Fast Computation with Linearized Neural Networks for Domain Adaptation

Andreas Damianou - **Alexa Shopping Science**

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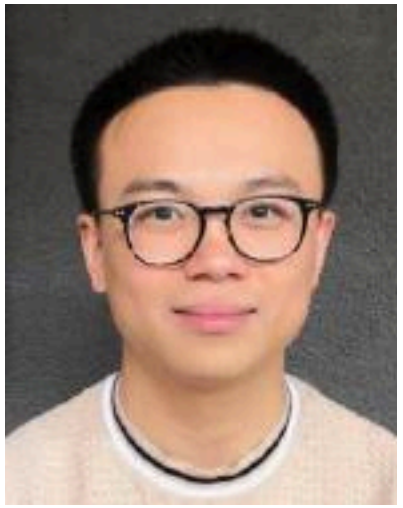
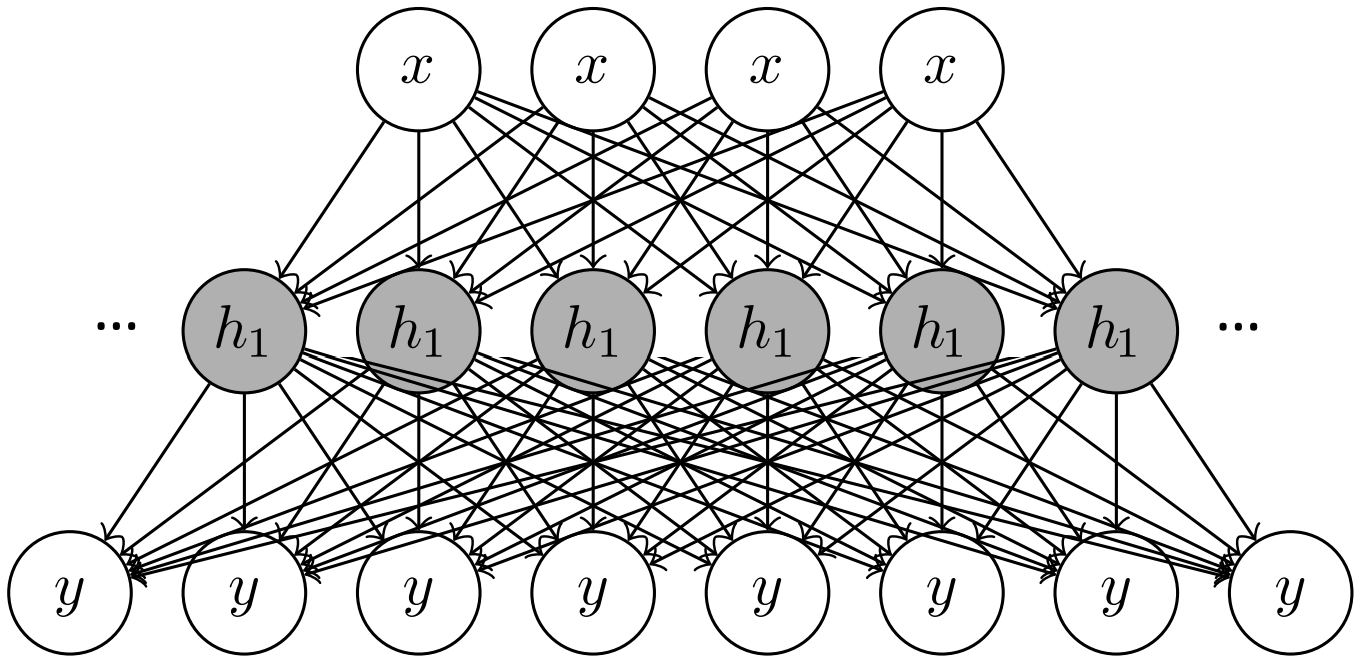


W. Maddox, S. Tang, P. G. Moreno, A. G. Wilson, A. Damianou:
Fast Adaptation with Linearized Neural Networks. 2019

Infinite width NN → GP

Also assuming Gaussian *i.i.d* noise for weights and biases



GP

Neal 1994; Williams 1997

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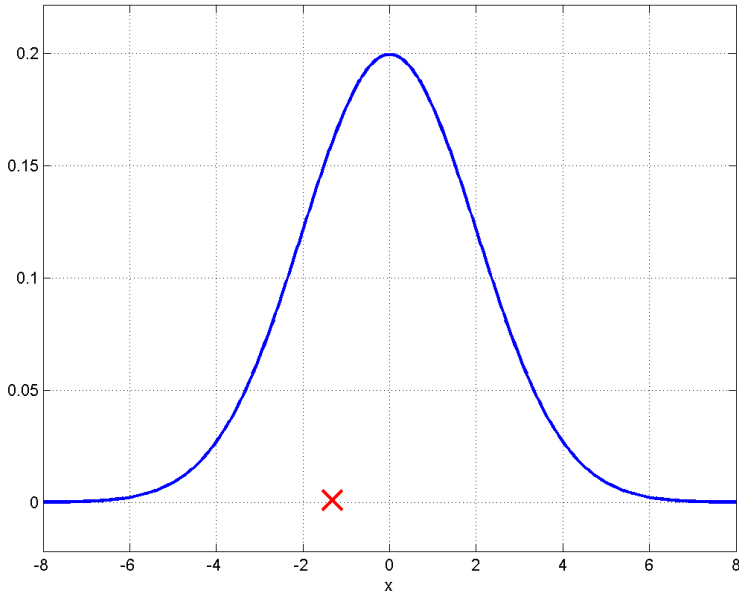
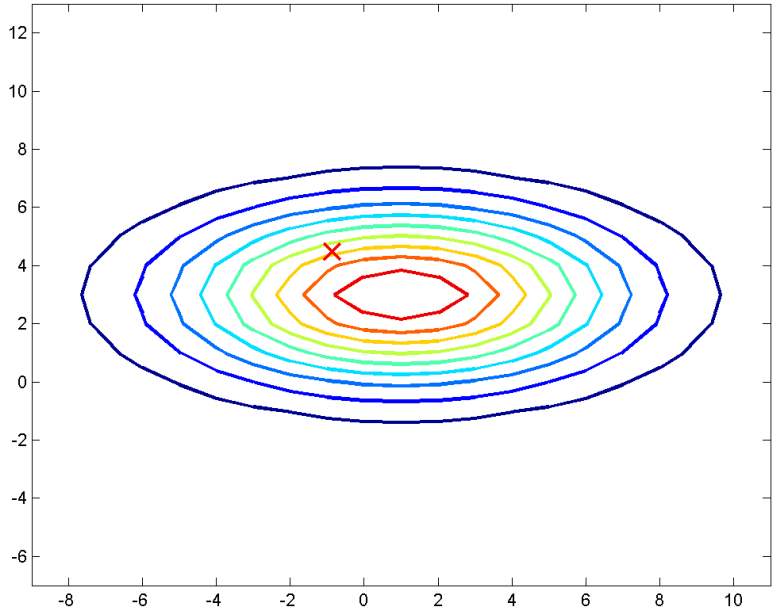
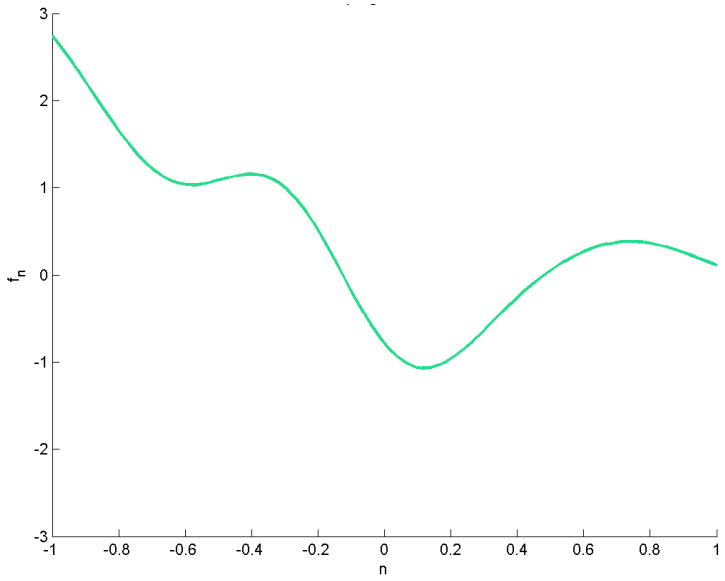
GP: Infinite dimensional Gaussian distribution



1-dim



2-dim



∞-dim

A GP is a distribution over functions.

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Gaussian process

- A Gaussian **distribution** depends on a covariance **matrix**.
- A Gaussian **process** depends on a covariance **function**.

$$p(f_1, f_2, \cdots, f_n) \sim \mathcal{N}(0, \mathbf{K})$$

$$p(f_1, f_2, \cdots, f_n, \cdots, f_\infty) \sim \mathcal{GP}(0, \underbrace{k(x, x')})$$

covariance function

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Neural networks:

- Require a large number of data and, even then, are fooled by out-of-distribution examples
- Do not have good uncertainty calibration $p(y|f(\hat{w}_D))$ vs $\int_f p(y|f)p(f|D)$
- Are not easy to compose together (black-boxes) $f([w_1, w_2])$ vs $f_1 \circ f_2$

But they are easy to learn and work well in practice!

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Defining the model != learning the model

ML in a nutshell:

STEP 1: Define the model
STEP 2: Learn the model

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ML in a nutshell:

STEP 1: Define the model
STEP 2: **Learn** the model

"Did we throw the baby out with the bathwater? (MacKay 2002)"

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Our Motivation

- Use neural networks in the situations where they work well.
- Encode them in function space through a GP with Neural Tangent Kernel (NTK).
- Manipulate the resulting function e.g. for domain adaptation.

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*We encode inductive biases from the **trained** DNN (leveraging learnability), **not** from the DNN architecture (which would defeat the purpose).*

W. Maddox, S. Tang, P. Moreno, A. Wilson, A. Damianou: *Fast Adaptation with Linearized Neural Networks*. 2019

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Adaptation in parameter vs function space

If $f_1(w_1)$ solves task 1 and $f_2(w_2)$ (unknown) solves task 2:

- Fine-tuning: Take an arbitrary subset of (the vast) w_1, move it for an arbitrary number of steps towards (hopefully) w_2.
- Our method: Take the whole f_1 and move it towards f_2 in the function space - closed-form (for regression) with accompanying uncertainty.

A GP encodes smoothness assumptions: task 1 close to task $2 \Rightarrow f_1$ close to f_2.

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GP with NN inductive biases

- Fit DNN's parameters $\mathbf{w}$ on data $\mathbf{x}$.
- Consider a GP f with kernel: $k(x, x') = J(x; \mathbf{w})^\top J(x'; \mathbf{w})$.
- Adaptation: $p(f_*|x_*, \mathbf{x}, \mathbf{f}) = \mathcal{N}(\boldsymbol{\mu}_*, k_{**} - \mathbf{k}_{*\mathbf{x}}\mathbf{K}_{\mathbf{xx}}^{-1}\mathbf{k}_{\mathbf{x}*})$

  where e.g. $\mathbf{k}_{*\mathbf{x}} = k(x_*, \mathbf{x}) = J(x_*; \mathbf{w})^T J(\mathbf{x}; \mathbf{w})$.
- Equivalent to Bayesian generalized linear model with Jacobians as features.

Efficient computations

$$\boldsymbol{\mu}_* = \mathbf{k}_{*\mathbf{x}}\mathbf{K}_{\mathbf{xx}}^{-1}\mathbf{f}$$
$$k_* = k_{**} - \mathbf{k}_{*\mathbf{x}}\mathbf{K}_{\mathbf{xx}}^{-1}\mathbf{k}_{\mathbf{x}*}$$

- Observation 1: Difficult parts can be cached.
- Observation 2: We can turn inversion into optimization:

$g(\mathbf{a}) = \frac{1}{2}\mathbf{a}^\top\mathbf{K}\mathbf{a} - \mathbf{a}^\top\mathbf{f}$ has maximum at $\hat{\mathbf{a}} = \mathbf{K}^{-1}\mathbf{f}$

- For t iterations the covariance expressed in terms of matrices with t columns.
- Allows to access $\mathbf{K}^{-1}\mathbf{f}$ lazily using fast MVP.

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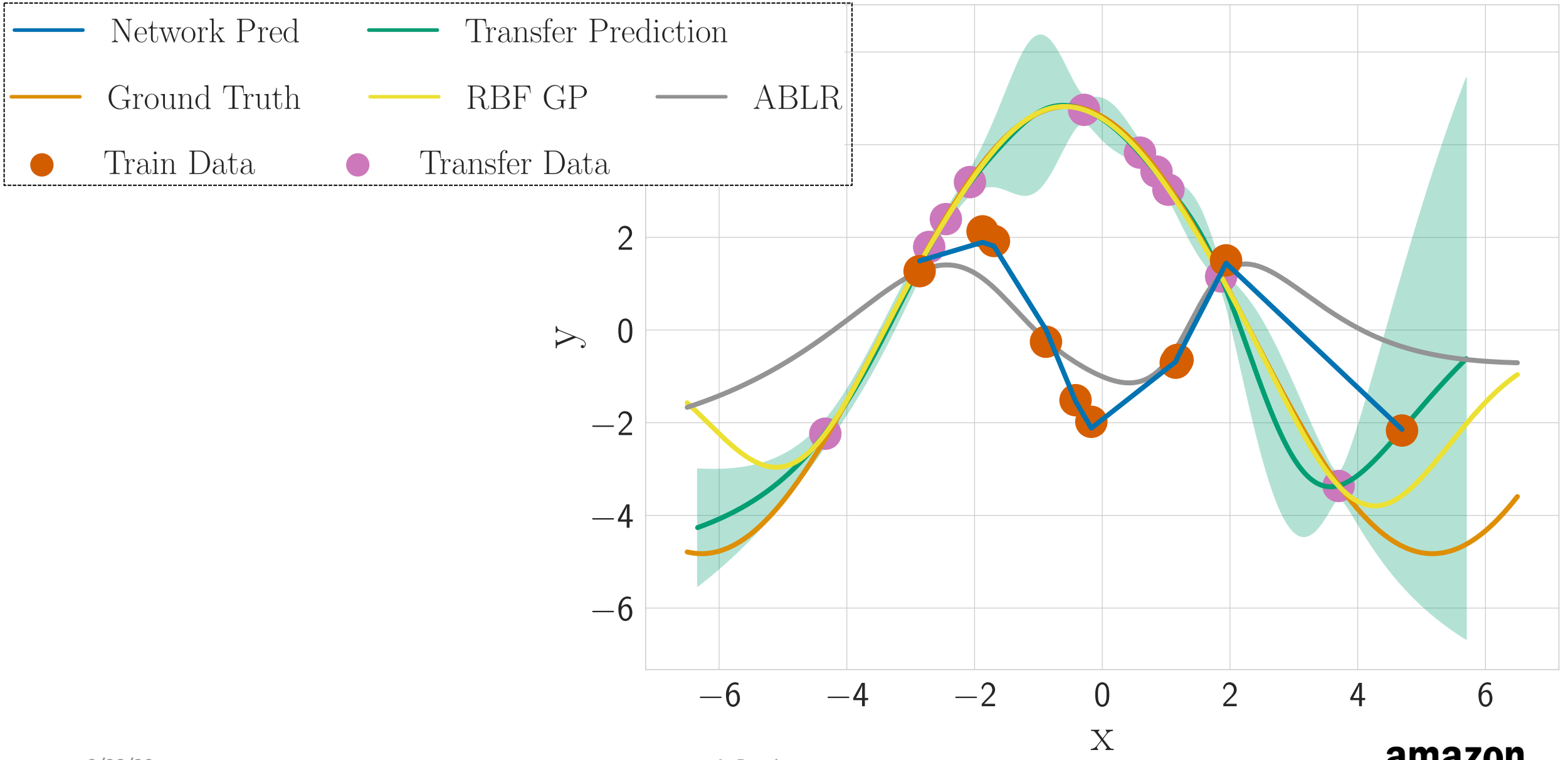
Transfer learning (toy regression data)



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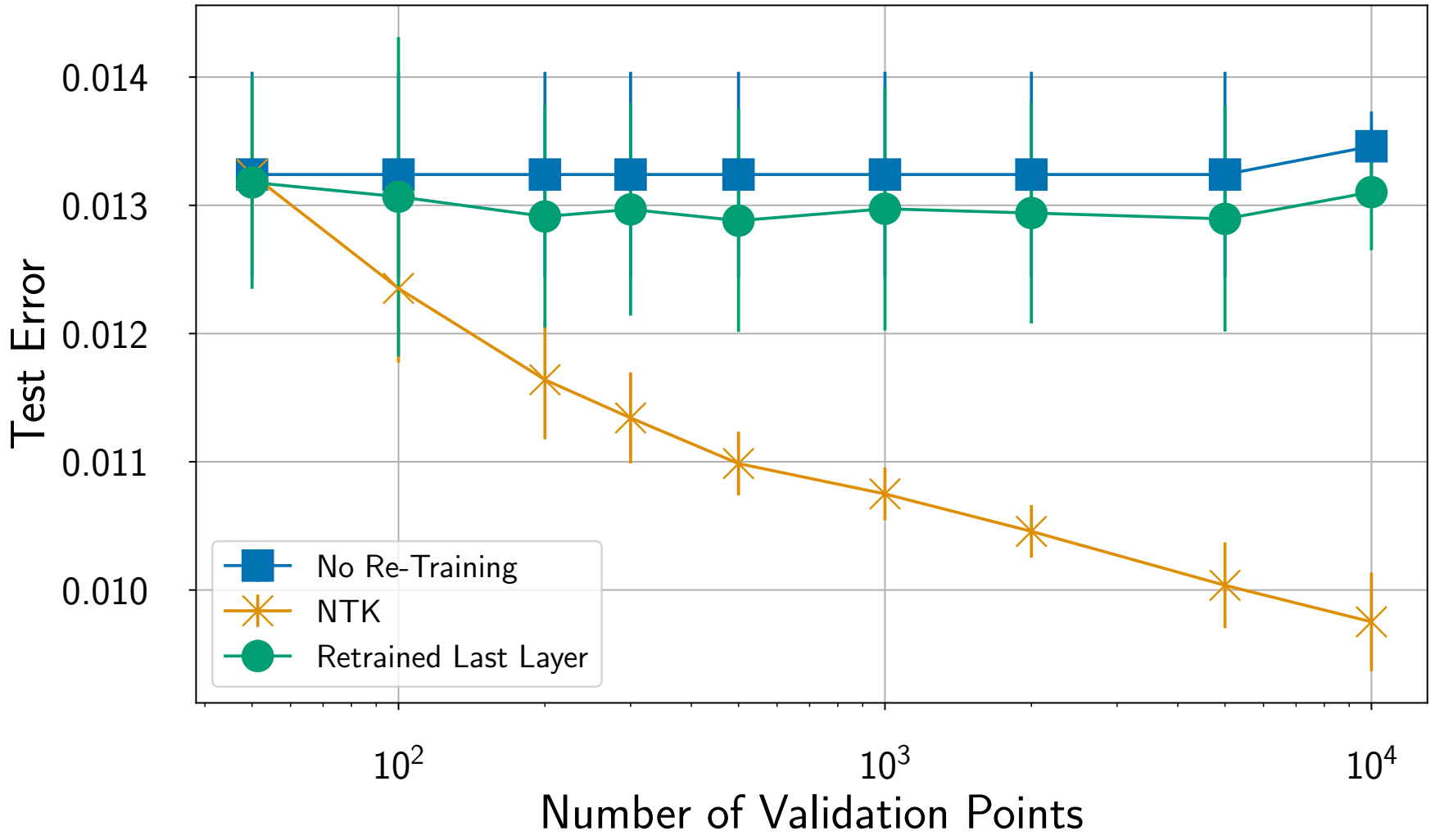
Malaria spread data



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What I don’t have time to show

- Theory from DNN training dynamics across GD justifies the approach.
- Justifying the assumption about Jacobian similarity across tasks.
- Framework for working in the parameter space (Bayesian GLM) or the function space (GP).
- Fast computations through MVP.

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Thanks!

Questions?

Appendix

DNN training dynamics in GD

$$\frac{\mathrm{d}f(x)}{\mathrm{d}t} = -\eta \mathbf{J}_{\mathbf{w}}(x)^{\top} \mathbf{J}_{\mathbf{w}}(x) \nabla_f \log p(y|f,x)$$

Neural Tangent Kernel (NTK)

- The NTK governs the dynamics of f throughout the GD training of $\mathbf{w}$.
- Taylor expand: $f(x, \mathbf{w}) \approx f(x, \mathbf{w}_0) + J_{\mathbf{w}}(x, \mathbf{w}_0)^T (\mathbf{w} - \mathbf{w}_0)$
- Linear in $\mathbf{w}$, non-linear in inputs (because of J)
- Linear model using feature map (kernel) $J_{\mathbf{w}}(x, \mathbf{w}_0)^{\top} J_{\mathbf{w}}(x, \mathbf{w}_0)$

Lee et al. *arXiv:1902.06720*

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DNN training dynamics in GD

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DNN -> GP through NTK

- For linearized networks around w0, the network output becomes a linear model with NTK.
- For non-linearized networks and small learning rate, same behavior arises with GD.

DNN -> GP through NTK

- For linearized networks around *w0*, the network output becomes a linear model with NTK.
- For non-linearized networks and small learning rate, same behavior arises with GD.
- We leverage this to linearize the network at convergence, *w_final*, and use it within a GP with the NTK.
- This also allows us to do DNN transfer learning analytically with GPs: we transfer neural network parameters (= kernel parameters) across tasks.

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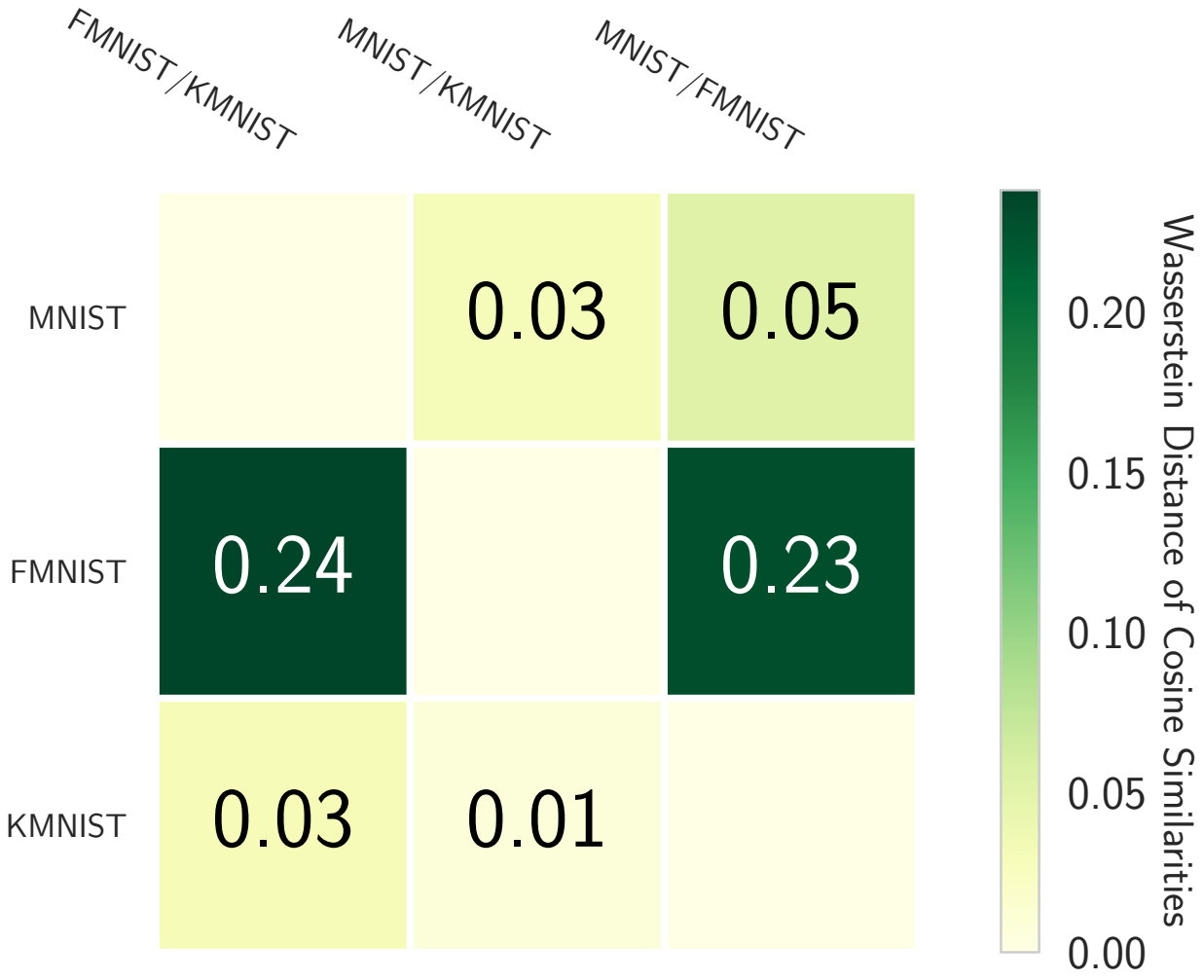
Similar tasks have similar Jacobians



See also Fisher Matrix similarity assumptions by Lian et al. '17, Achille et al. '19

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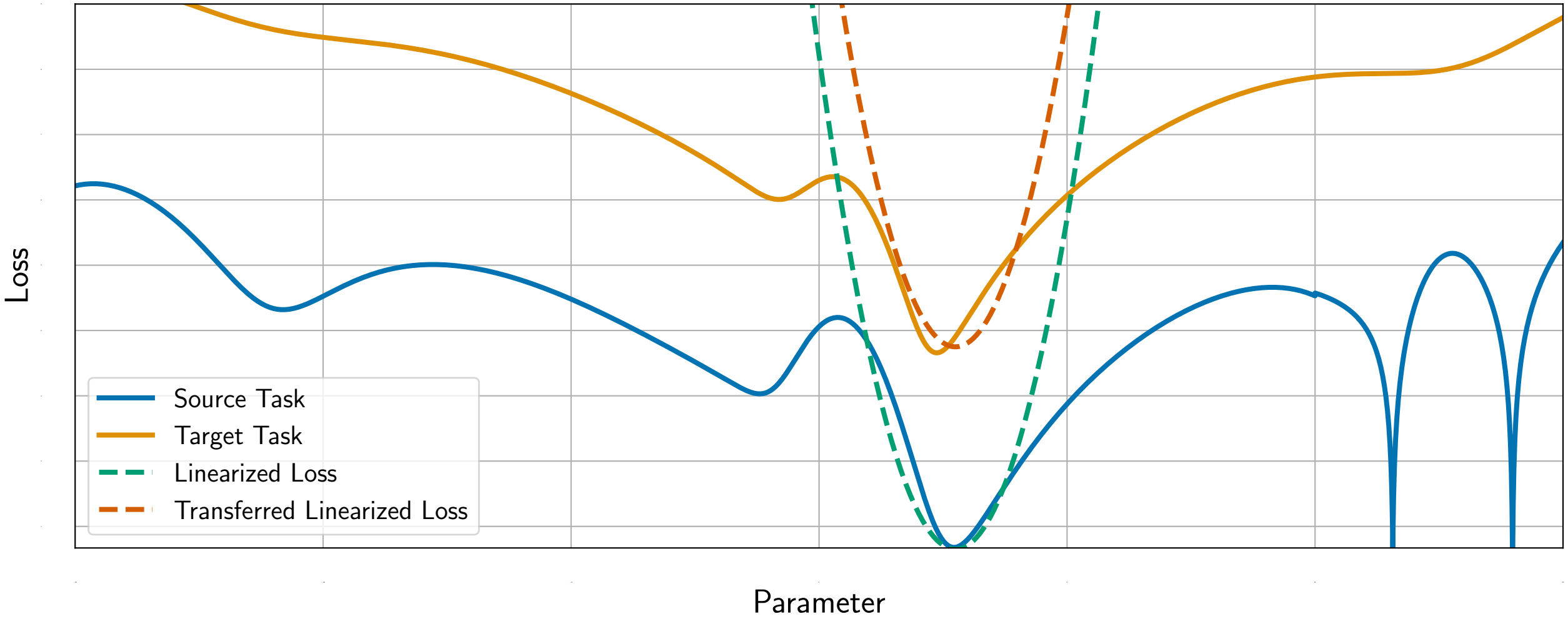
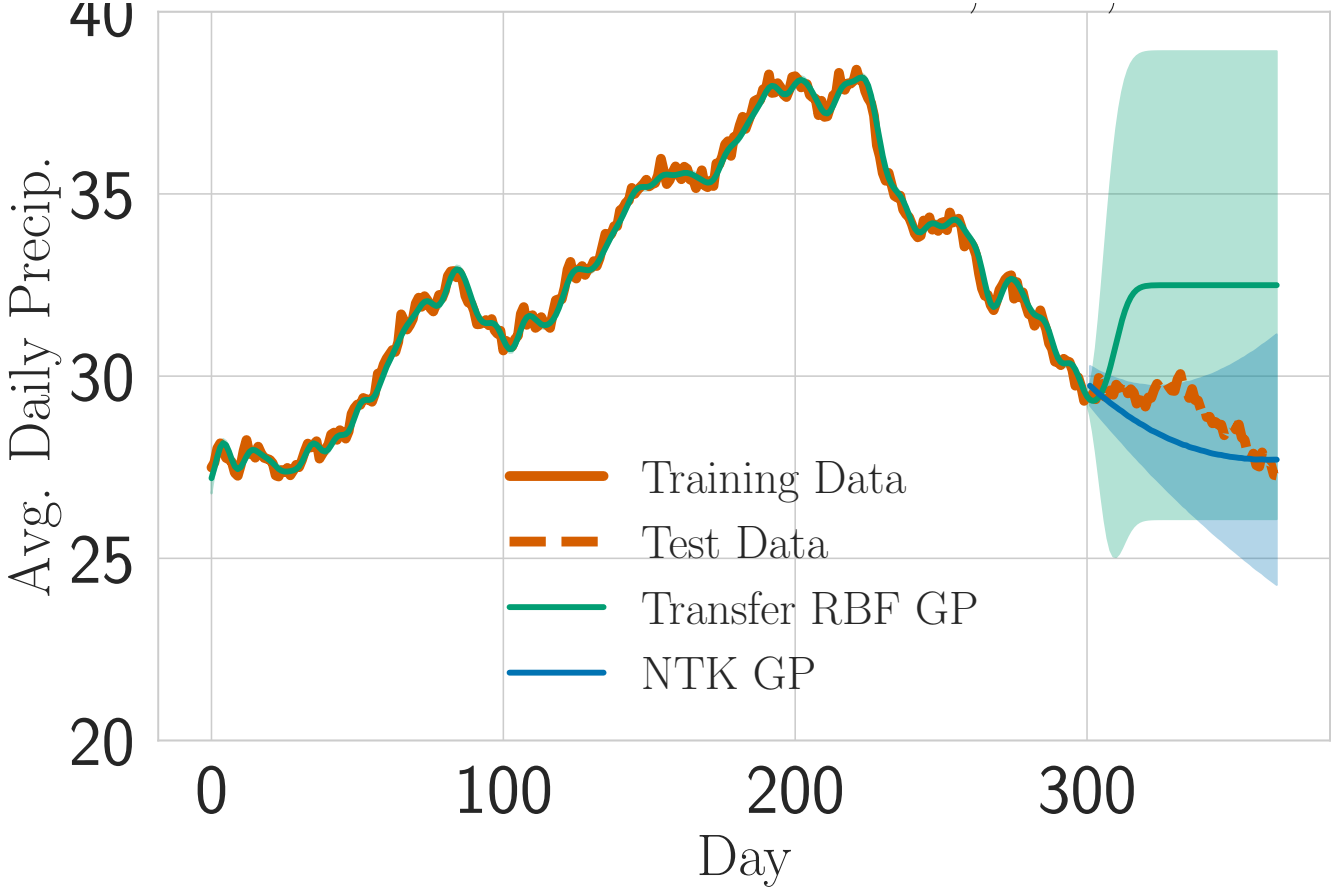
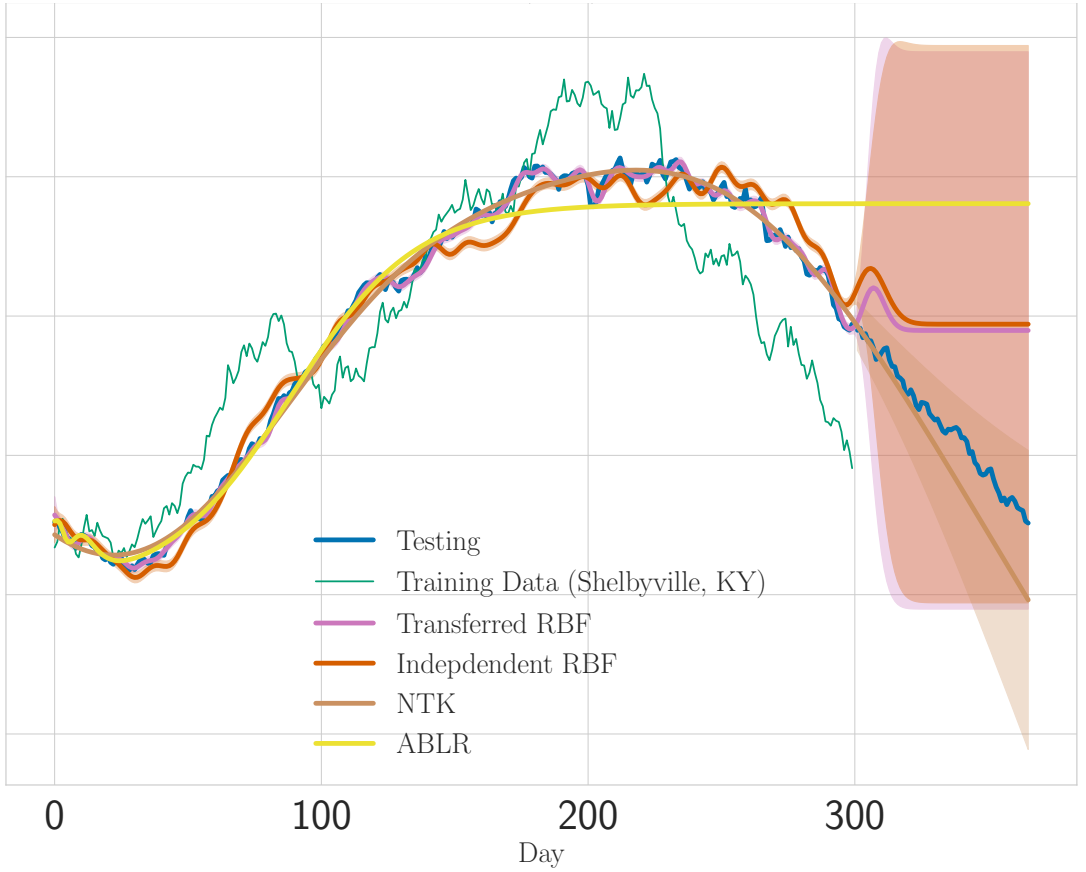

Loss
Parameter
Source Task
Target Task
Linearized Loss
Transferred Linearized Loss

Transfer learning for precipitation data

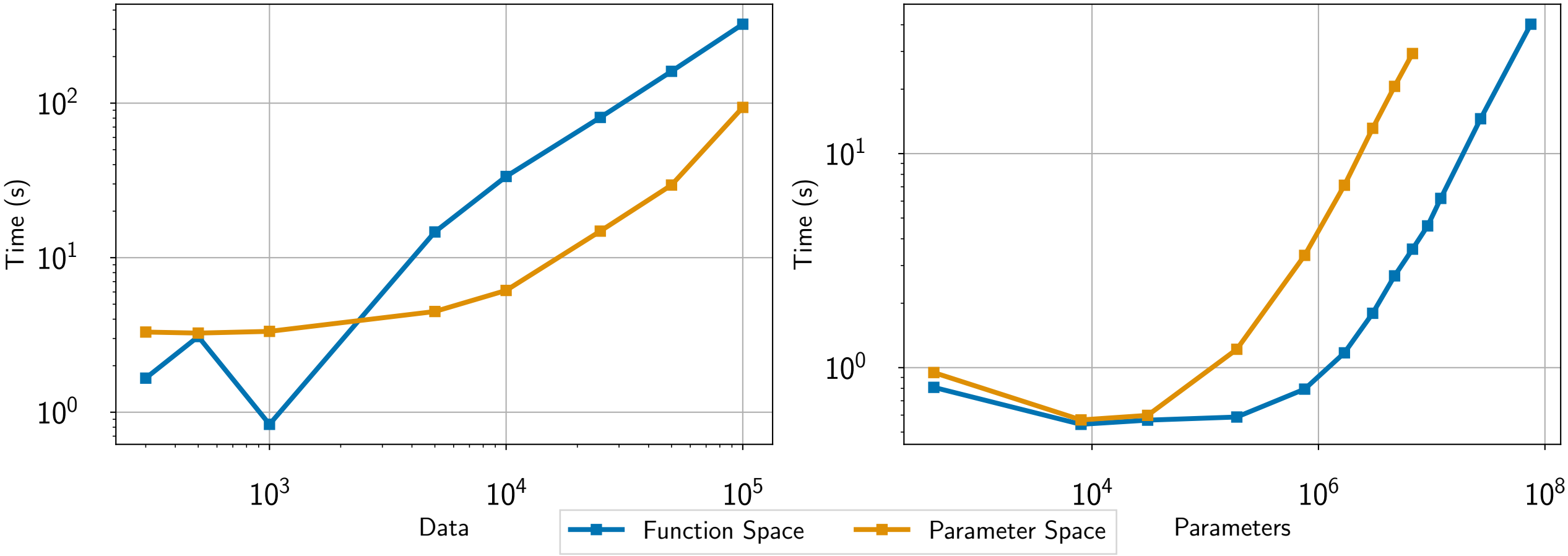
Source task



Target task



Scaling


Time (s)
10^2
10^1
10^0
10^3
10^4
10^5
Data
Function Space
Parameter Space
Time (s)
10^1
10^0
10^4
10^6
10^8
Parameters