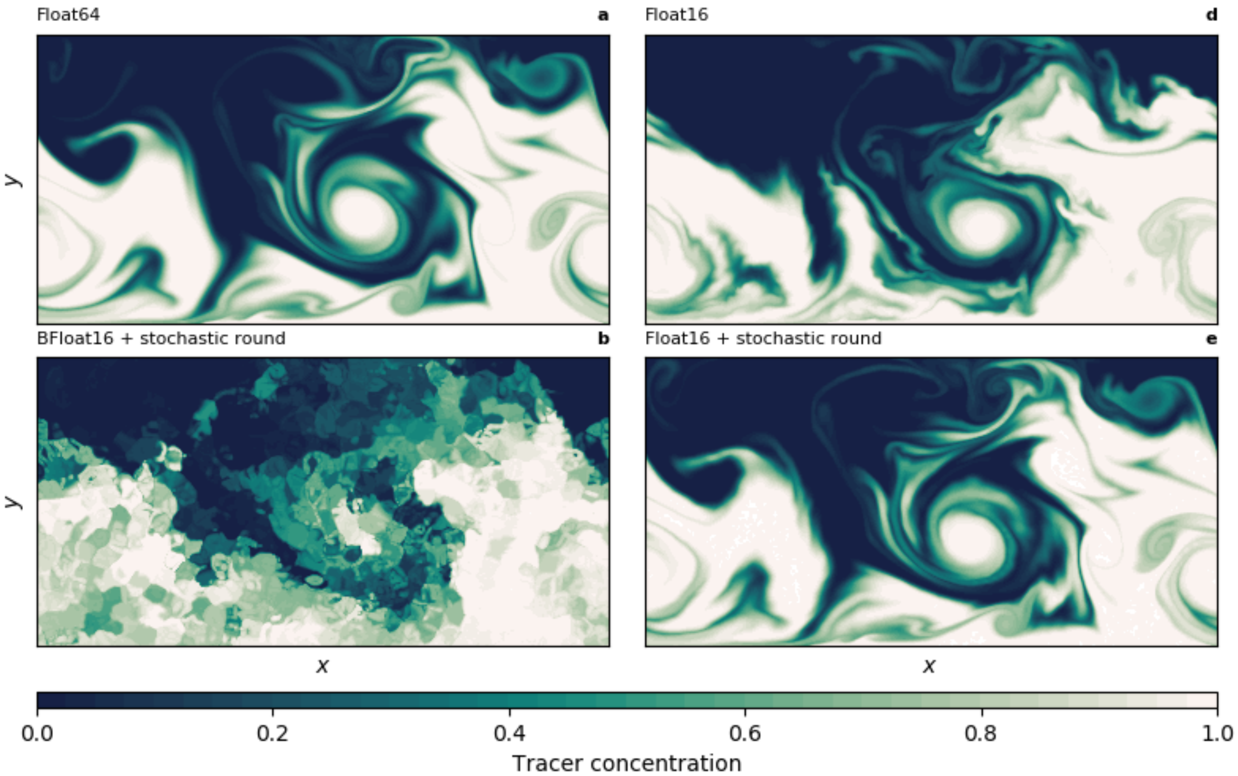
$h(x,y,t) = H(x) + \eta(x,y,t)$ layer depth

$\mathbf{F}(x,y,t) = (f(y), 0)$ wind forcing

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\,\mathbf{u} + f\mathbf{z} \times \mathbf{u} = -g\nabla \mathbf{u} + \mathbf{D}(\mathbf{u}, \nabla \mathbf{u}) + \mathbf{F}$$

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (h\mathbf{u}) = 0$$

- Finite difference scheme, 100×50 spatial grid



We want to estimate the Shallow Water model climatology (i.e. invariant measure).

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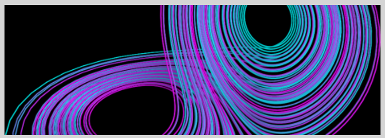
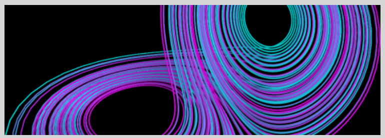
Some problems arise:

- We have time evolution in a $100 \times 50 = 5000$ dimensional space.
- Working with high-dimensional probability distributions is non-trivial.
- Data-binning becomes stupid. Looking at just one parameter u and assigning just 2 bins per spatial coordinate would lead to 2^{5000} bins. (number of atoms in observable universe $\approx 2^{270}$)



- One strategy: project down onto lower-dimensional subspaces.



- One strategy: project down onto lower-dimensional subspaces.
- This is what I have seen done so far.

Ranking IPCC Models Using the Wasserstein Distance

G. Vissio[1], V. Lembo[1], V. Lucarini[1,2,3] and M. Ghil[4,5]

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[2]Department of Mathematics and Statistics, University of Reading, Reading, UK

[3]Centre for the Mathematics of Planet Earth, University of Reading, Reading, UK

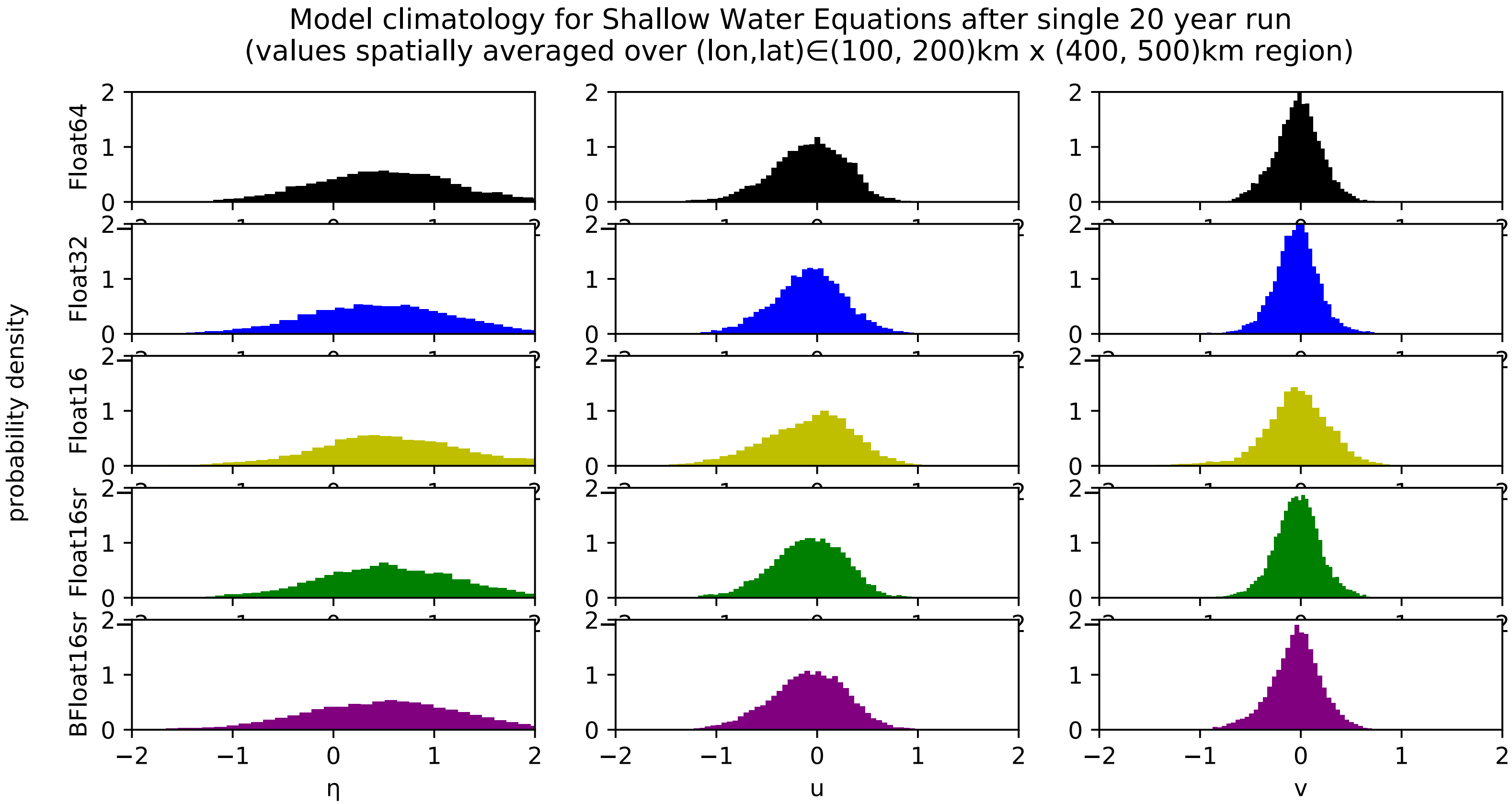
[4]Geosciences Department and Laboratoire de Météorologie Dynamique (CNRS and IPSL), Ecole Normale Supérieure and PSL University, Paris, France

[5]Department of Atmospheric & Oceanic Sciences, University of California at Los Angeles, Los Angeles, USA

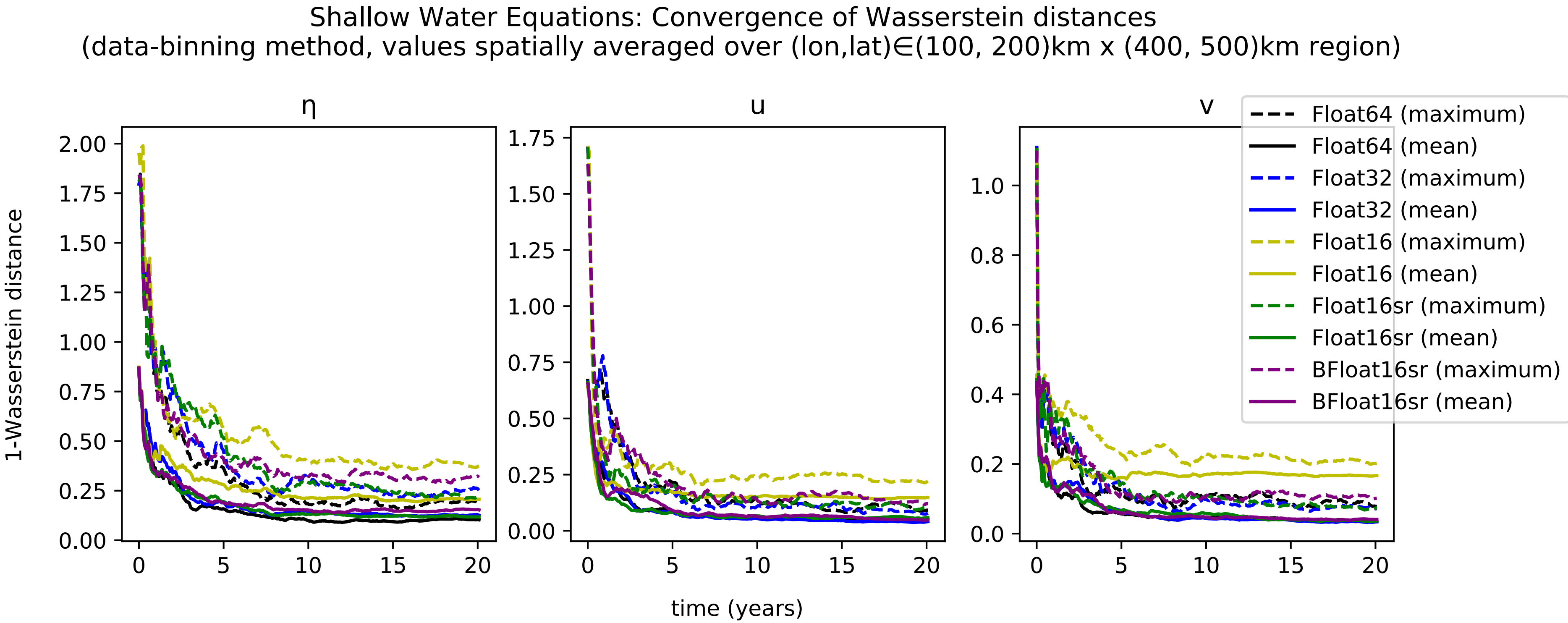
Key Points:

- Evaluation of climate model performance by benchmarking with reference datasets
- Climate model ranking related to the choice of variables of interest
- Highlighting model deficiencies through emphasis on climatic regions and variables

We can do this for Shallow Waters. Take spatial average over some (arbitrary) region (100,200)km x (400,500). Do 1D data-binning.



- We can compute Wasserstein distances between these 1D distributions.
- Same experiment as before (5-member ensembles, one Control ensemble).



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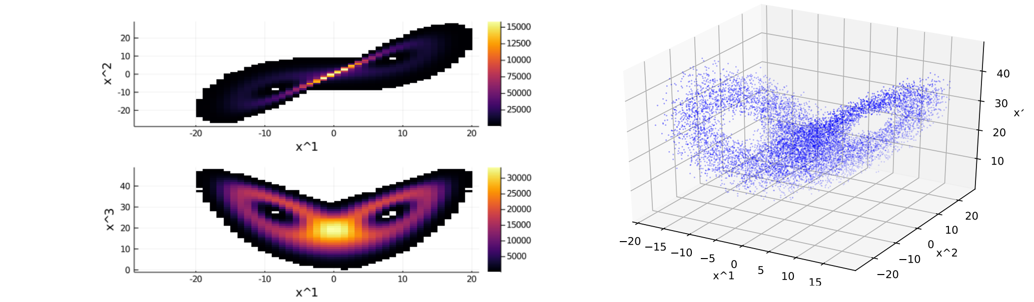
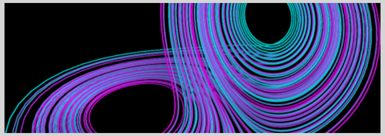
Recall: (a) data-binning, (b) scatter-plotting





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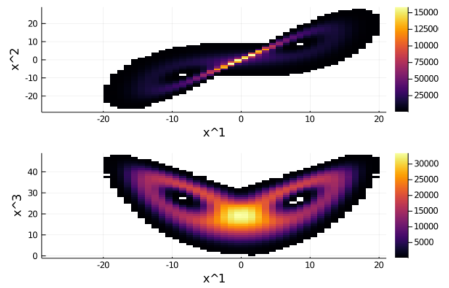

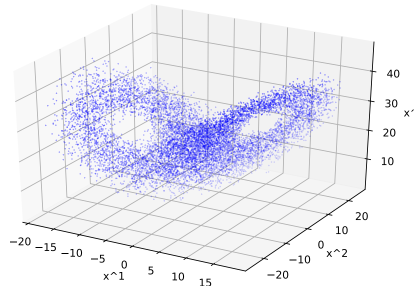

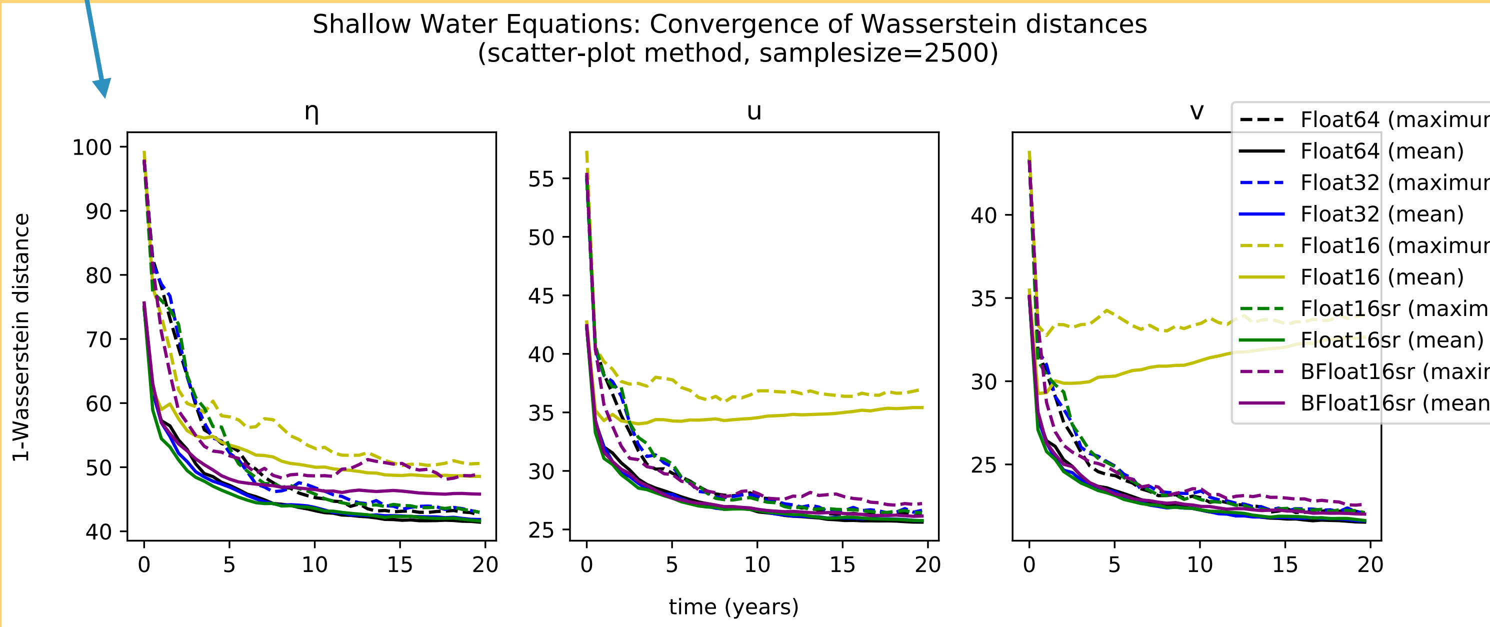

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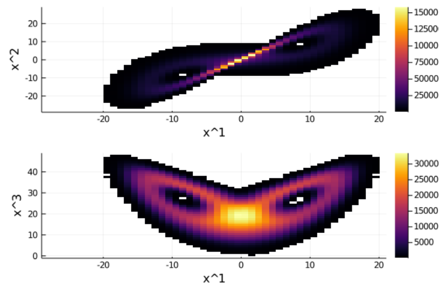

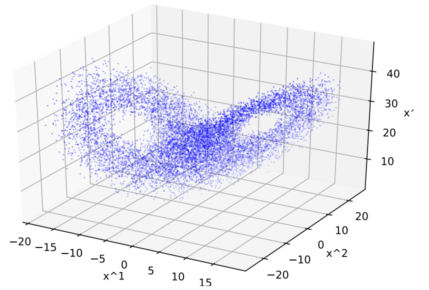

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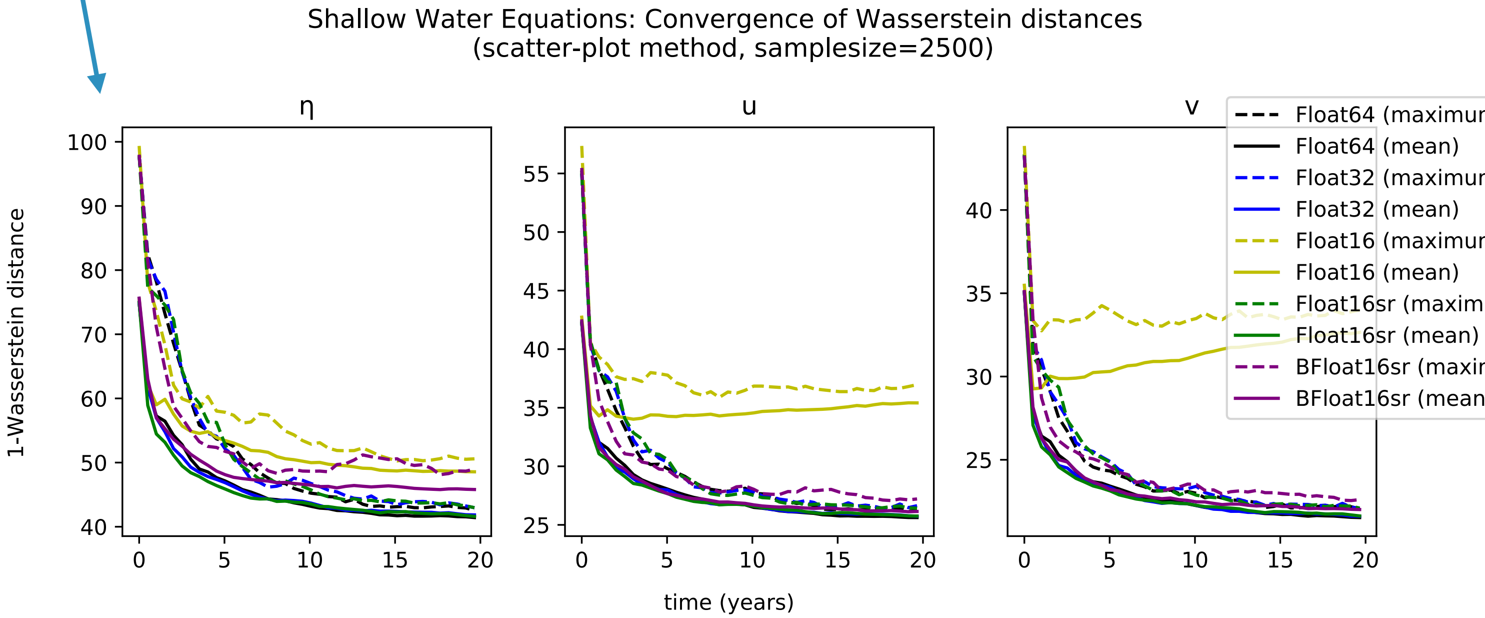
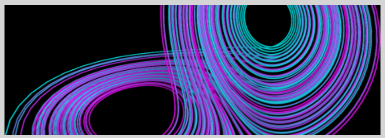


nb. This method is dimension agnostic (roughly the moral of Monte-Carlo methods)

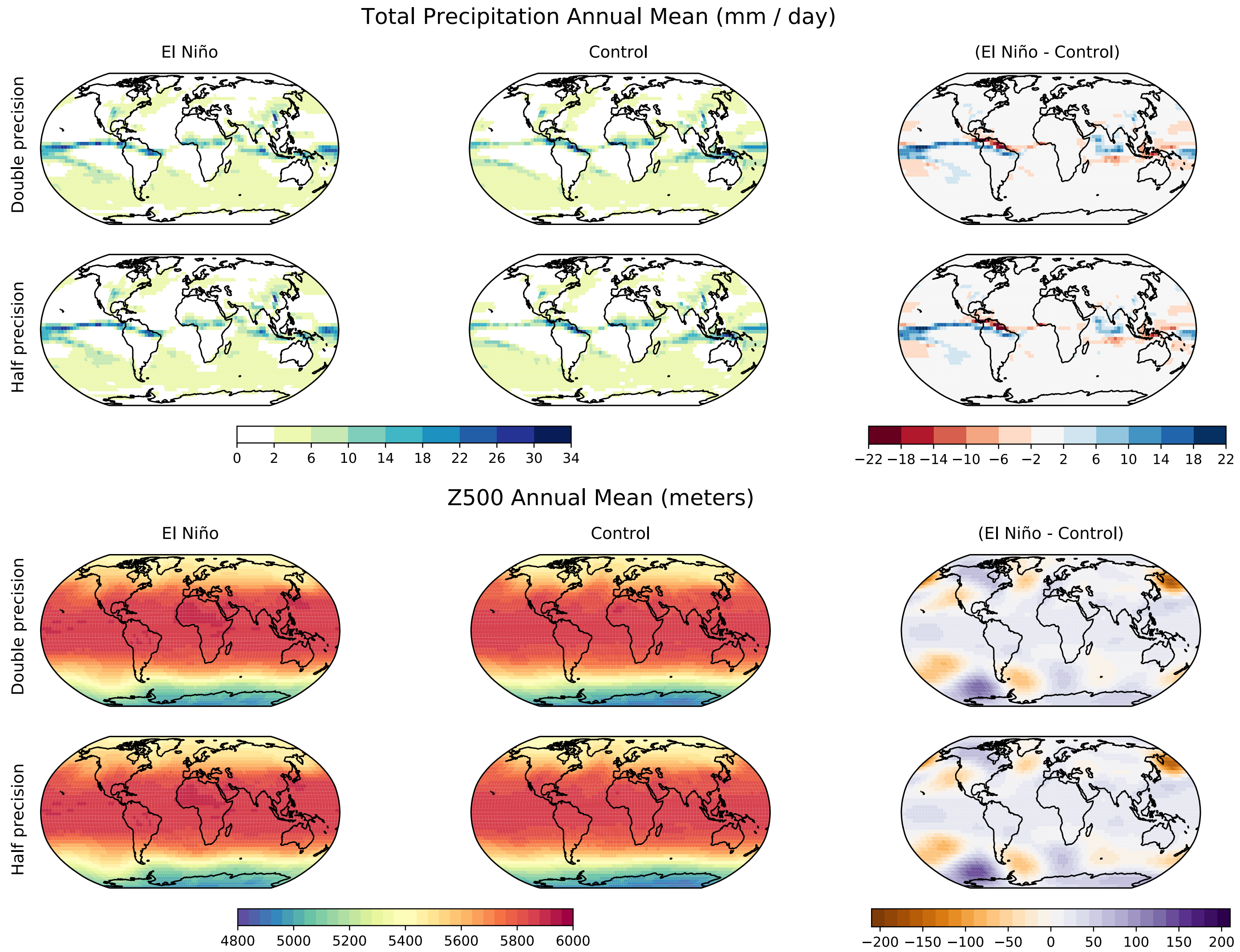
Conclusion of experiment.

The results provide strong evidence that the effects of rounding error on the shallow water model climatology, when compared with initial condition variability & discretisation error are:

1. *Negligible for **Float32** and **Float16sr**.*
2. *Significant for **Float16** and **BFloat16sr**.*

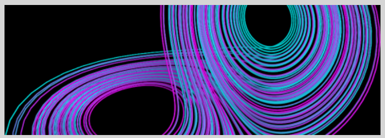


- Next steps: performing the same analysis to reduced precision SPEEDY.
- A coarse resolution ($3.75° \times 3.75°$) atmosphere only, primitive equation model (prescribed SSTs) with simplified parameterisations.
- Leo's 16-bit (deterministic) version of the code has held up to the first tests.



Summary of talk:

- The Wasserstein metric gives a notion of distance between probability distributions.
- It has excellent properties.
- It's computation presents challenges.
- Nonetheless it is a powerful tool for exploring high-dimensional probability distributions.
- Using the WD, the ensemble method, and ideas from sampling theory we have designed an experiment to test effects of rounding error on model climatology.
- Half-precision with stochastic-rounding is a suitable arithmetic for climate modelling with both of the L63 and Shallow Water models investigated so far.



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Thank-you!!! :)

... Any questions/thoughts/suggestions?