BSc Informatics & Telecommunications

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MSc Informatics & AI

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PhD Machine Learning

- BSc Informatics & Telecommunications
- MSc Informatics & AI
- PhD Machine Learning
- **Researcher ML & Robotics**

- BSc Informatics & Telecommunications
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- **Start-up**

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ATI Fellowship

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- PhD Machine Learning
- Researcher ML & Robotics
- Start-up

  ATI Fellowship
- **Amazon**

What this talk is about

- Deep Bayesian learning over functions.

• Adding prior knowledge/assumptions	$p(f) \quad \text{vs} \quad p(w)$
• Generalization/generation by averaging hypotheses	$\int_f p(y\|f)p(f) \quad \text{vs} \quad p(y\|f(\hat{w}))$
• Unsupervised learning for generation	$p(\text{generated\_speech} \mid \text{latent\_style})$
• Intuitive composition of signals	$f_1 \circ f_2 \quad \text{vs} \quad f([w_1, w_2])$

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• Intuitive composition of signals	$f_1 \circ f_2 \quad \text{vs} \quad f([w_1, w_2])$

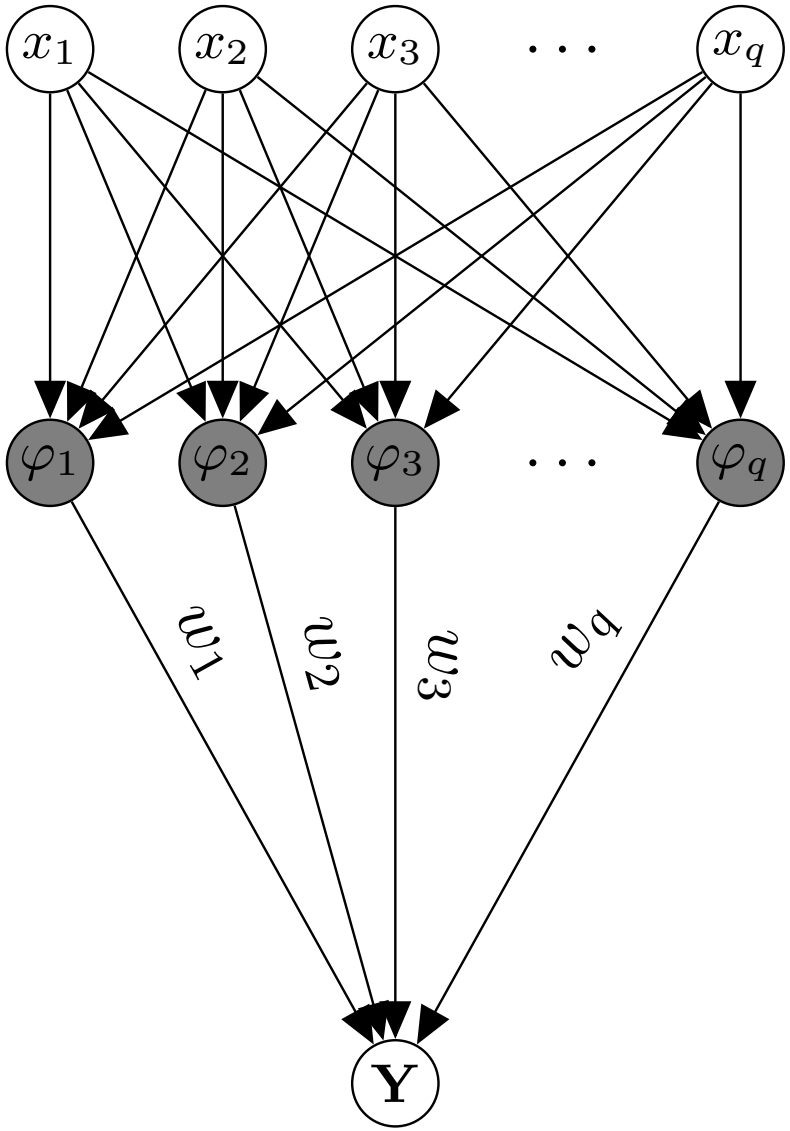
- Particularly important for:
  - Generative modeling
  - Domain adaptation

What this talk is ***not*** about

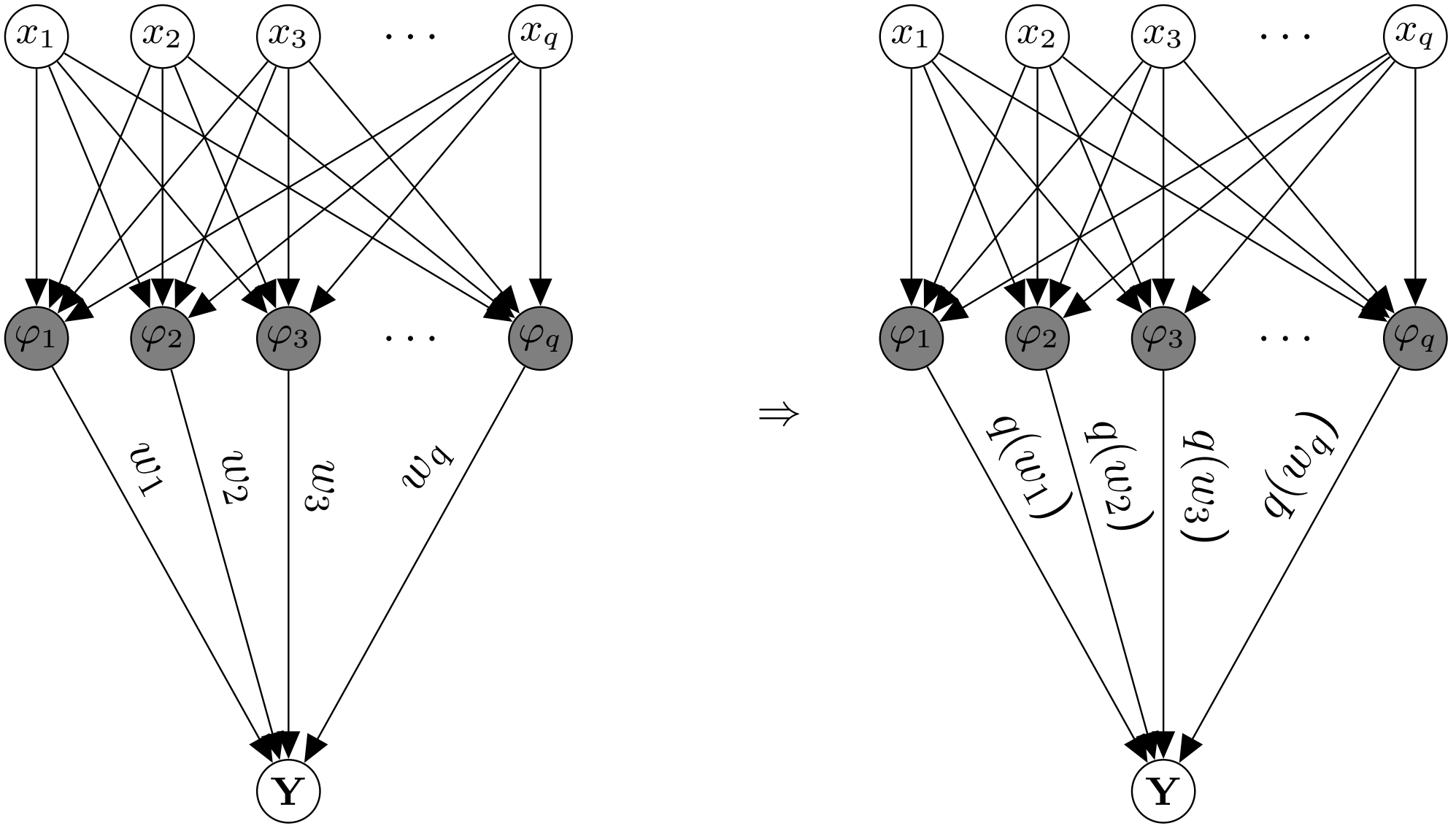
Reverend T. Bayes

- We don't dogmatically motivate Bayesian methods.
- In fact, Bayesian methods lack the practical *learnability* of DNNs.
- *Hence, we wish to combine function space modeling with the learnability of DNNs.*

A standard neural network



BNN with priors on its weights



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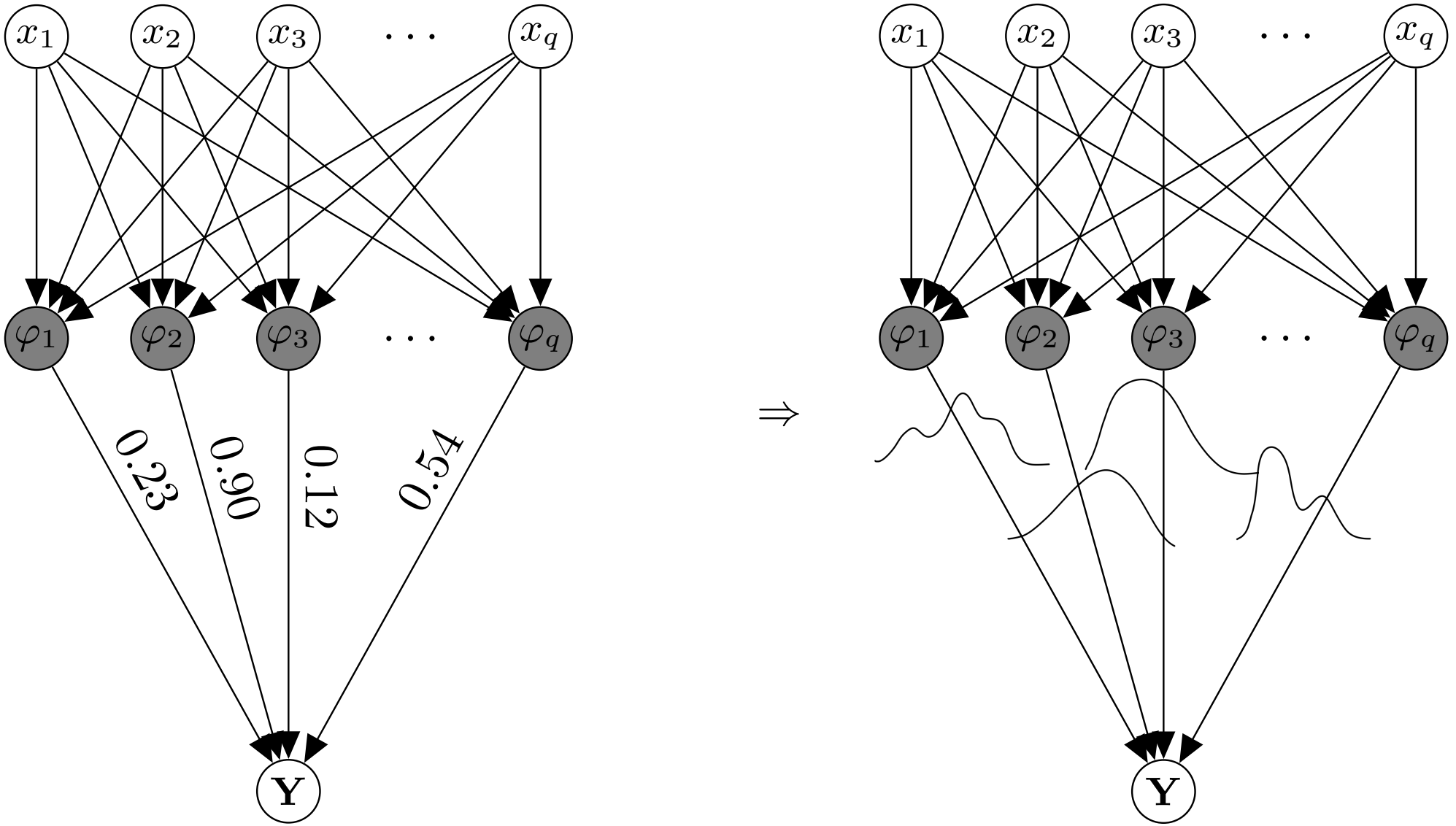

Learning in function space

Given training data $\mathbf{D}$, predict test outputs $\mathbf{y}_*$ from test inputs $\mathbf{x}_*$:

$$\textit{parametric}: \quad p(\mathbf{y}_*|\mathbf{x}_*, \hat{\mathbf{w}}_\mathbf{D}) \quad = \phi(\mathbf{x}_*; \hat{\mathbf{w}}_\mathbf{D})$$

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$$\textit{Bayesian parametric}: \quad p(\mathbf{y}_*|\mathbf{x}_*) = \int_\mathbf{w} p(\mathbf{y}_*|\phi(\mathbf{x}_*; \mathbf{w}))p(\mathbf{w}|\mathbf{D})$$

Learning in function space

Given training data $\mathbf{D}$, predict test outputs $\mathbf{y}_*$ from test inputs $\mathbf{x}_*$:

$$\begin{aligned}
\textit{parametric}: \quad & p(\mathbf{y}_*|\mathbf{x}_*, \hat{\mathbf{w}}_\mathbf{D}) && = \phi(\mathbf{x}_*; \hat{\mathbf{w}}_\mathbf{D}) \\
\textit{Bayesian parametric}: \quad & p(\mathbf{y}_*|\mathbf{x}_*) && = \int_\mathbf{w} p(\mathbf{y}_*|\phi(\mathbf{x}_*; \mathbf{w}))p(\mathbf{w}|\mathbf{D}) \\
\textit{Gaussian process} : \quad & p(\mathbf{y}_*|\mathbf{x}_*) && = \int_{\mathbf{f}_*} \; p(\mathbf{y}_*|f_*(\mathbf{x})) \quad p(f_*|\mathbf{D})
\end{aligned}$$

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\end{aligned}$$

Infinite model... but we *always* work with finite sets!

Multivariate Gaussian for all $f_i = f(\mathbf{x}_i)$:

$$p(\underbrace{f_1, f_2, \cdots, f_n}_{\mathbf{f}_n}, \underbrace{f_{n+1}, f_{n+2}, \cdots, f_s}_{\mathbf{f}_s}) = p(\mathbf{f}_n, \mathbf{f}_s) \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{K}).$$

with:

$$\boldsymbol{\mu} = \begin{bmatrix} \boldsymbol{\mu}_n \\ \boldsymbol{\mu}_s \end{bmatrix} \text{ and } \mathbf{K} = \begin{bmatrix} \mathbf{K}_{nn} & \mathbf{K}_{ns} \\ \mathbf{K}_{sn} & \mathbf{K}_{ss} \end{bmatrix}$$

Marginalisation:

$$p(\mathbf{f}_n) = \int_{\mathbf{f}_s} p(\mathbf{f}_n, \mathbf{f}_s) \mathrm{d}\mathbf{f}_s = \mathcal{N}(\boldsymbol{\mu}_n, \mathbf{K}_{nn})$$

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Multivariate Gaussian for all $f_i = f(\mathbf{x}_i)$:

$$p(\underbrace{f_1, f_2, \cdots, f_n}_{\mathbf{f}_n}, \underbrace{f_{n+1}, f_{n+2}, \cdots, f_\infty}_{\mathbf{f}_\infty}) = p(\mathbf{f}_n, \mathbf{f}_\infty) \sim \mathcal{GP}(\boldsymbol{\mu}_\infty, \mathbf{K}_\infty).$$

with:

$$\boldsymbol{\mu}_\infty = \begin{bmatrix} \boldsymbol{\mu}_n \\ \cdots \end{bmatrix} \quad \text{and} \quad \mathbf{K}_\infty = \begin{bmatrix} \mathbf{K}_{nn} & \cdots \\ \cdots & \cdots \end{bmatrix}$$

Marginalisation:

$$p(\mathbf{f}_n) = \int_{\mathbf{f}_\infty} p(\mathbf{f}_n, \mathbf{f}_\infty) \mathrm{d}\mathbf{f}_\infty = \mathcal{N}(\boldsymbol{\mu}_n, \mathbf{K}_{nn})$$

Infinite model... but we *always* work with finite sets!

Multivariate Gaussian for all $f_i = f(\mathbf{x}_i)$:

$$\mathbf{K}_\infty = \begin{bmatrix} \mathbf{K}_{nn} & \cdots \\ \cdots & \cdots \end{bmatrix}$$

Infinite model... but we *always* work with finite sets!

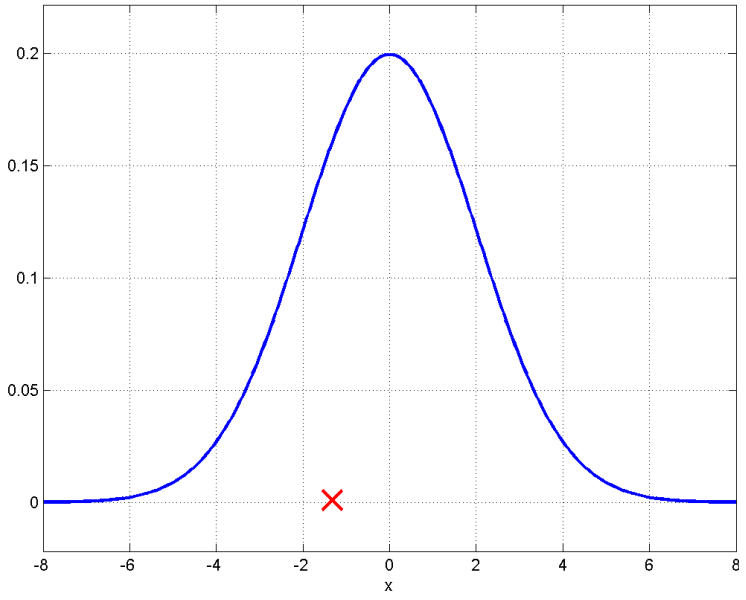
Multivariate Gaussian for all $f_i = f(\mathbf{x}_i)$:

$$\mathbf{K}_\infty = \begin{bmatrix} \mathbf{K}_{nn} & \cdots \\ \cdots & \cdots \end{bmatrix}$$

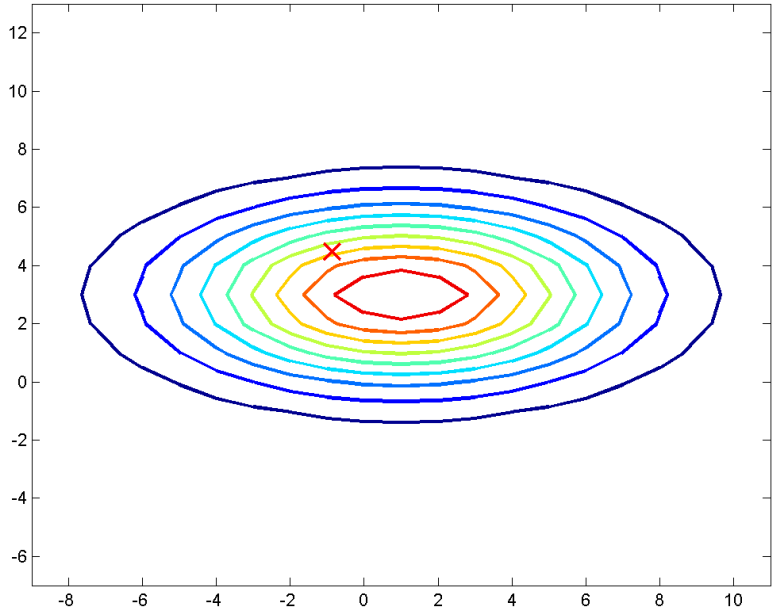
$$\mathbf{K}_{i,j} = k(\mathbf{x}_i, \mathbf{x}_j; \theta)$$

Train a GP means fitting θ

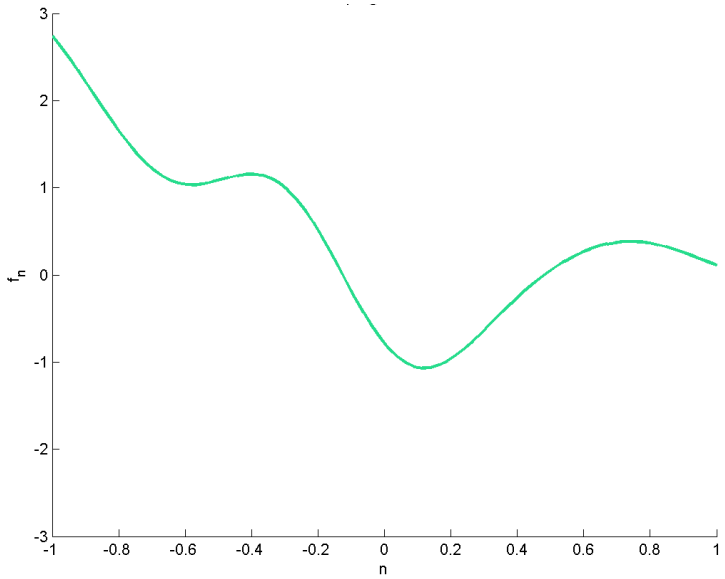
GP: Infinite dimensional Gaussian distribution



1-dim



2-dim



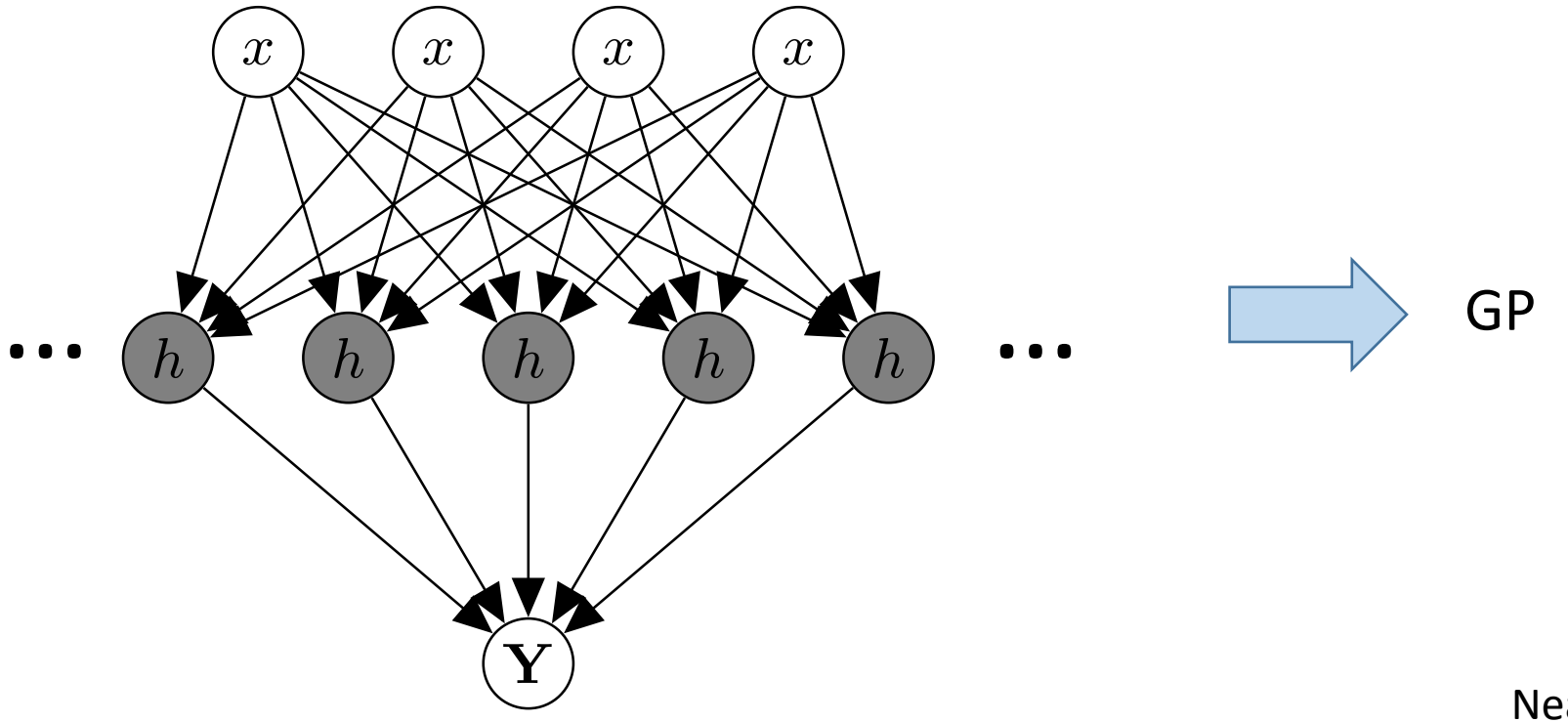
∞-dim

A GP is a distribution over functions.

GP as the limit of a Bayesian NN

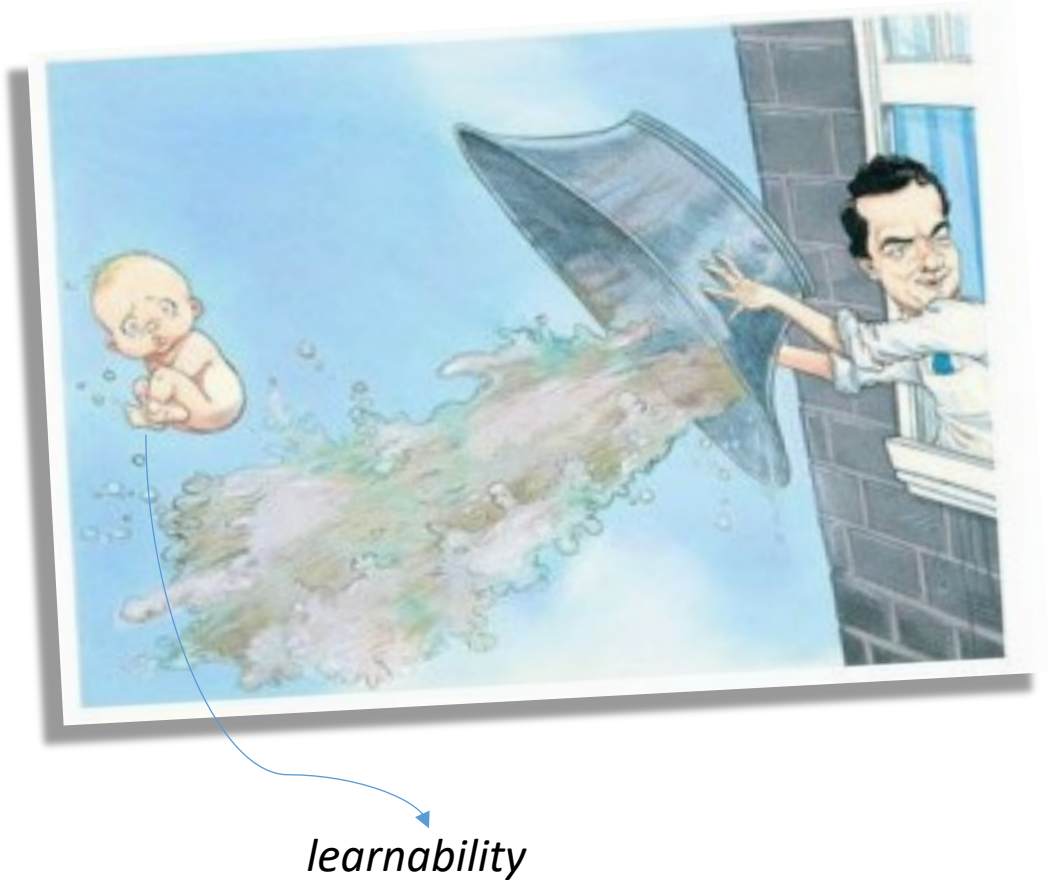
- Limit of infinite num. parameters:
  Optimization of finite num. parameters → Integration of infinite model

- *Closed form* solution for modelled function class!



Neal 1994; Williams 1997

Did we throw the baby out with the bathwater? (D. MacKay)



learnability

- In the presence of finite data the analytic solution might not be the best! Neural networks, instead, perform **hierarchical concept learning**.

For the rest of the talk…

Function space modeling
(benefits for tasks beyond supervised learning)

+

Hierarchical concept learning
(benefits for learnability)

Deep Gaussian process

Hierarchical feature learning *and* function space learning.

$$g(x) = f(f(f \cdots (x)))$$ where $$f \sim \mathcal{GP}$$

[Damianou, Lawrence. "Deep Gaussian processes", 2013]
[Damianou, "Deep Gaussian processes and variational propagation of uncertainty", PhD Thesis]
[Kumar, Singh, Srijith, Damianou, "Deep Gaussian processes with convolutional kernels", 2018]

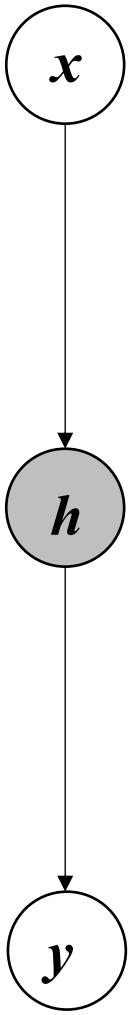
Deep Gaussian process

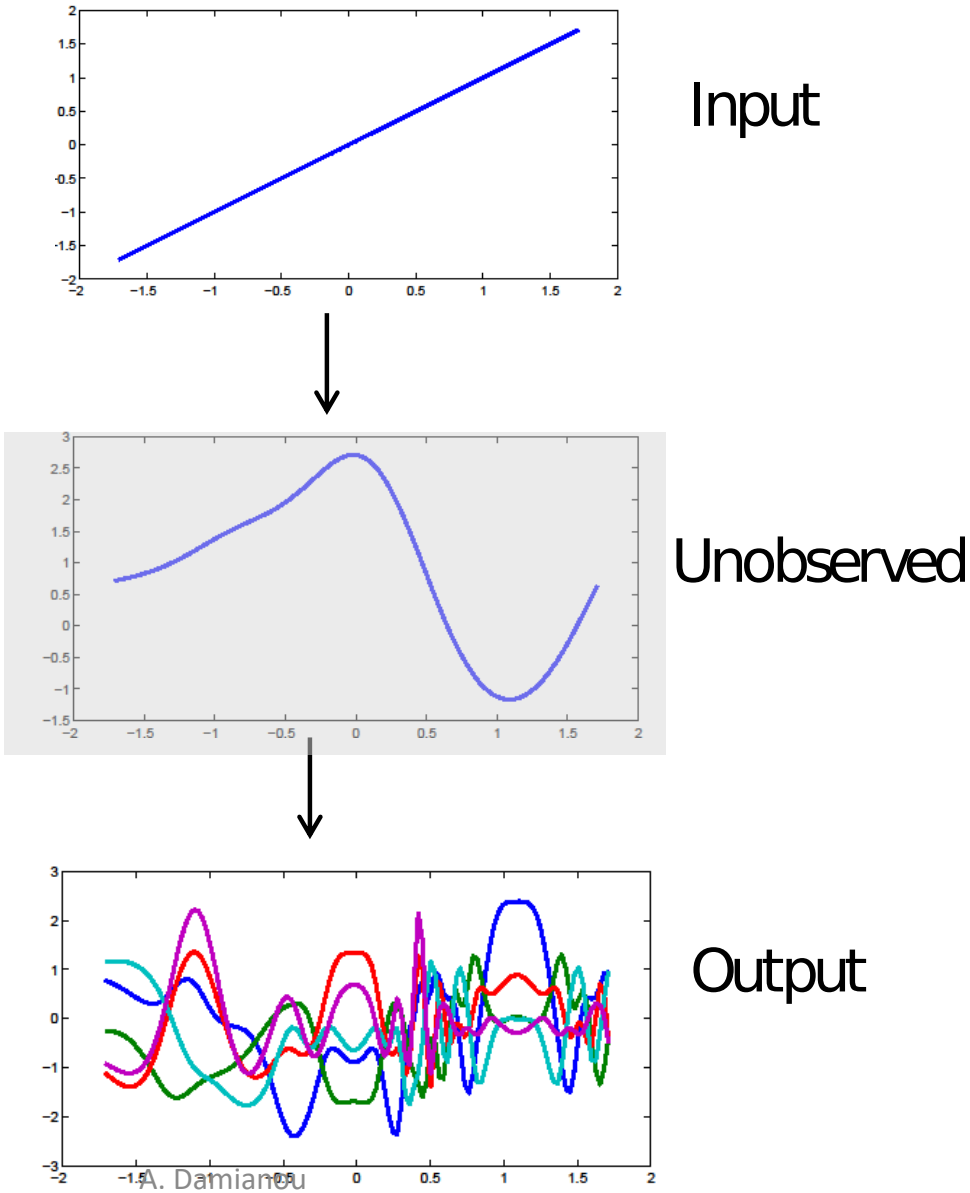
$$p(y|x) = \int_{f_3} p(y|f_3) \int_{f_2} p(f_3|f_2) \int_{f_1} p(f_2|f_1)p(f_1|x)$$

Damianou & Lawrence, 2013, Damianou, PhD Thesis 2015

Hierarchical function learning

[Damianou, PhD Thesis]

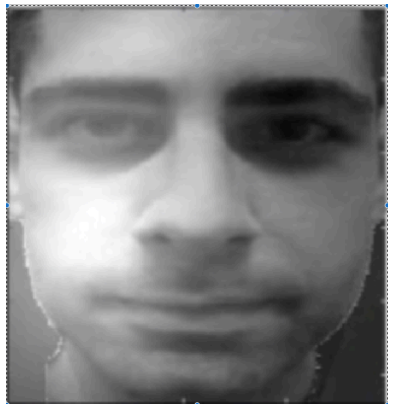




Function space ≈ the "*infinite data*" space

$\ldots \quad h \quad \ldots \quad h \quad \ldots \quad h \quad \ldots \quad h \quad \ldots$

$\ldots \quad f(h) \quad \ldots \quad f(h) \quad \ldots \quad f(h) \quad \ldots \quad f(h) \quad \ldots$

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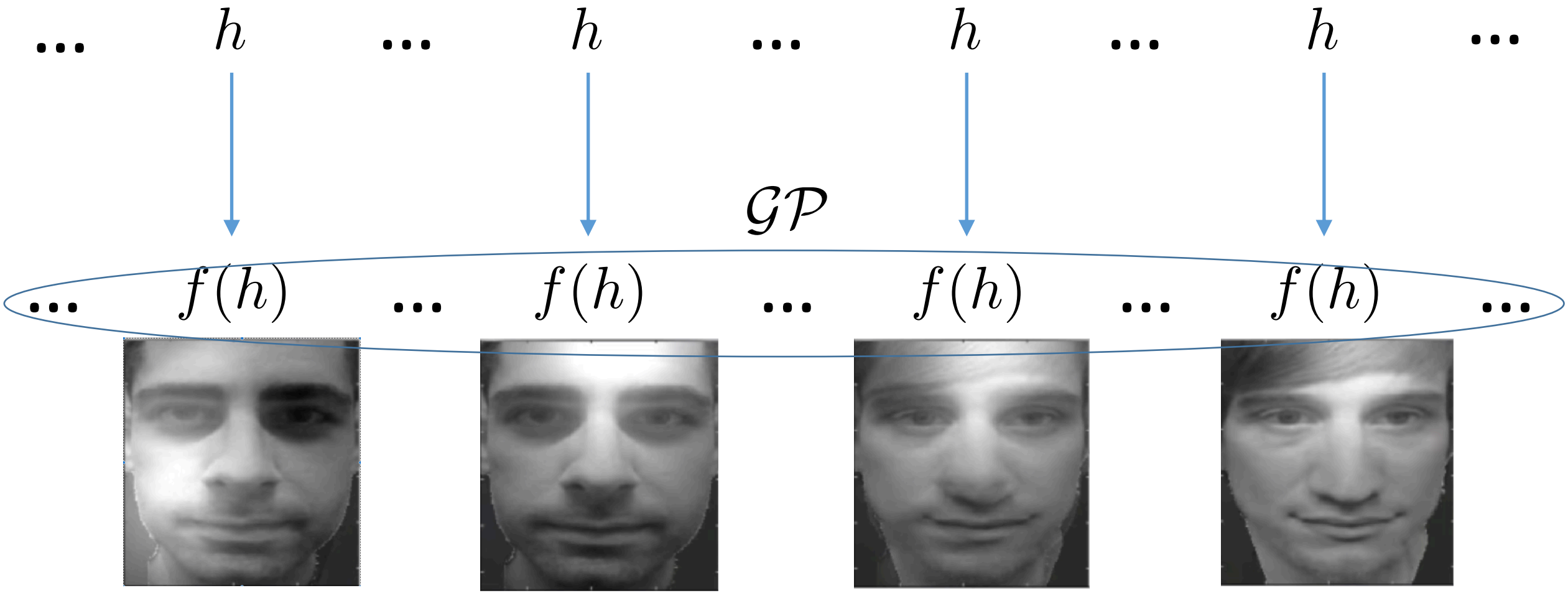

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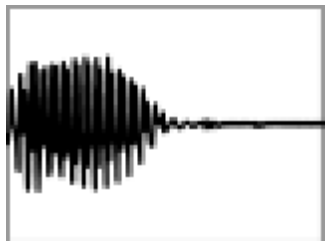
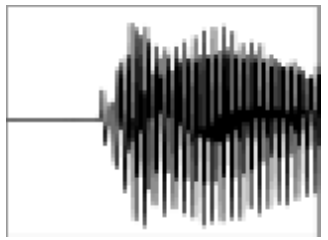

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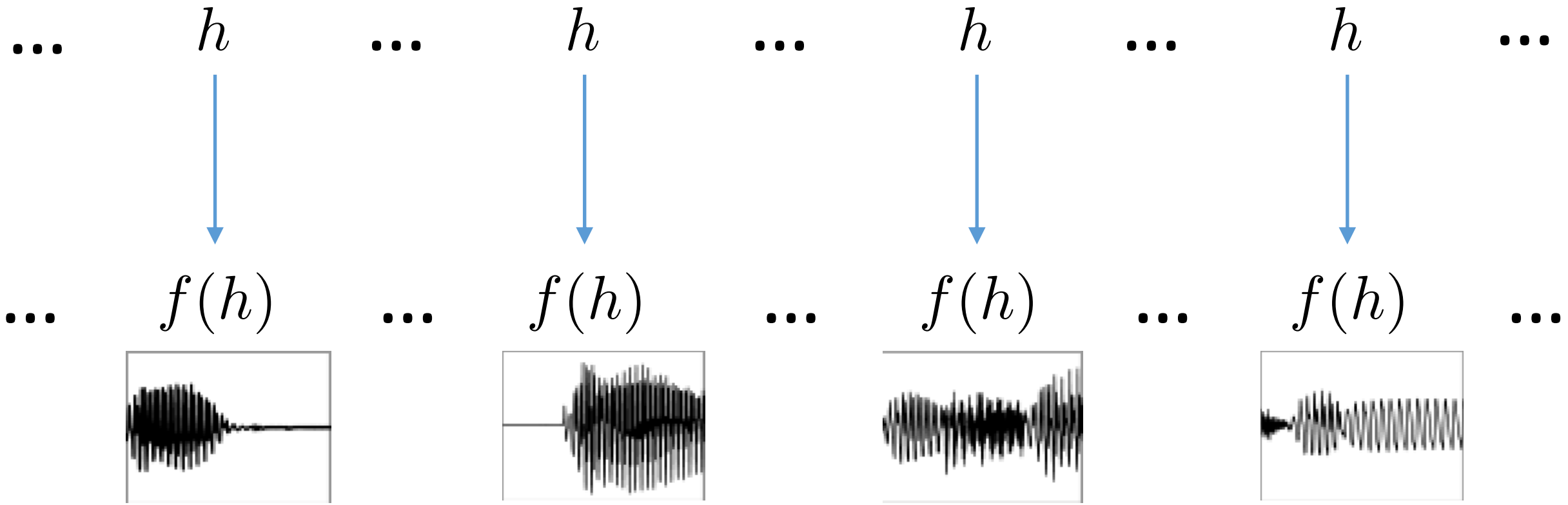
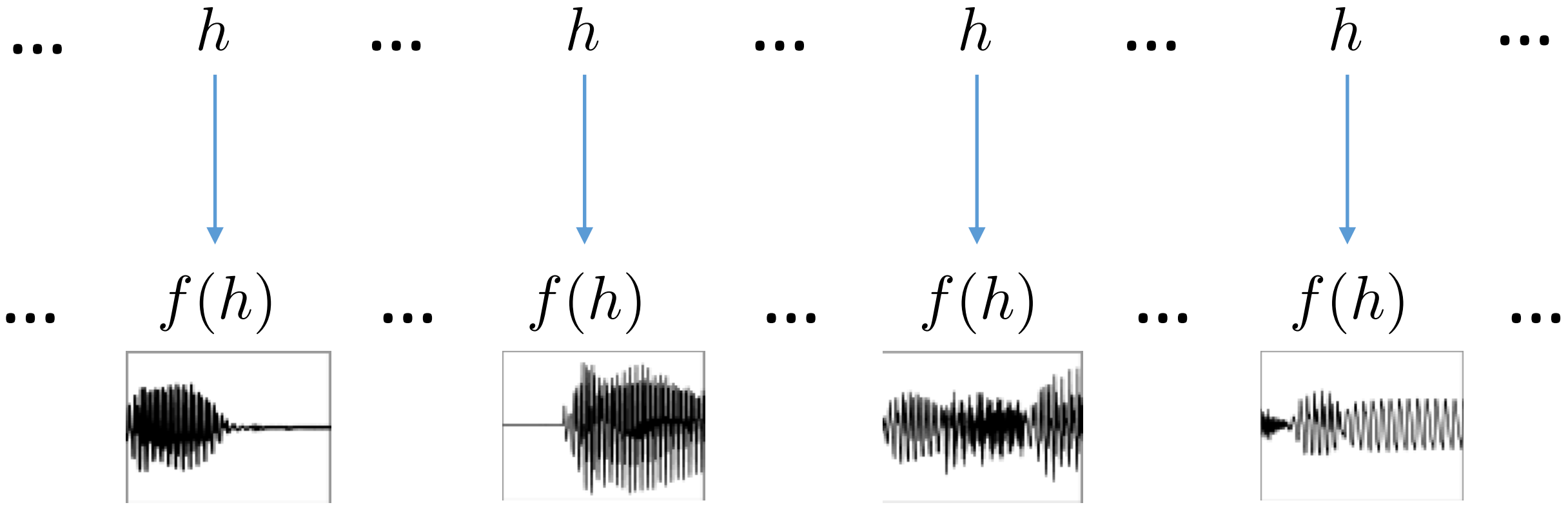


$$p(f_*|x_*, \mathbf{x}, \mathbf{f}) \sim \mathcal{N}(\mathbf{k}_{*\mathbf{x}}\mathbf{K}_{\mathbf{xx}}^{-1}\mathbf{f}, k_*)$$

Predictions: linear combination of training utterances

Function space ≈ the "*infinite data*" space



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Hybrid between "unit selection" and "parametric" (functional) generation?

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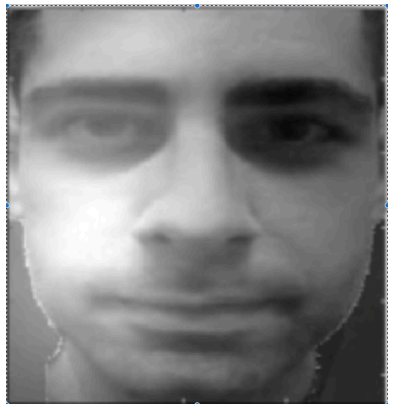
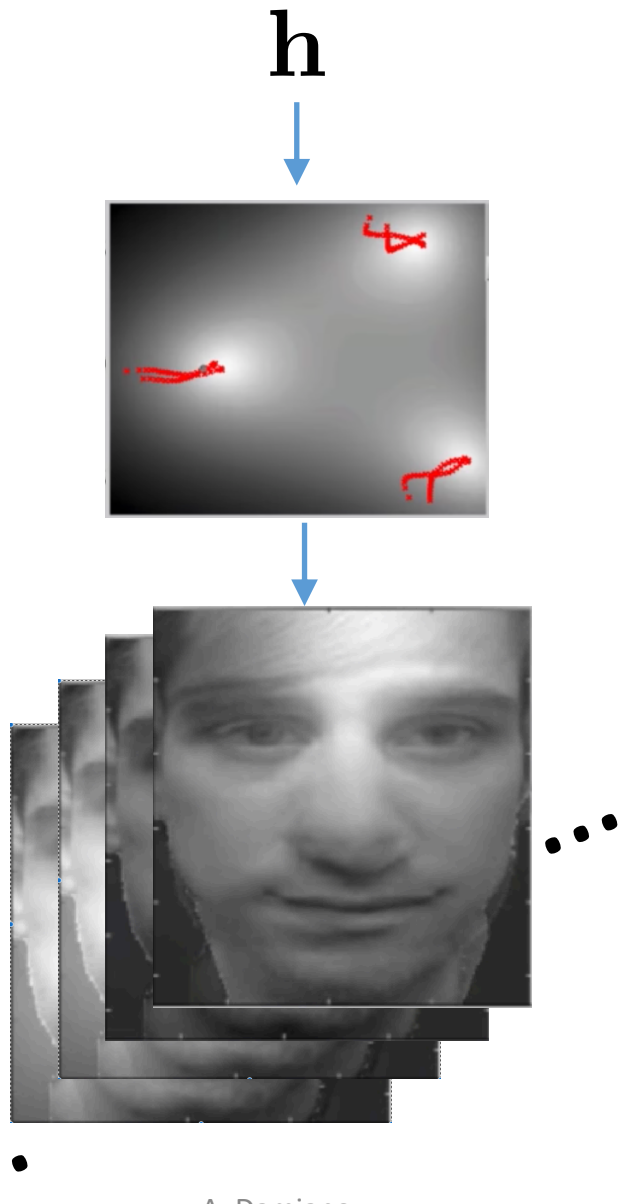



Function space ≈ the "*infinite data*" space

Intermediate layer
function space
(2-dim multivariate function)

Observation layer
(#pixels-dim multivariate function)



Generative modelling

- Training set: *150* images
- Raw pixels, no pre-processing
- No convolutions
- No explicit information about variables such as *“person_id”* or *“light_angle”*

https://youtu.be/rIPX3CIOhKY?t=91

Audio generation

https://youtu.be/Q3oBt2WhaXc

- Training set: ~ *200* short pieces of classical music
- No pre-processing

Function generative modeling advantages

- Controls are learned “automatically” in function space, where is easier to (de)compose because we work directly with the *function* rather than with *the parameter that induces the function*.

- Can learn from very small data by averaging hypotheses which is a useful property even when we have massive data, because it shows *we can cover the space of variability well*.

State-of-the-art for deep GPs

- Focus on extensions:
  - Recurrent DGPs *[Mattos, Dai, Damianou, Barreto, Lawrence, 2017]*
  - Convolutional DGPs *[Kumar et al. 2018; Blomqvist et al. 2018; Dutordoir et al. 2019]*
  - IRL-DGP *[Jin, Damianou, Abbeel, Spanos, 2015]*
  - Active learning/BO *[Yang et al. 2020; Fei et al. 2019]*
  - Physical sciences & Engineering (molecule dynamics, aerospace vehicle design, geospatial modeling)
  - ***Hybrids with DNNs*** *[Dai, Damianou, Gonzalez, Lawrence ICLR 2016; Tran et al. 2019]*

- Focus on approximations:
  - EP, MCMC etc. VI dominates *[Damianou NeurIPS workshop keynote 2017; Yu et al. 2019; Salimbeni et al. 2019]*

- Opinion: Time to re-visit generative modelling with functional models

Gaussian processes with trained neural network inductive biases

(best of both worlds?)

- Train neural networks in situations where they are superior.
- Encode them in function space through a GP.
- Manipulate the resulting function e.g. for domain adaptation in function space.
  - *Transfer inductive biases from the **trained** DNN, not its architectural structure!*

GP with NN inductive biases

[Maddox, Tang, Moreno, Wilson, Damianou (2020)]

- 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. $\mathbf{k}_{*\mathbf{x}} = k(x_*, \mathbf{x}) = J(x_*; \mathbf{w})^T J(\mathbf{x}; \mathbf{w})$.

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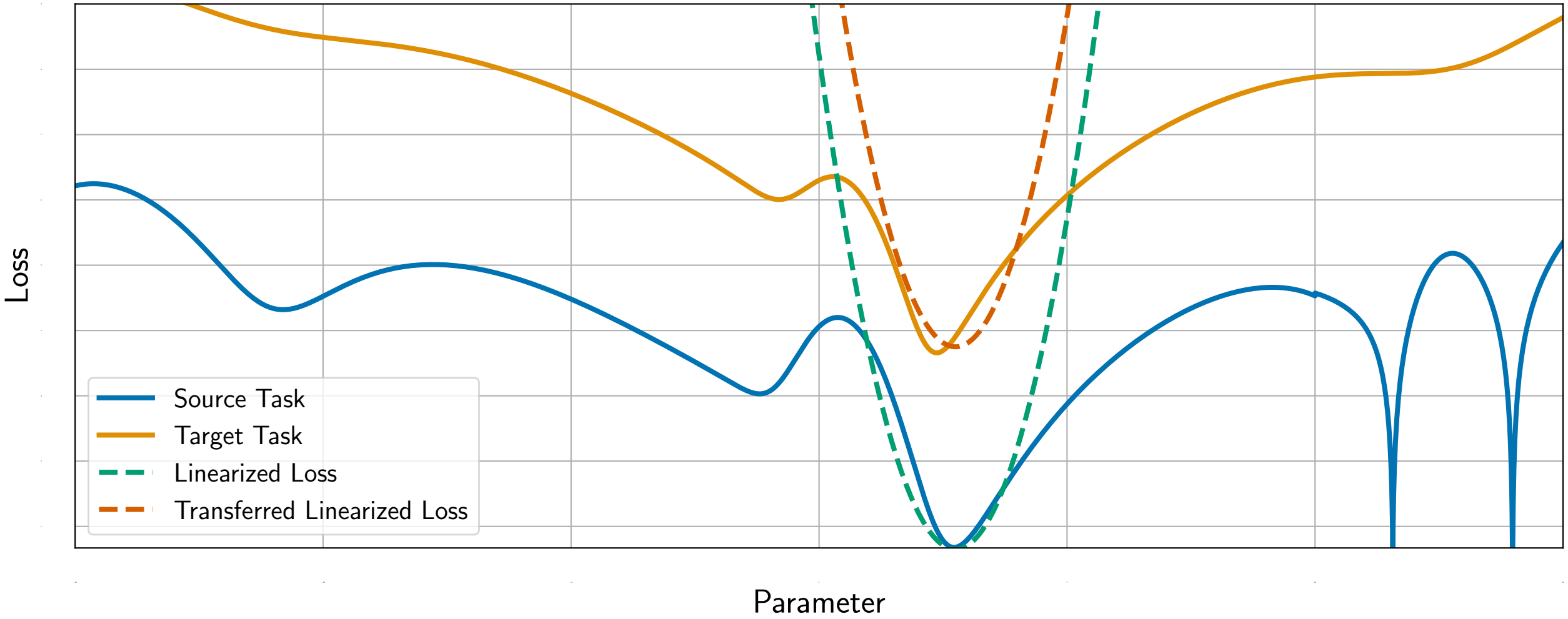
Fast, closed-form adaptation in the functional space with uncertainty!

DNN training dynamics in GD

$$w_{t+1} = w_t - \eta \nabla_w L(f(w_t)) \Rightarrow$$
$$\frac{w_{t+1} - w_t}{\eta} = -\nabla_w L(f(w_t)) \Rightarrow$$
$$\frac{dw(t)}{dt} = -\nabla_w f(w_t) \nabla_f L(f(w_t))$$

Then:

$$\frac{d\ f(w(t))}{dt} = -\underbrace{\nabla_w^\top f(w_t) \nabla_w f(w_t)}_{\text{NTK}} \nabla_f L(f(w_t))$$


Loss
Parameter
Source Task
Target Task
Linearized Loss
Transferred Linearized Loss

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.

Efficient computations

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

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

- 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.

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:

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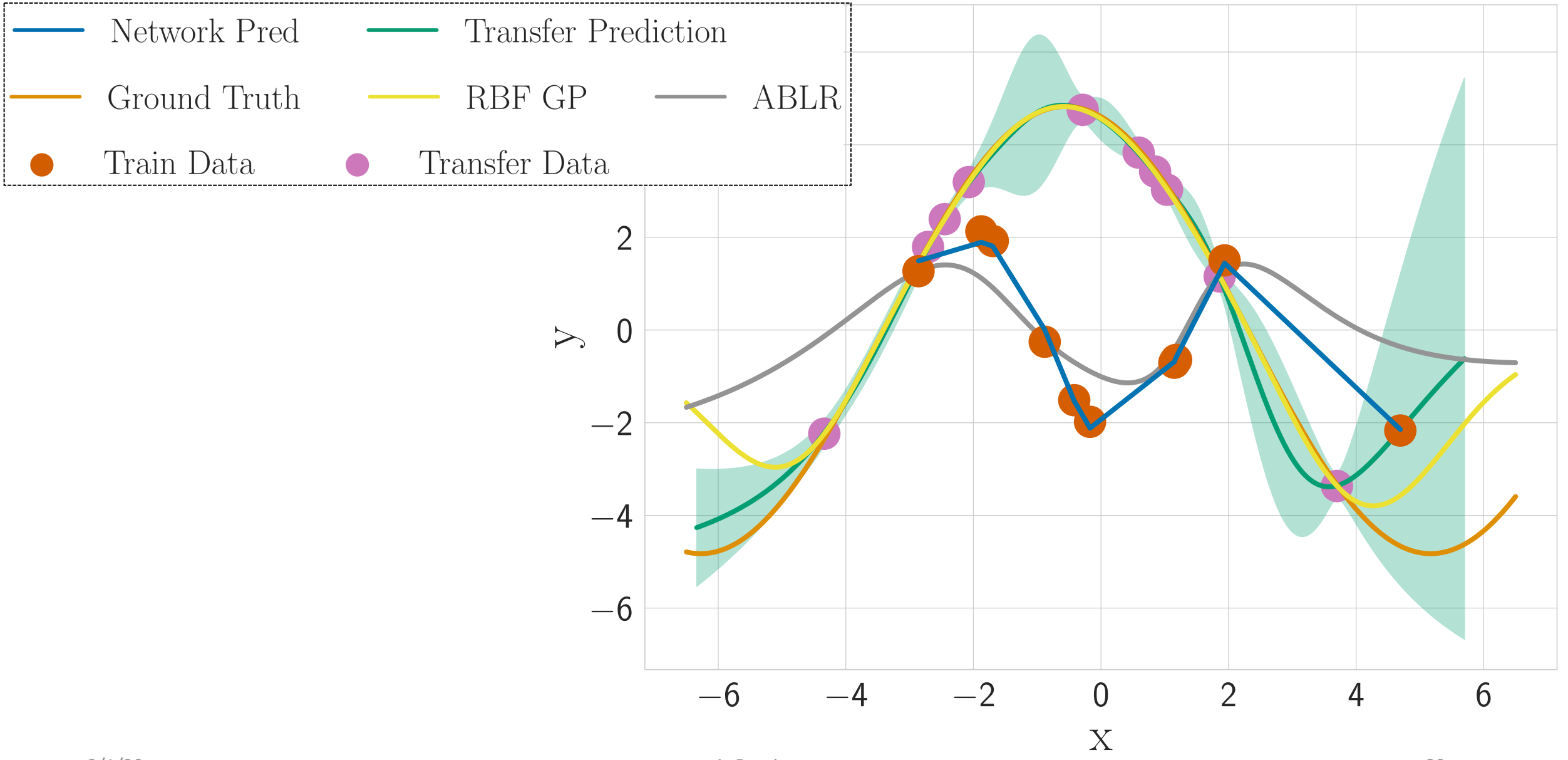
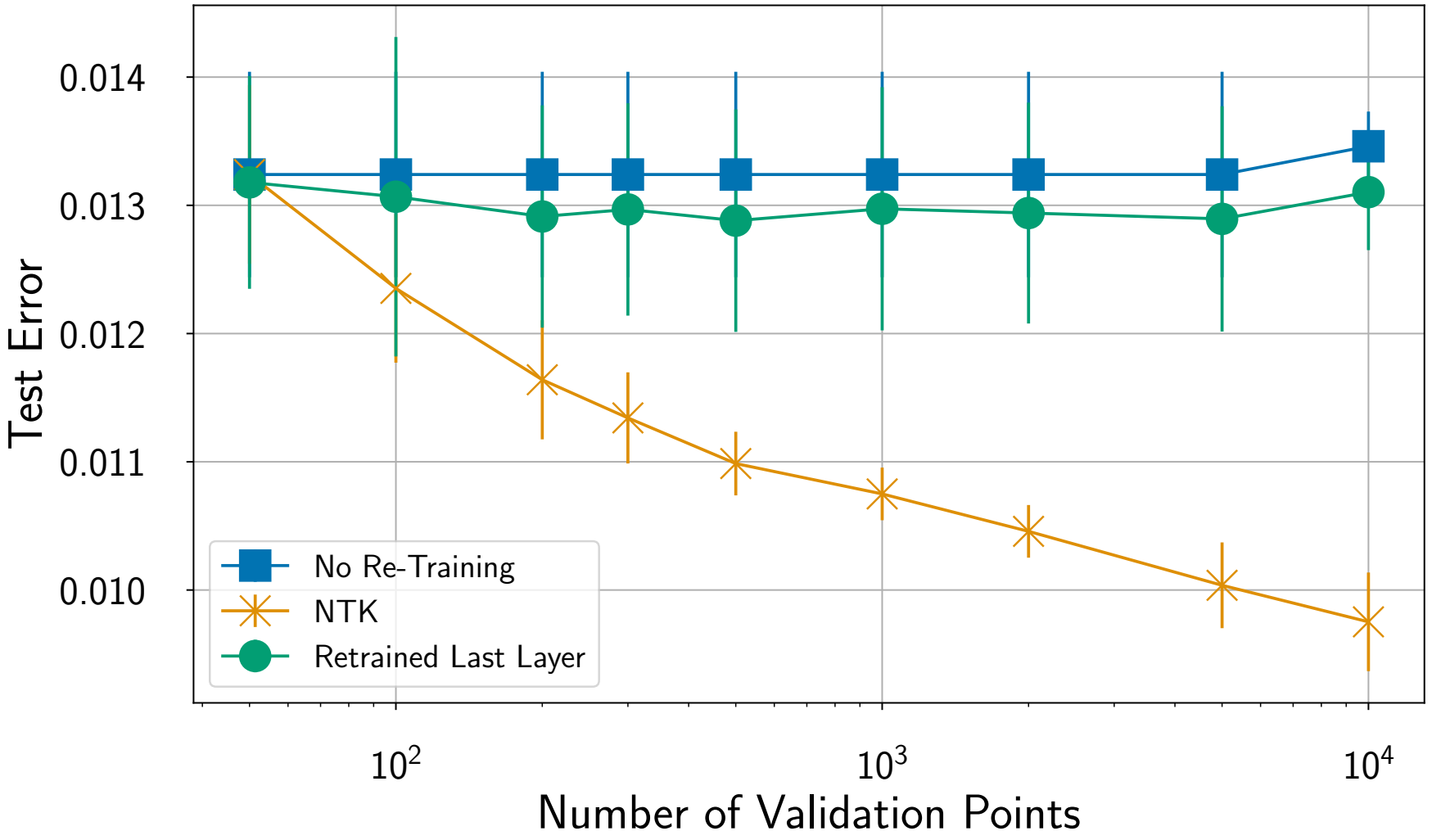
- For t iterations the covariance expressed in terms of matrices with t columns.
- Allows to access $\mathbf{K}^{-1}\mathbf{f}$ lazily using fast MVP.

Transfer learning (toy regression data)



Malaria spread data



Conclusions

- DNNs are great predictors (supervised learning), thanks to learning algorithms.
- Beyond supervised learning: modelling in function space offers an alternative.
- Leverage hierarchical concept learning together with function space modelling:
  - NNs as inductive biases for GPs
  - Deep Gaussian process (stack of GPs)
- Demonstrated success in transfer learning.
- Re-visiting hybrid functional/DNN models for generation might be timely.

Questions?

See also:

- *adamian.github.io/talks/Damianou_deep_learning_rss_2018.pdf*
- *adamian.github.io/talks/Damianou_GP_tutorial.html*

Appendix

NTK

GP ⟷ DNN beyond initialization (and practical use)

Initialization	During training	**Convergence**
Neal ‘94 Lee et al. ‘18 Matthews et al. ‘18	Jacot et al. ‘18 NTK Lee et al. ‘19 Hayou et al. ‘19	Maddox et al. ‘19

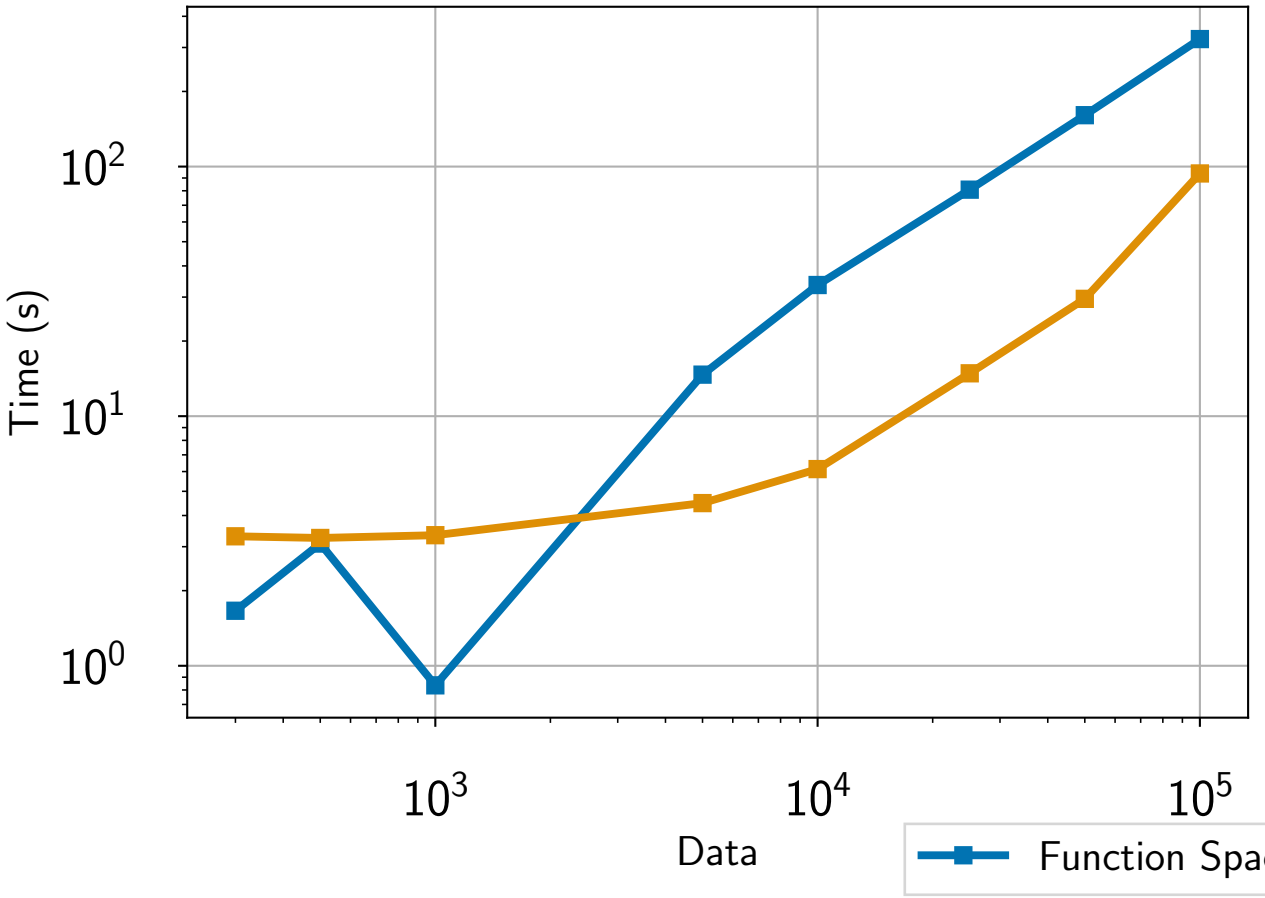
Model: A degenerate GP from DNNs obtained at convergence.

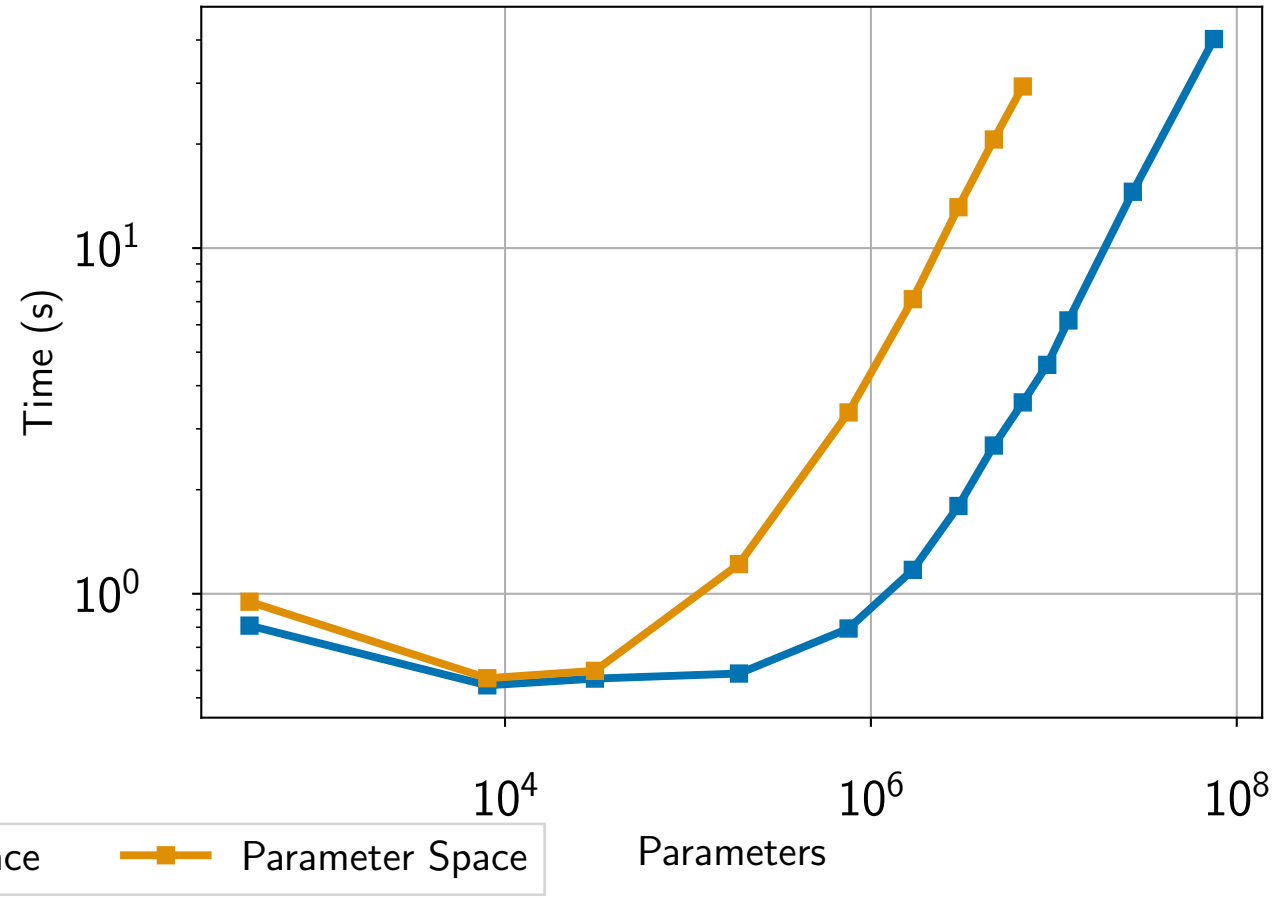
W. Maddox, S. Tang, P. Moreno, A. Wilson, A. Damianou: *Fast Adaptation with Linearized Neural Networks*. 2019

Other relevant works

- Perrone et al. 2018: Explicitly uses output features of DNN (we use NTK with Jacobian information from all layers)
- Wilson et al. 2015: DKL (whole NN embedded in kernel)
- Jaakkola et al. 1998 and others: gradients as features

Scaling

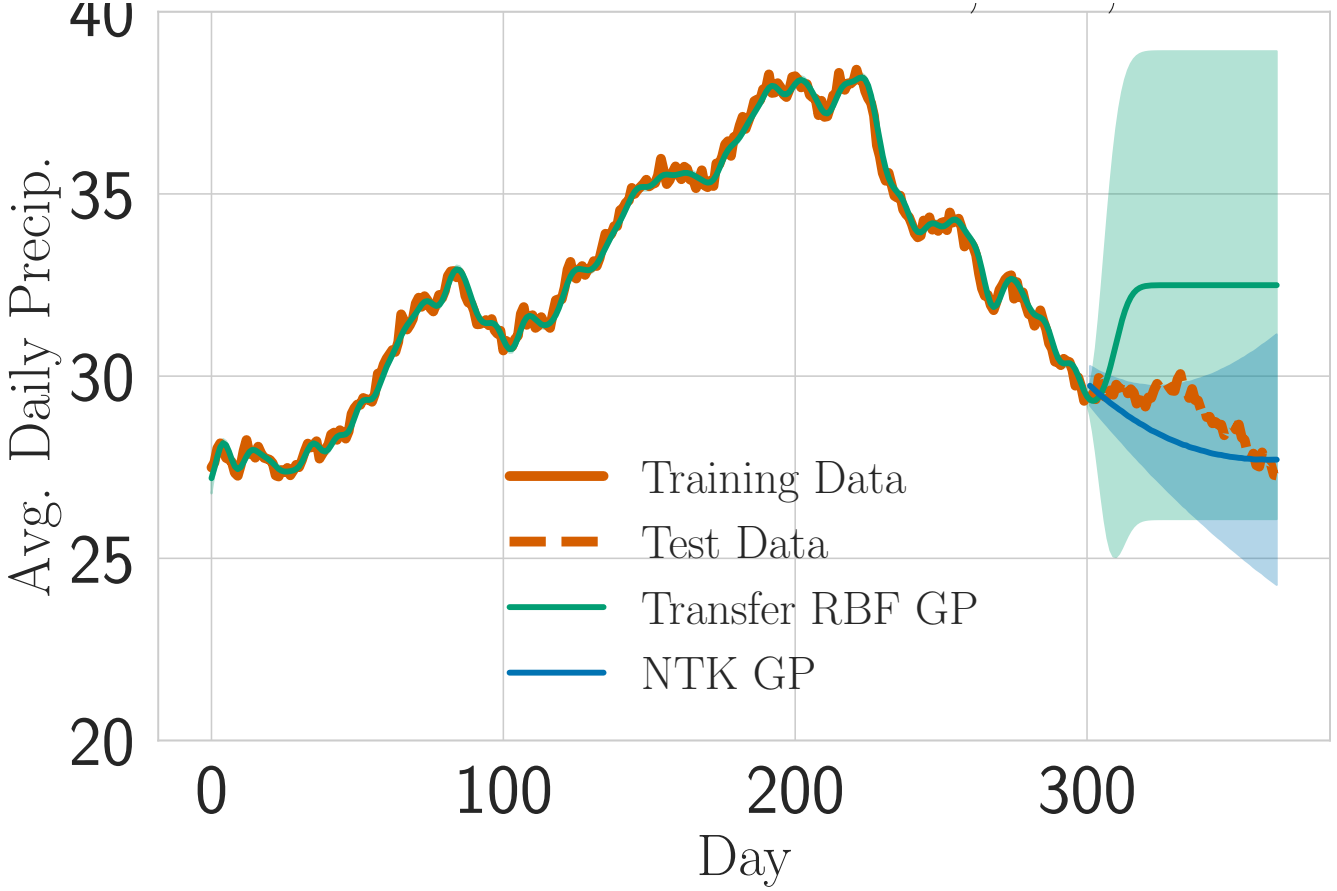

10^2
10^1
10^0
Time (s)
10^3
10^4
10^5
Data


10^1
10^0
Time (s)
10^4
10^6
10^8
Parameters

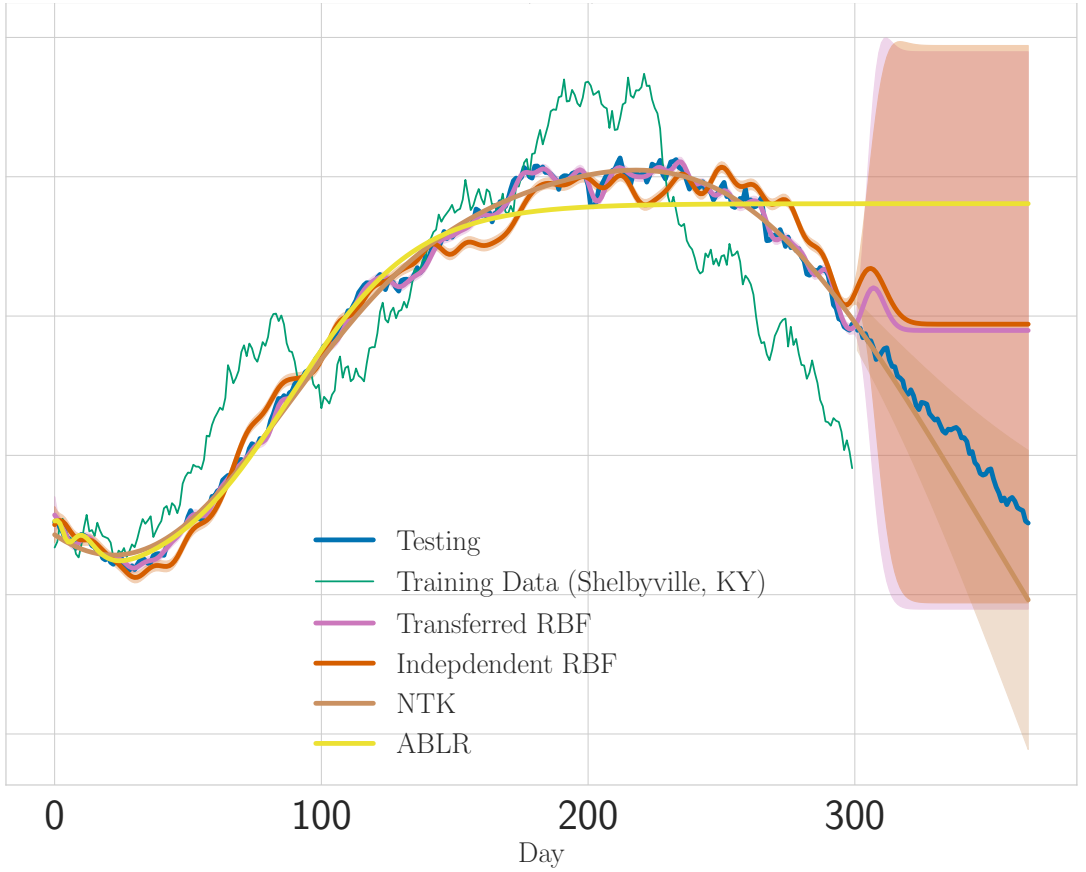
Function Space
Parameter Space

Transfer learning for precipitation data

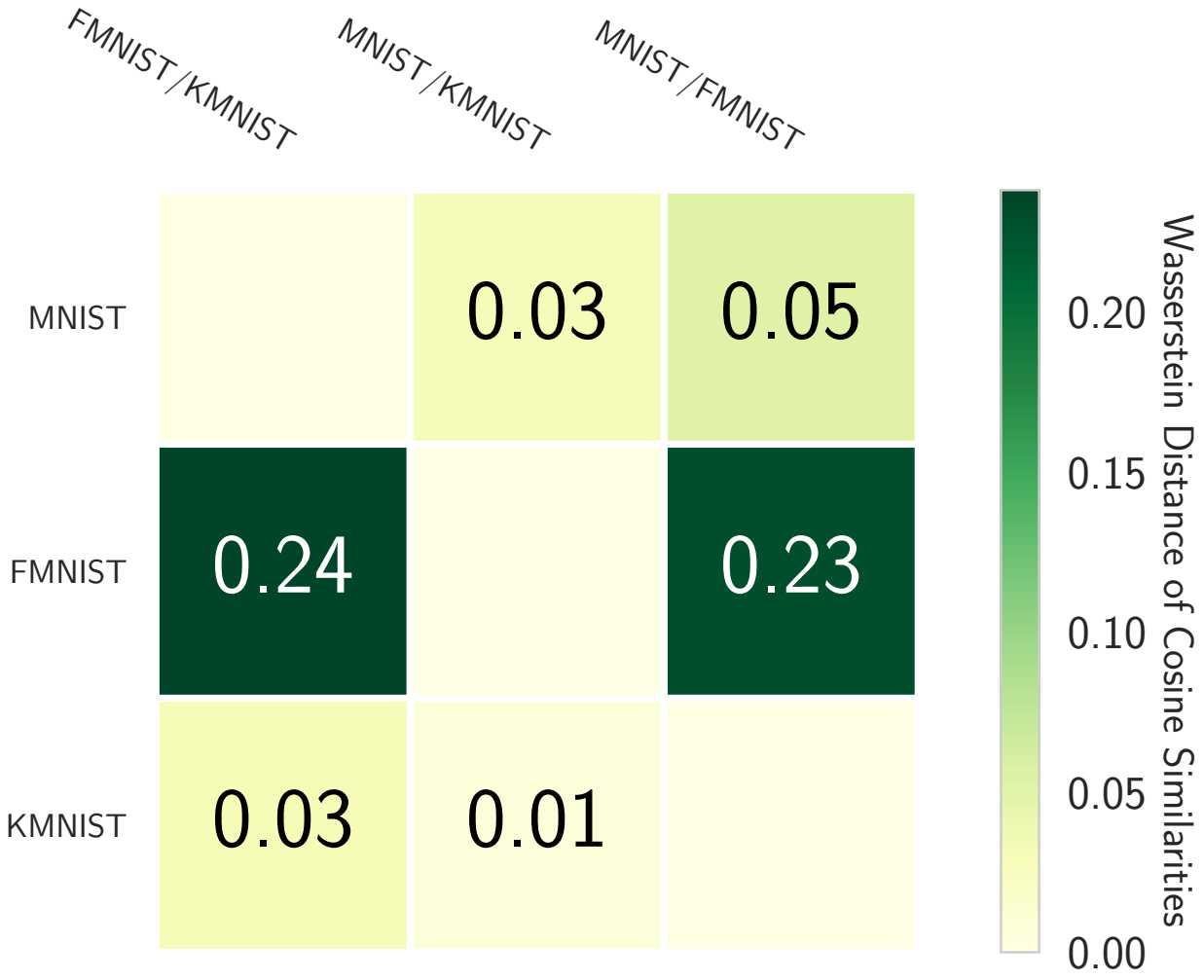
Source task



Target task



Similar tasks have similar Jacobians



DNN training dynamics in GD

$$w_{t+1} = w_t - \eta \nabla_w \underbrace{L(f(x; w_t))}_{\log p(y|f(x;w))} \Rightarrow \frac{w_{t+1} - w_t}{\eta} = -\nabla_w L(f(w_t)) \Rightarrow$$

$$\frac{dw(t)}{dt} = -\nabla_w L(f(w_t)) \tag{1}$$

But: $\frac{dL(f(w_t))}{dw_t} = \frac{L(f(w_t))}{df} \frac{df(w_t)}{dw_t}$ (chain rule). So writing nabla notation, (1) becomes:

$$\frac{dw(t)}{dt} = -\nabla_w f(w_t) \nabla_f L(f(w_t)) \tag{2}$$

Then: $\frac{d\ f(w(t))}{dt} = \frac{df(w(t))}{dw(t)} \frac{dw(t)}{dt} = -\underbrace{\nabla_w^\top f(w_t) \nabla_w f(w_t)}_{\text{NTK}} \nabla_f L(f(w_t))$

Notation, $\nabla_w f(x; w_t) = J_w(x)$

Finite-NTK complexity

Computational complexities

- exact-GP : O(n^2)
- KISS-GP+Lanczos : O(t).
- exact-GP+Lanczos : O(tn) but k is very small
- sparseGP : O(m^2) but m is typically large
- sparseGP+Lanczos : O(km)

Storage costs

- exact-GP : O(n^2)
- KISS-GP+Lanczos : O(tm)
- exact-GP+Lanczos : O(tn) [but parallelizable]
- sparseGP : O(m^2)
- sparseGP+Lanczos : O(tm)

Complexities

- In training, $\mathbf{K}_{XX}$ is computed by $k(\mathbf{X}, \mathbf{X}; \theta)$. During optimization we change θ and thus have to compute the inverse in each optimization step. Cholesky is $O(n^3)$ and with ind. pts it can be done $O(nm^2)$. With KISS-GP it can be $O(n + m \log m)$ but requires grid.
- In predictions θ and hence $\mathbf{K}_{XX}$ is fixed. If we precompute whatever doesn't include $*$, then we have a standard vector-vector mult. for the mean, i.e. (O(n)). No linear solves required, so it can be done in a single GPU. For variance, if we precompute again, the remainder still costs $O(n^2)$ or $O(m^2)$ for Sparse GP or $O(k(n + mlogm))$ for KISS-GP.
- WIth KISS-GP + Lanczos (KISS-GP LOVE), instead of $\mathbf{k}_{*X}const$ we have $\mathbf{w}_{\mathbf{x}_*}$ which has only 4 nonzero elements, hence mean pred. is O(1). Pred. variance can then be O(k) with k very small, so they consider it O(1).
- With just Lanczos (and no KISS-GP), the variance goes back to O(nk) or O(mk) if used with sparse GPs. In the exact gp paper they say O(n), possibly because k is typically small. The mean remains O(n), I think, but can be parallelized.

Fast predictive variances

$$\tilde{\mathbf{k}}_{X\mathbf{x}_i^*} = W_X^\top K_{UU} \mathbf{w}_{\mathbf{x}_i^*}, \qquad \tilde{K}_{XX} = W_X^\top K_{UU} W_X$$

Approximate covariance using points in grid with weight W

$$k_{f|\mathcal{D}}(\mathbf{x}_i^*, \mathbf{x}_j^*) \approx k_{\mathbf{x}_i^*\mathbf{x}_j^*} - \tilde{\mathbf{k}}_{X\mathbf{x}_i^*}^\top (\tilde{K}_{XX} + \sigma^2 I)^{-1} \tilde{\mathbf{k}}_{X\mathbf{x}_j^*}. \quad (7)$$

By fully expanding the second term in (7), we obtain

$$\mathbf{w}_{\mathbf{x}_i^*}^\top \underbrace{K_{UU} W_X (\tilde{K}_{XX} + \sigma^2 I)^{-1} W_X^\top K_{UU}}_{C} \mathbf{w}_{\mathbf{x}_j^*} \quad (8)$$

Replace in GP predictive equation. Precomputing C with Lanczos.

$$C = K_{UU} W_X \underbrace{(\tilde{K}_{XX} + \sigma^2 I)^{-1}}_{\text{Apply Lanczos}} W_X^\top K_{UU}$$

$$\approx K_{UU} W_X (Q_k T_k^{-1} Q_k^\top) W_X^\top K_{UU}$$

$$= \underbrace{K_{UU} W_X Q_k}_{R^\top} \underbrace{T_k^{-1} Q_k^\top W_X^\top K_{UU}}_{R'}$$

C precomputed with t iterations, giving us structure R^T R

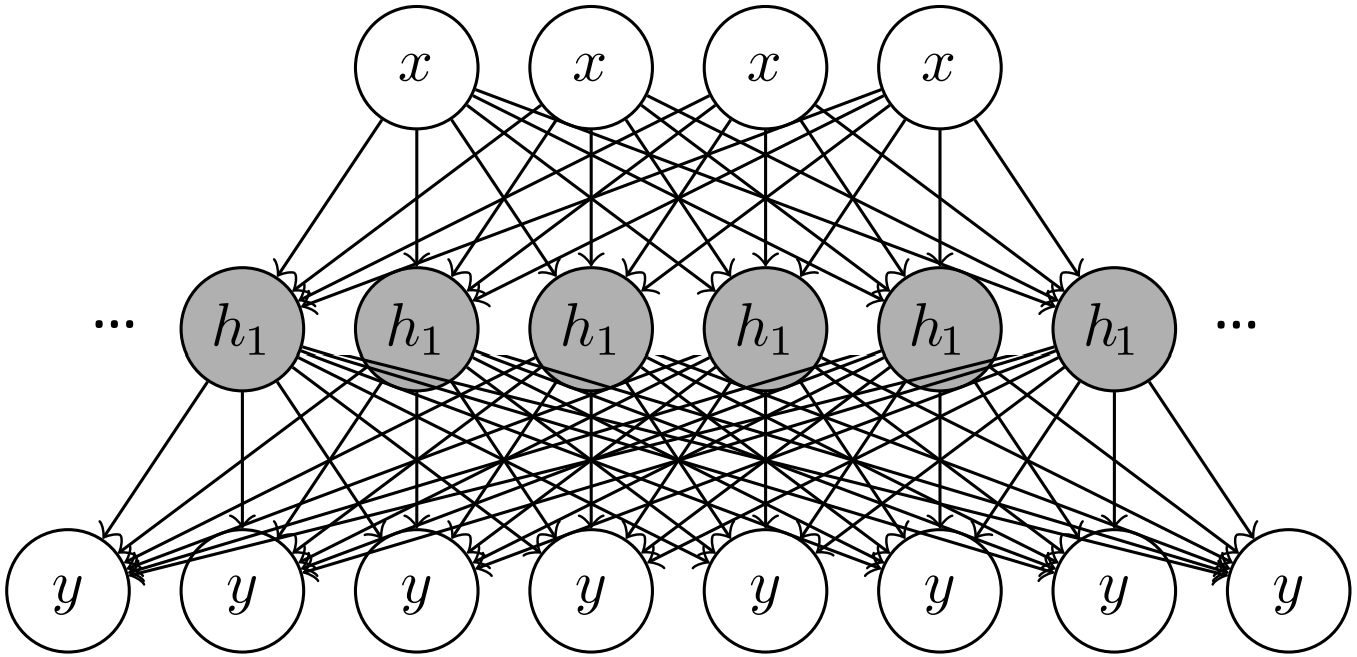
To compute R and R', we perform k iterations of Lanczos to achieve $(\tilde{K}_{XX} + \sigma^2 I) \approx Q_k T_k Q_k^\top$ using the av-

R is *m x t*

GP Limit properties

Single layer, infinite width NN → GP

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



GP

Neal 1994; Williams 1997

Conditions for limit results

- Independence (i.i.d. noise)
- Bounded variance
- #nodes → Inf

Then use multivariate Central Limit Theorem.

Analytic covariance function (1 layer)

Single layer network:

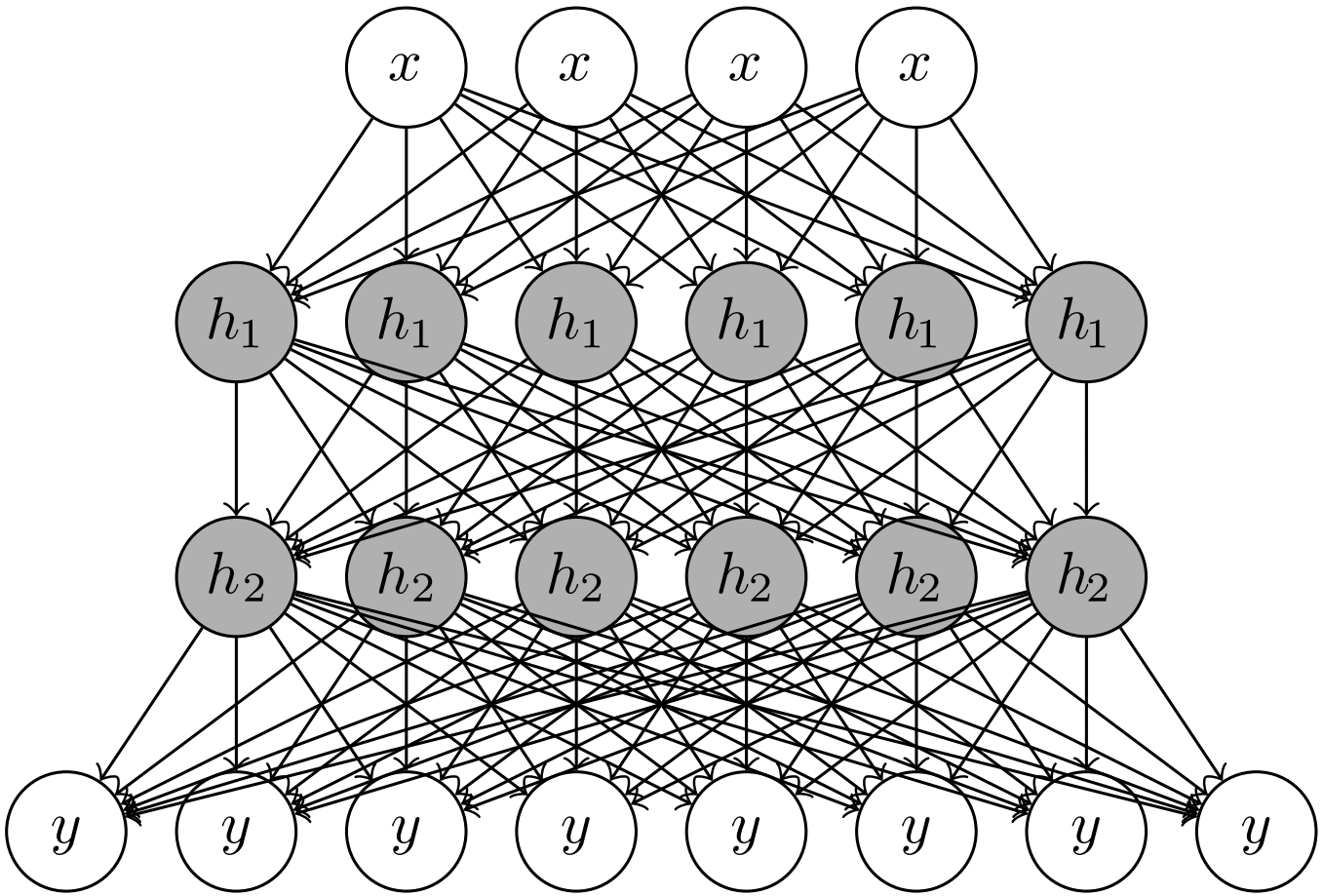
$$z_i^l(x) = b_i^l + \sum_{j=1}^{N_l} W_{ij}^l x_j^l(x), \quad x_j^l(x) = \phi(z_j^{l-1}(x)).$$

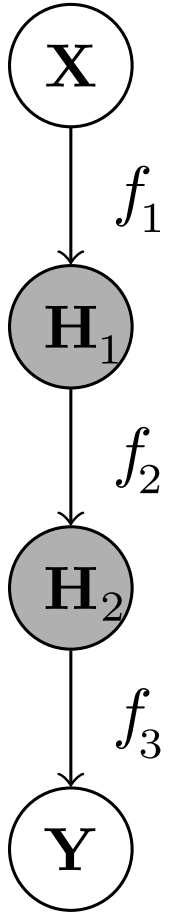
Corresponding GP cov. function:

$$K^1(x, x') \equiv \mathbb{E}\left[z_i^1(x) z_i^1(x')\right] = \sigma_b^2 + \sigma_w^2 \, \mathbb{E}\left[x_i^1(x) x_i^1(x')\right] \equiv \sigma_b^2 + \sigma_w^2 C(x, x').$$

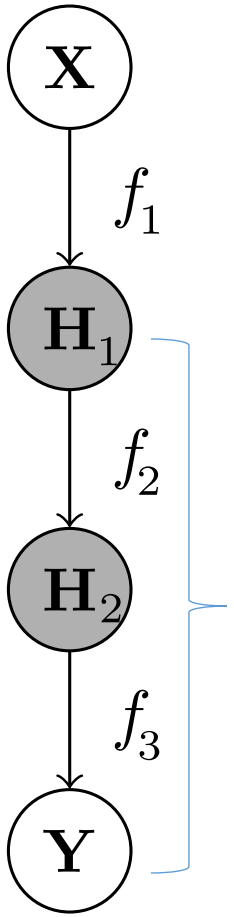
Lee et al. 2018, Matthews et al. 2018

Extension to deep models





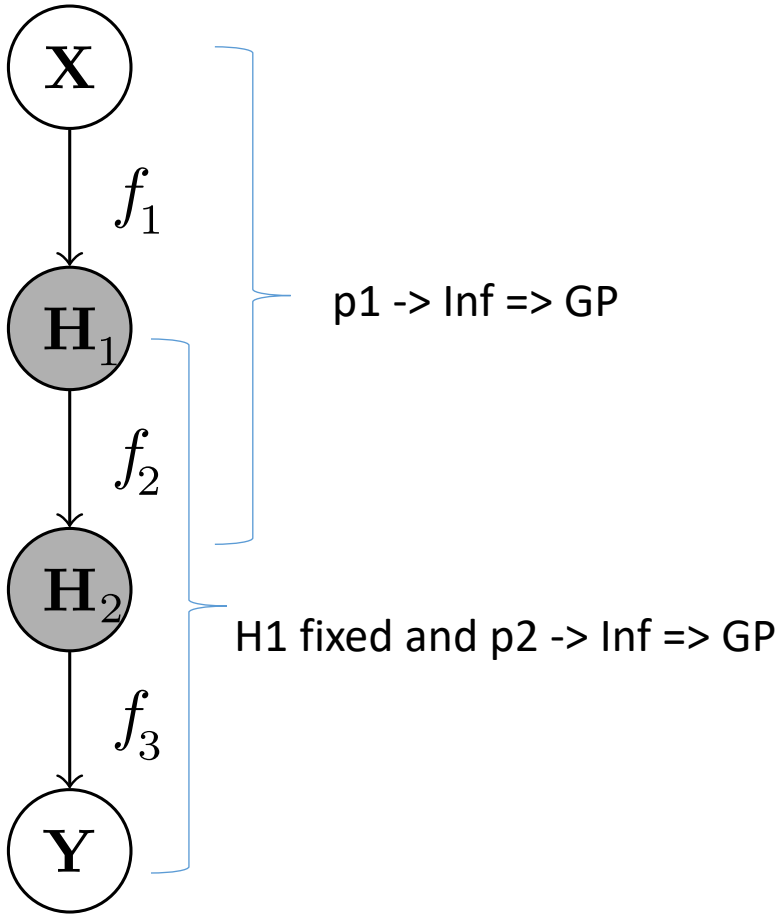
How to generalize the argument for >1 layers?



H1 fixed and p2 -> Inf => GP

(Neal 1994)

How to generalize the argument for >1 layers?



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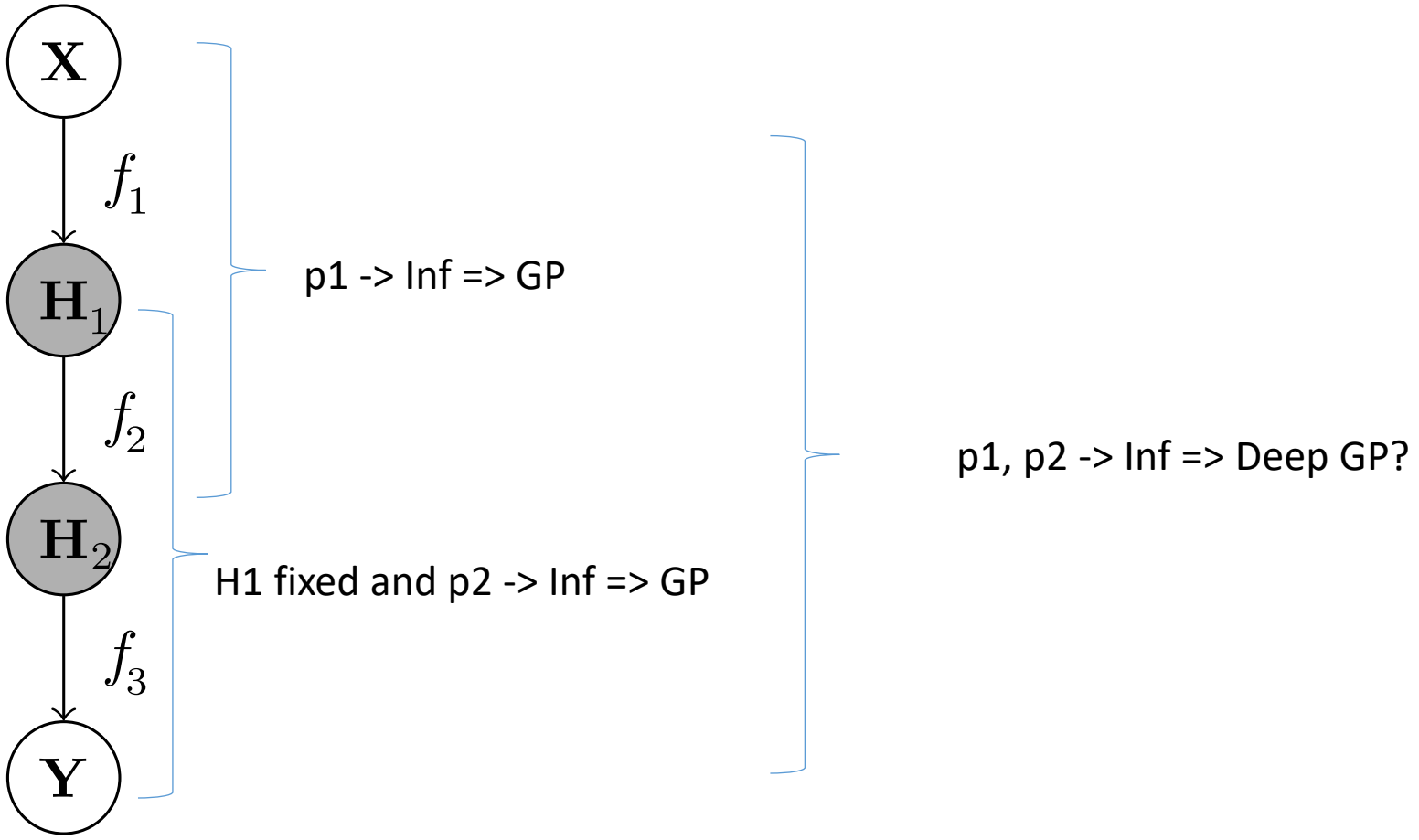

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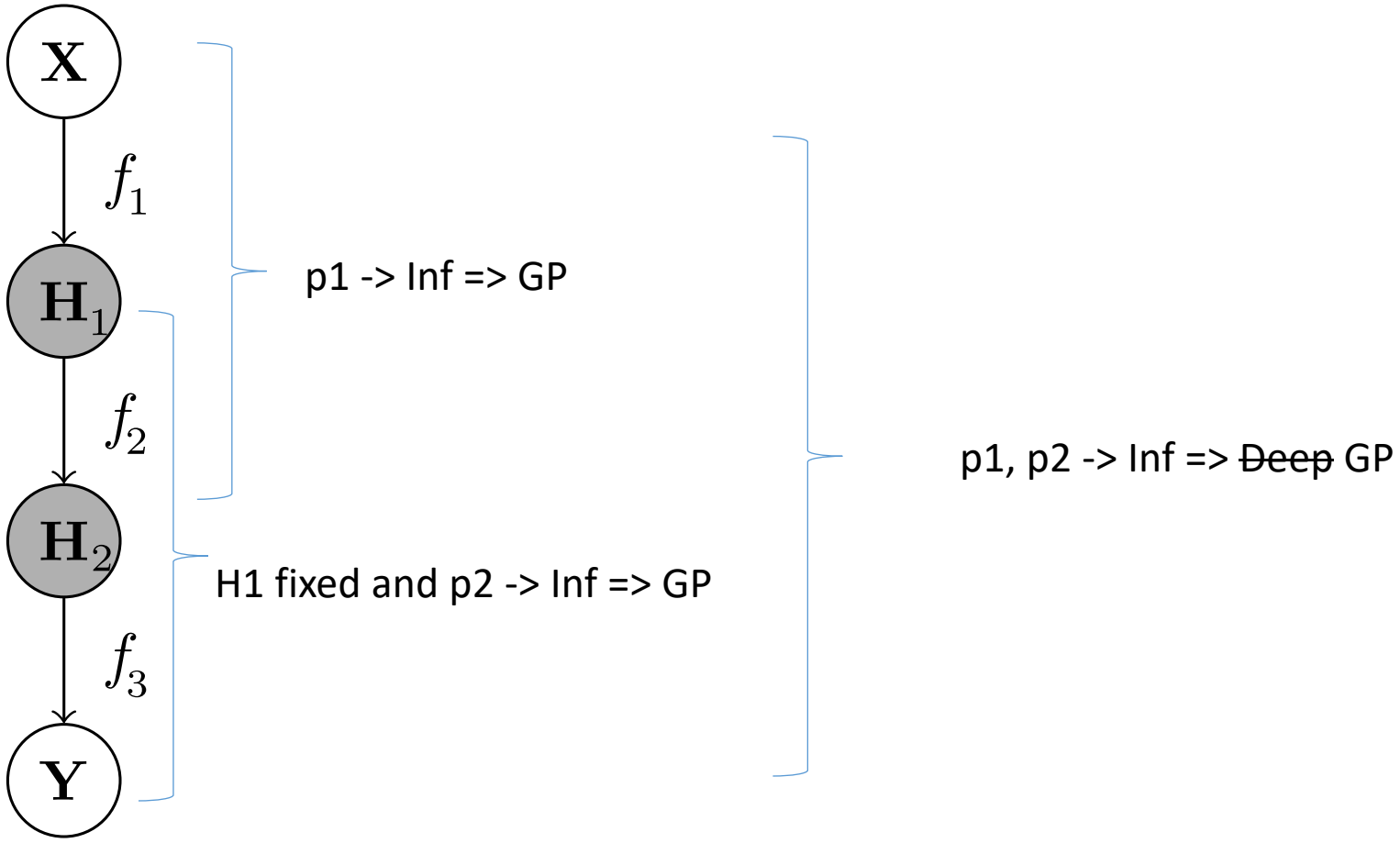


Lee et al., Matthews et al.

Recursive cov. function formulation

$$K^l(x, x') \equiv \mathbb{E}\left[z_i^l(x) z_i^l(x')\right]$$

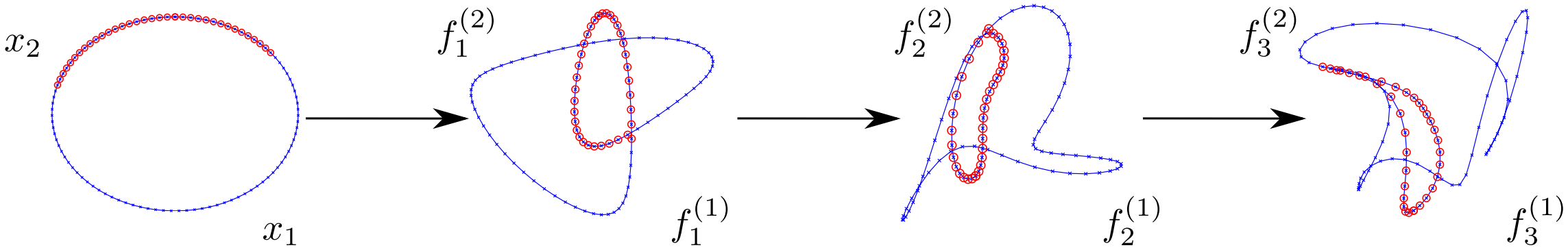
$$= \sigma_b^2 + \sigma_w^2 \, \mathbb{E}_{z_i^{l-1} \sim \mathcal{GP}(0, K^{l-1})}\left[\phi(z_i^{l-1}(x))\phi(z_i^{l-1}(x'))\right]$$

$$= \sigma_b^2 + \sigma_w^2 \, F_\phi\Big(K^{l-1}(x, x'),\, K^{l-1}(x, x),\, K^{l-1}(x', x')\Big)$$

DEEP GP

Feature learning

Features are learned as “knots” in the latent space, carried over from layer to layer.



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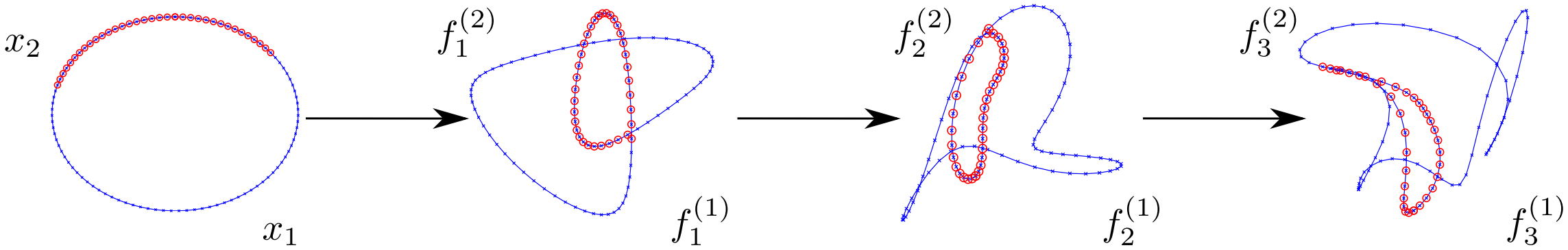

Narrow intermediate layers do give hierarchical feature learning.

DNN vs DGP

- Shallow NN → GP
- Deep NN → GP

DNN vs DGP

- Shallow NN → GP
- Deep NN → GP

Deep GP > Deep NN?
(Discussion)

Analysing DGPs

Limit properties

- Distribution of derivatives in deep models [Duvenaud et al. ‘14]
- How are effective depth and ergodicity connected? [Dunlop et al. ’18]

Few layers analysis through approximation:

- DGP moments and approximation of DGP with GP [Lu et al. ‘19]

Analysing DGPs

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- How are effective depth and ergodicity connected? [Dunlop et al. ’18]

Few layers analysis through approximation:

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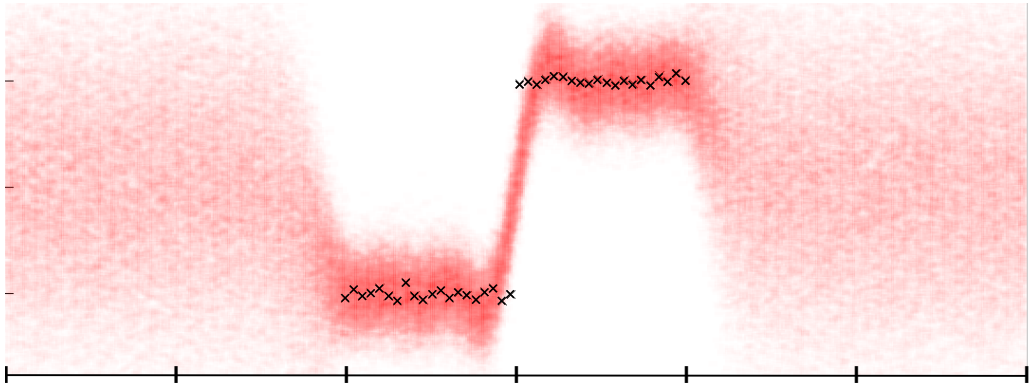
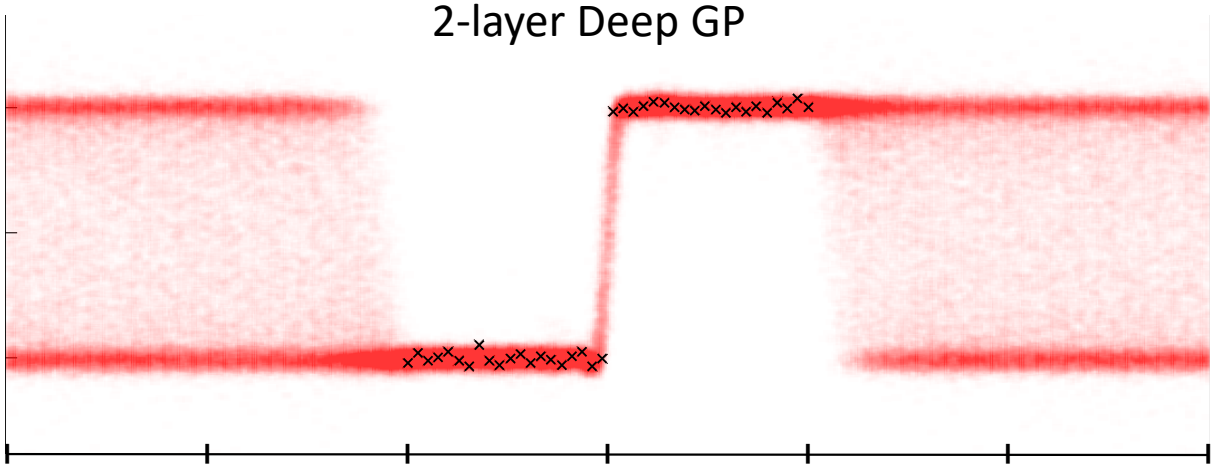
Discussion: What does a DGP with > 2 layers mean?

Step function example

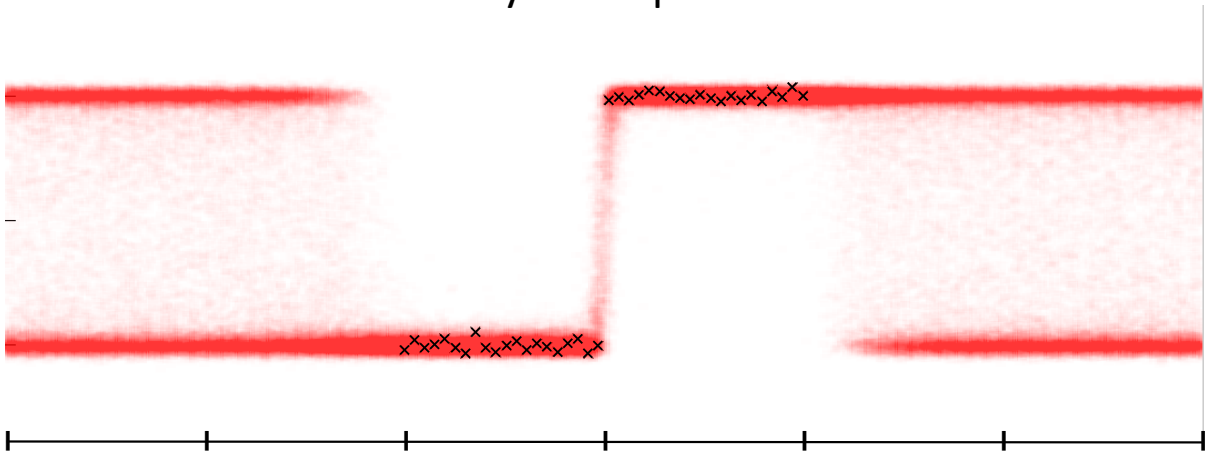
Single GP



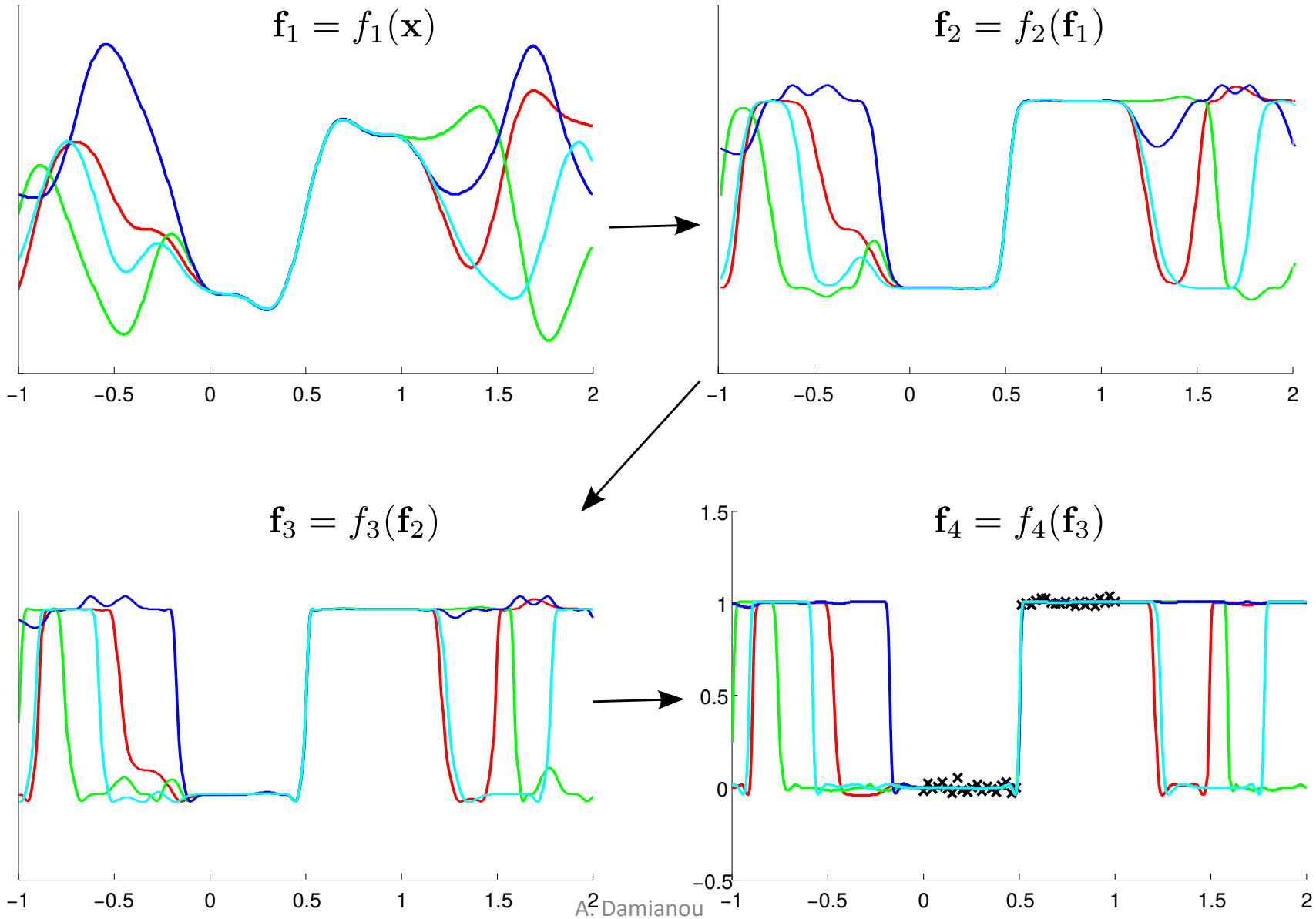
2-layer Deep GP



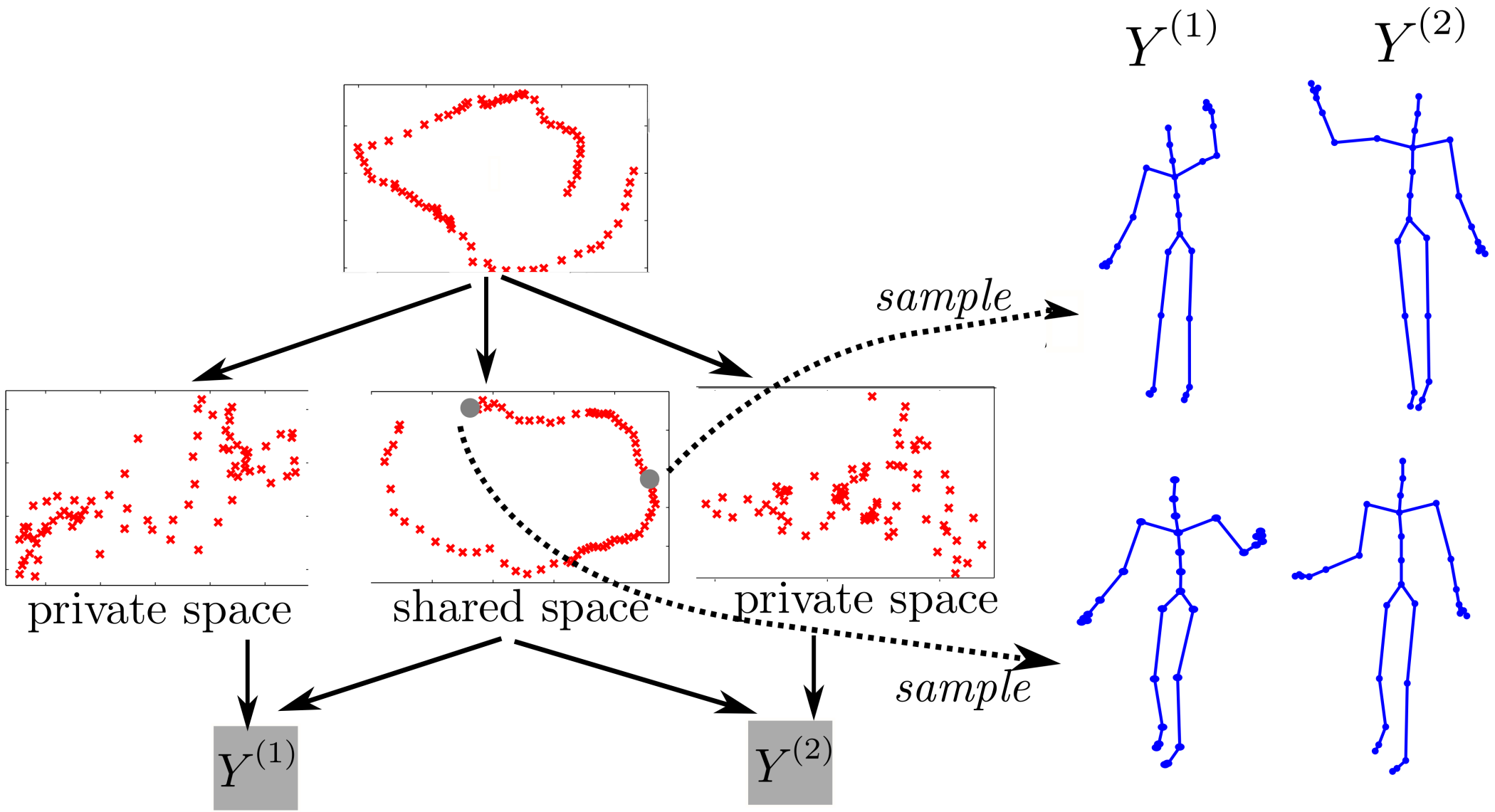
4-layer Deep GP



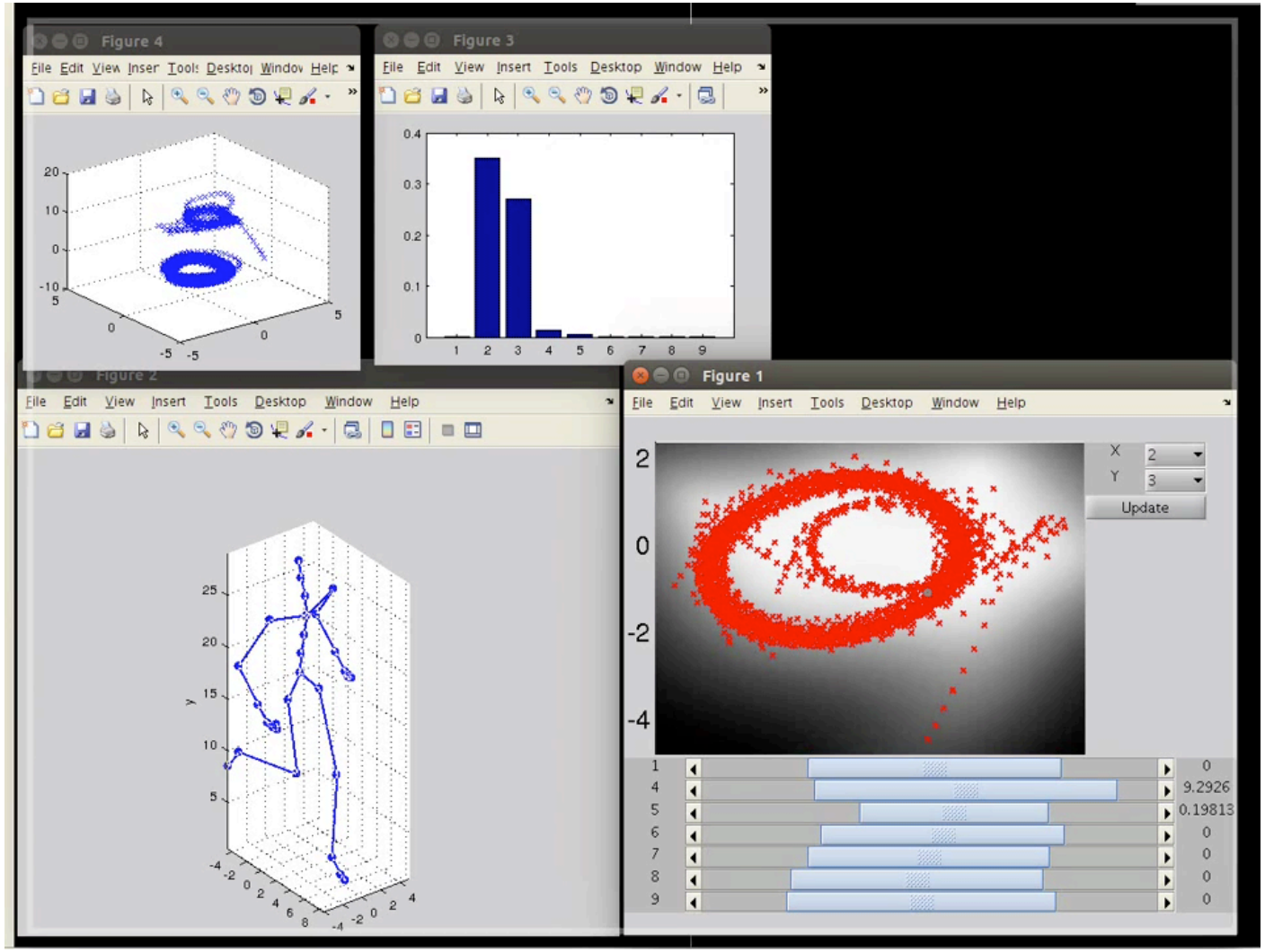
Successive warping to learn the step function



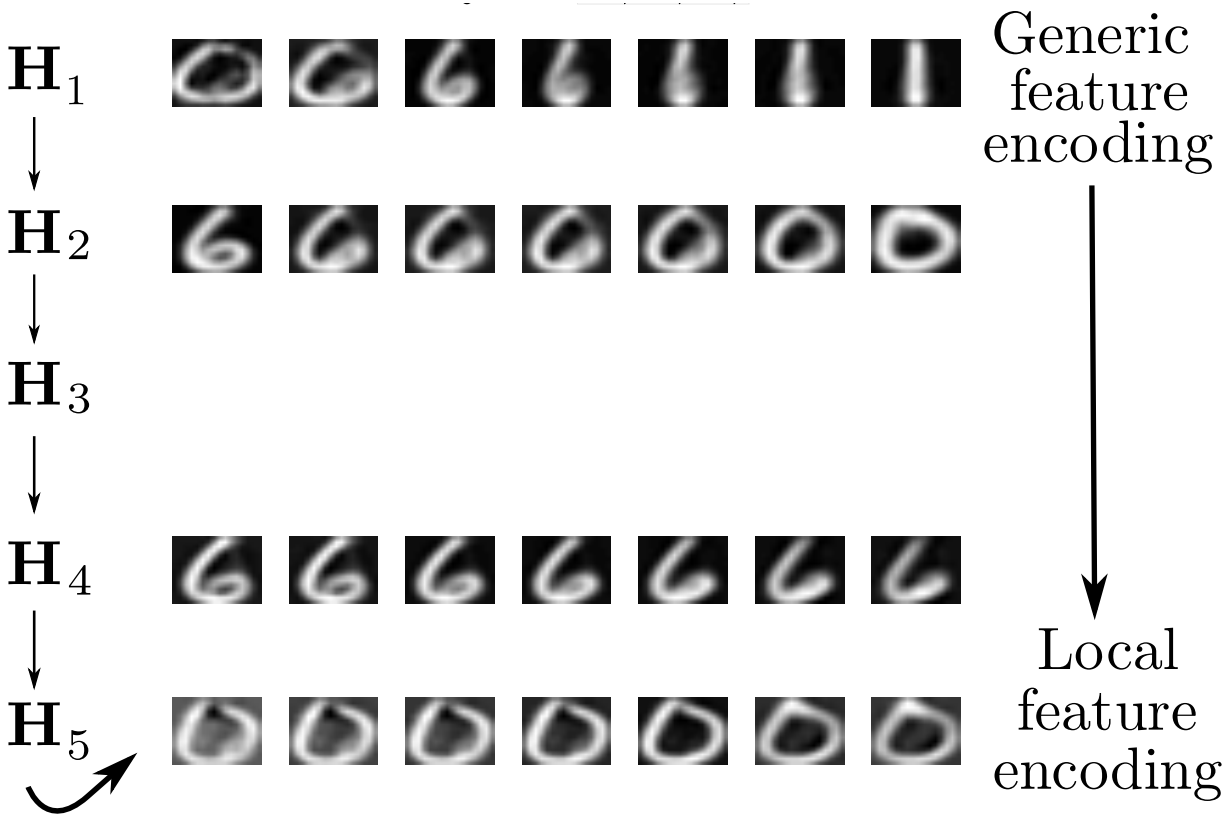
Unsupervised learning for multiple views



Generative modelling



https://youtu.be/fHDWloJtgk8


H1
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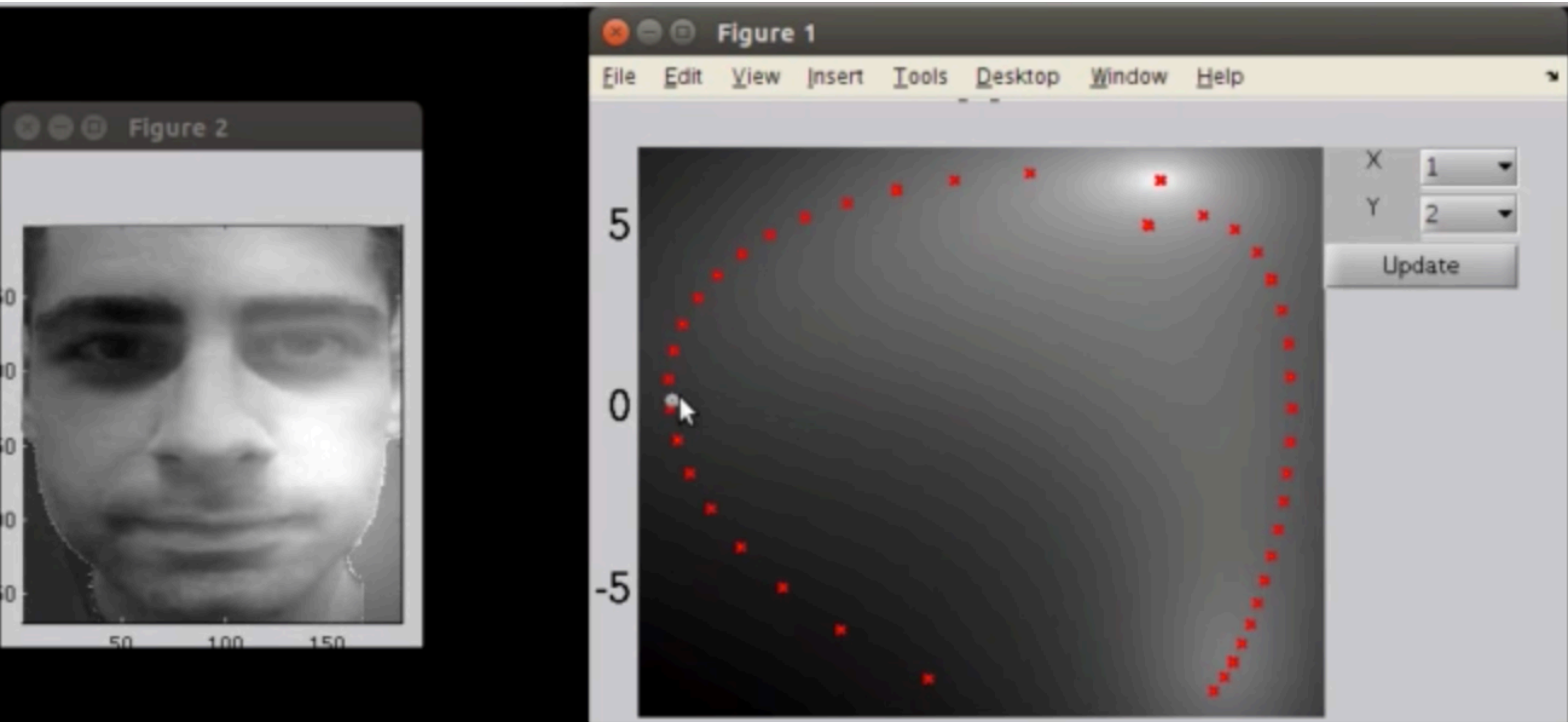
H4
H5
Generic feature encoding
Local feature encoding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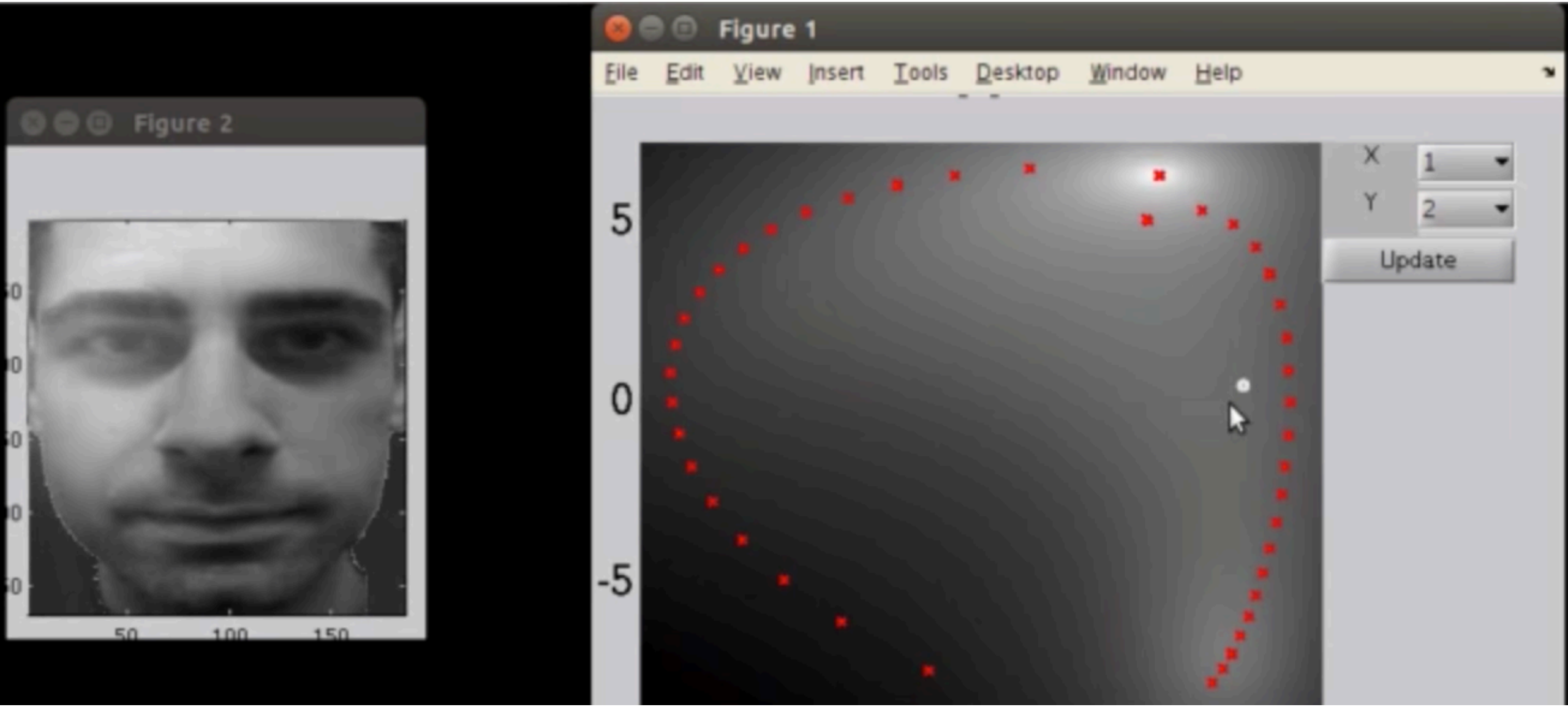
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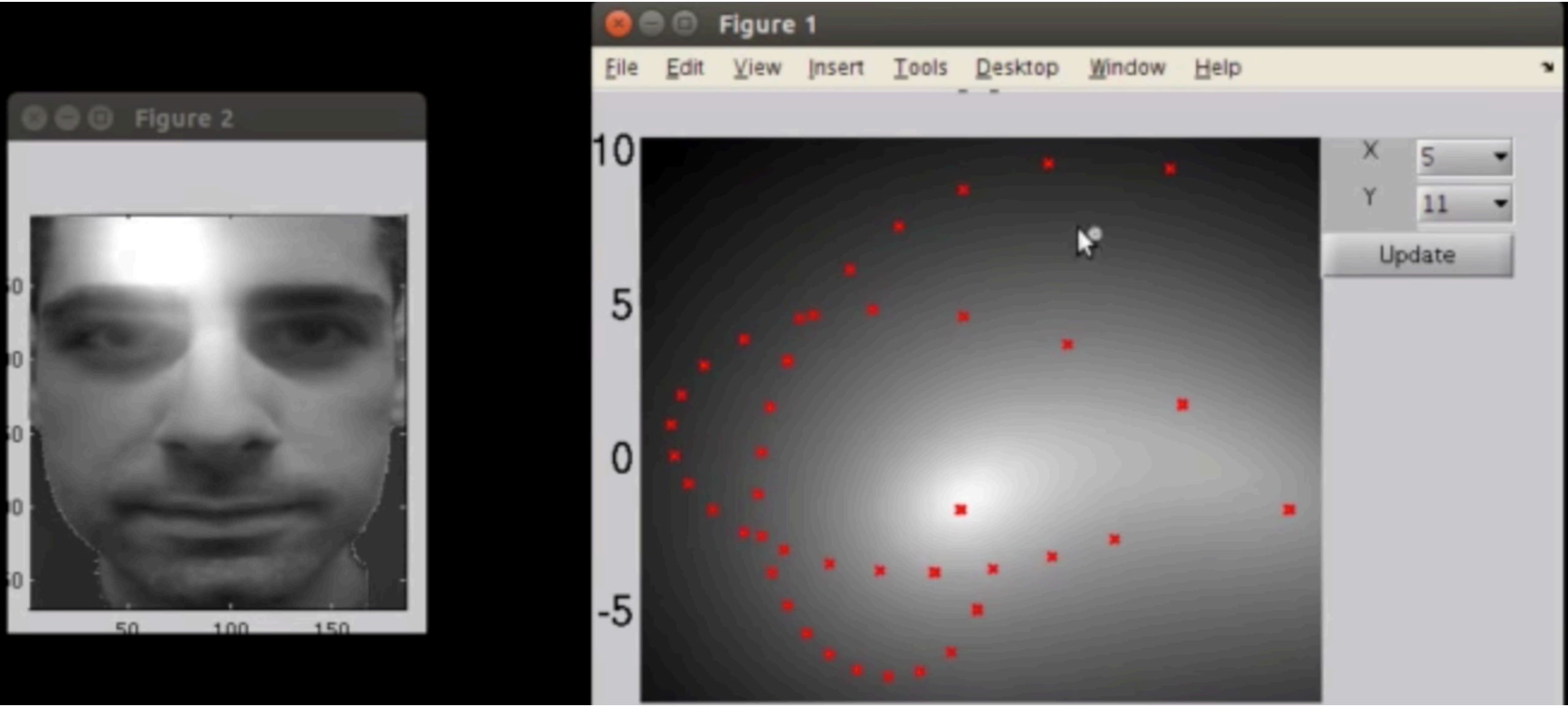
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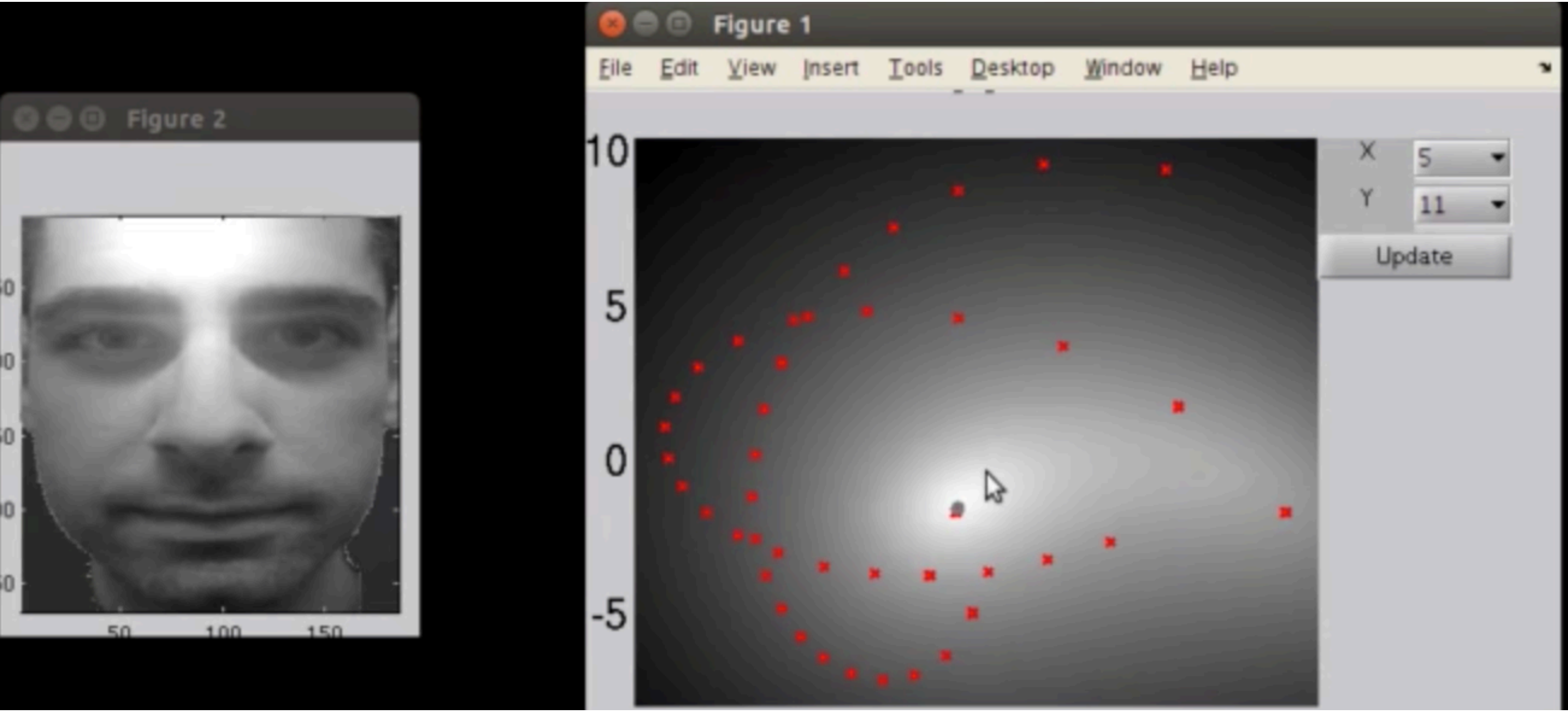
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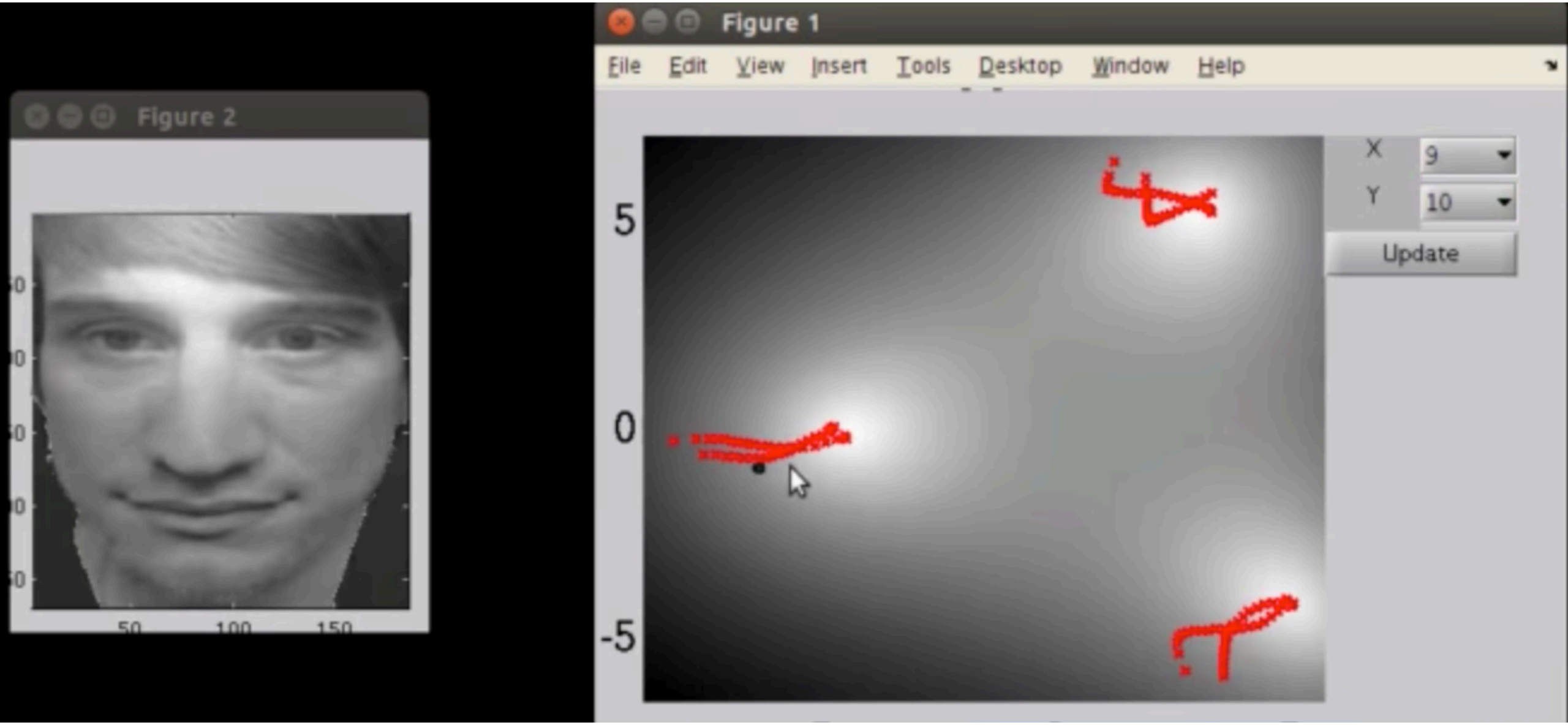
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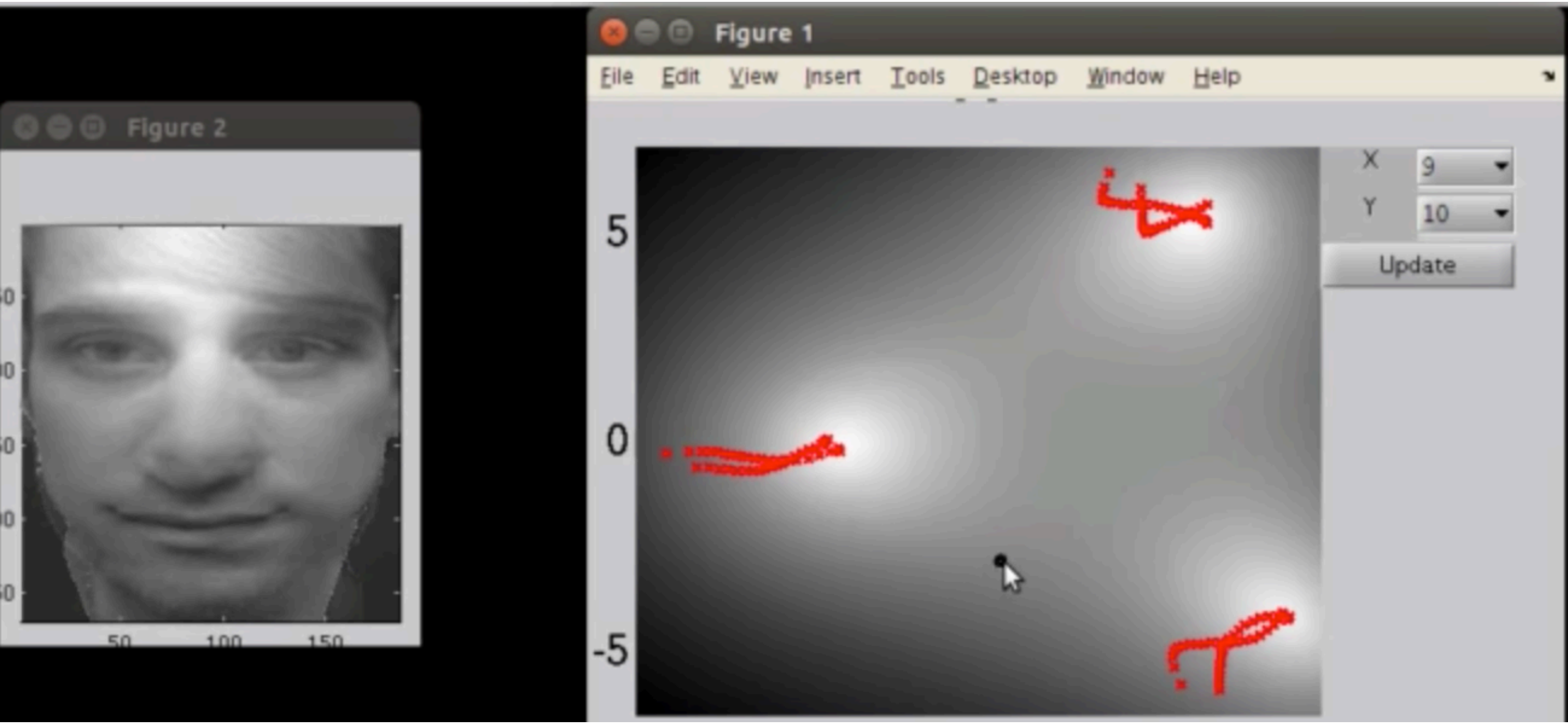
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Update

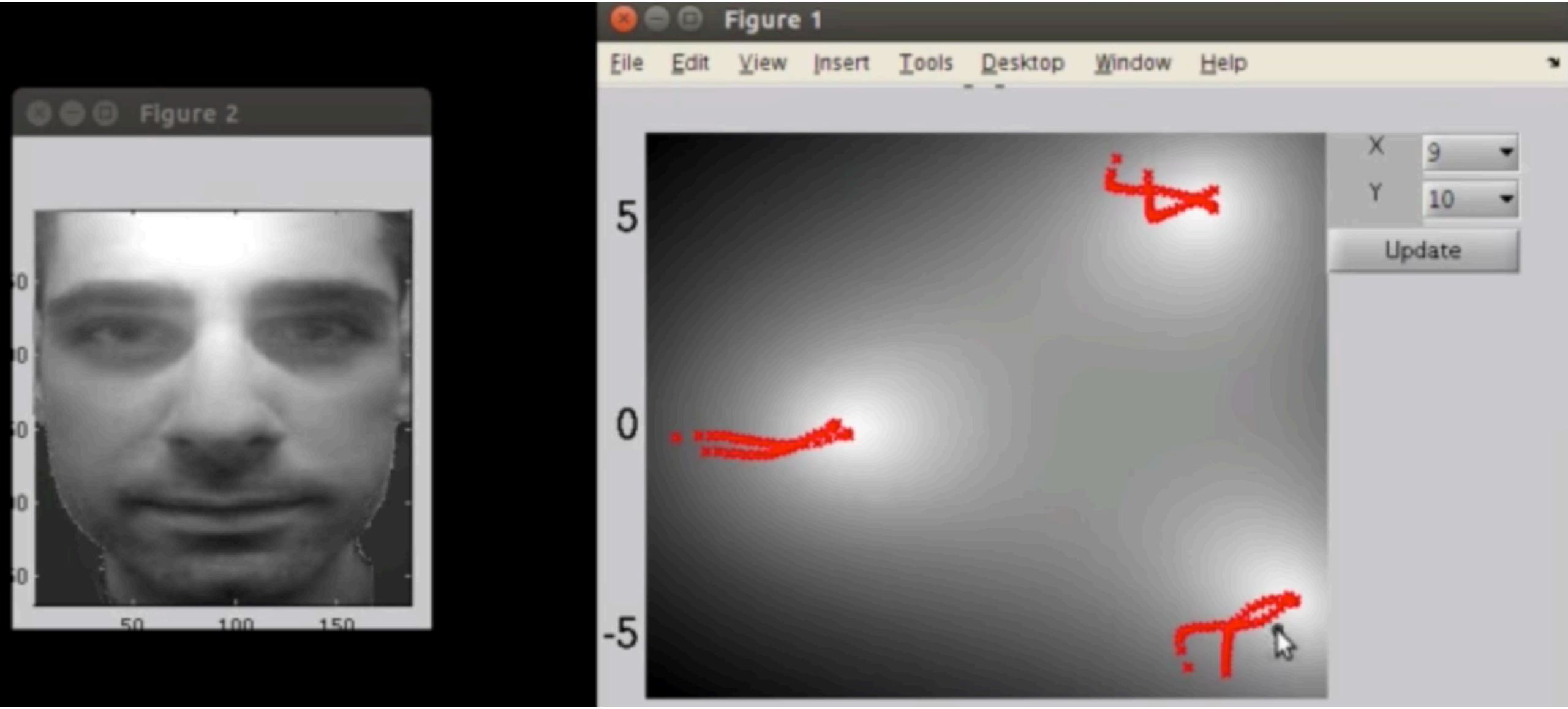
Figure 2
50
100
150
Figure 1
File
Edit
View
Insert
Tools
Desktop
Window
Help
5
0
-5
X
9
Y
10
Update

Properties

- Unsupervised learning possible due to Bayesian regularization
- Very data efficient
- Scalability also possible with newer techniques

- Intractable objective
- Classification is more challenging

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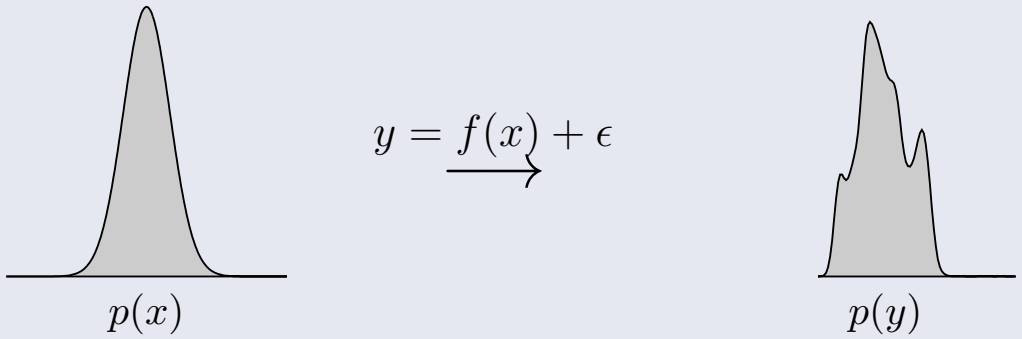
Inference in Deep GPs: uncertainty propagation

- Objective: $p(y|x) = \int_{h_2} \left(p(y|h_2) \int_{h_1} p(h_2|h_1) p(h_1|x) \right)$

- $p(h_2|x) = \int_{h_1, f_2} p(h_2|f_2) \underbrace{p(f_2|h_1)}_{\text{contains } (k(h_1, h_1))^{-1}} p(h_1|x)$

Propagating uncertainty through non-linearities:



Multi-fidelity

Multi-fidelity data

High fidelity observations

Low fidelity observations

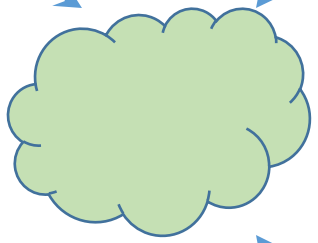
High fidelity simulations

Low fidelity simulations

Multi-fidelity data

High fidelity observations

Low fidelity observations



High fidelity simulations

Low fidelity simulations

X_H

Y_H =

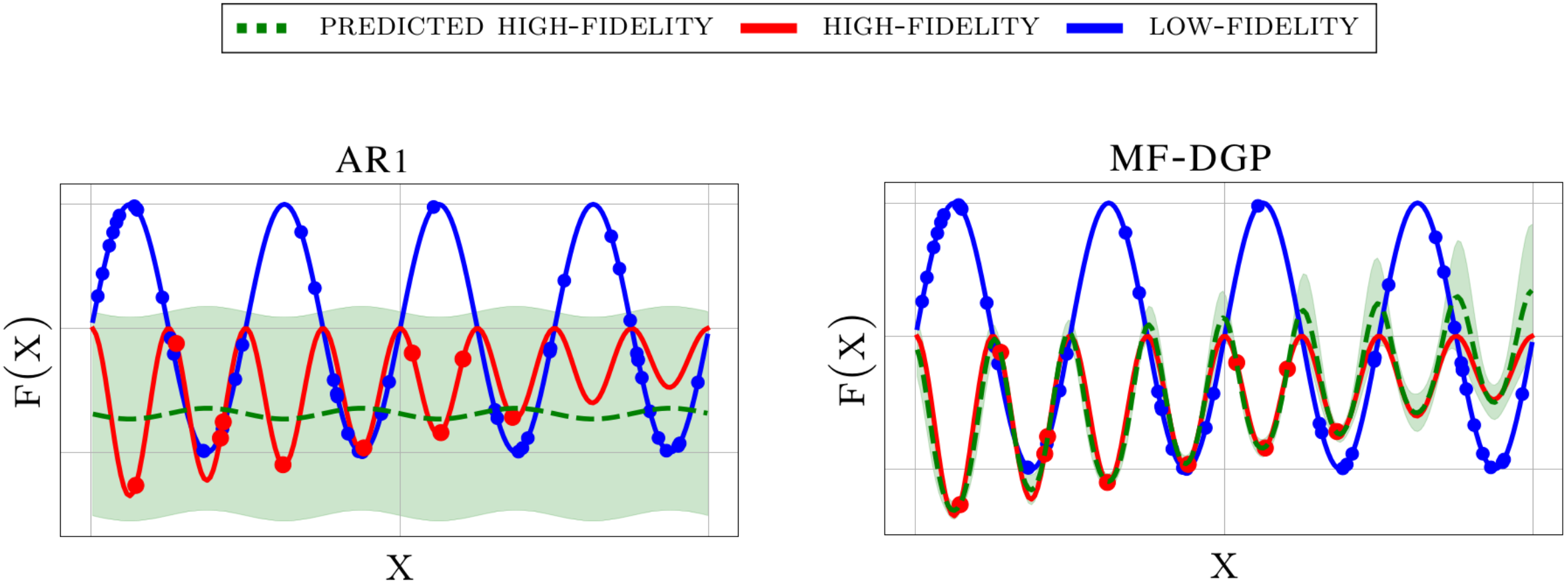
OK
OK
OK
OK
ERROR!
OK
OK

X_L

Y_L =

OK
OK
ERROR!
OK
ERROR!
OK
ERROR!

Fusing information from multiple fidelities



We want to trust the high-fidelity data, where we have them, and where we don't have them to learn how to reason based on low-fidelity data.

Linear GP multi-fidelity

$$f_H(x) = \rho_H f_L(x) + \delta_H(x)$$

f_H High fidelity function (GP)

ρ_H Contribution of low fidelity (const)

f_L Low fidelity function (GP)

δ_H Bias between fidelities (GP)

Kennedy & O'Hagan 2000, Le Gratiet & Garnier 2014

Non-linear multi-fidelity GP => Deep GP

$$f_H(x) = \rho_H f_L(x) + \delta_H(x)$$

Linear relationship between fidelities

$$f_H(x) = \rho_H(f_L(x), x) + \delta_H(x)$$

Non-linear relationship between fidelities
(if ρ is a GP -> overall a deep GP!)

Non-linear multi-fidelity GP => Deep GP

$$f_H(x) = \rho_H f_L(x) + \delta_H(x)$$

Linear relationship between fidelities

$$f_H(x) = \rho_H(f_L(x), x) + \delta_H(x)$$

Non-linear relationship between fidelities
(if ρ is a GP -> overall a deep GP!)

$$\Downarrow$$

$$f_H(x) = g_H(f_L^*(x), x)$$

δ absorbed into g

$f_L^*(x)$ denotes the posterior of the GP modeling the low-fidelity data.

Perdikaris et al., Proc. Royal Society, 2017

Algorithm

1. Train f_L on (X_L, Y_L)
2. Compute $f_L^*(X_H)$
3. Train f_H on $((X_L, Y_L), f_L^*(X_H))$

Predictions

$$p(f_H^*(x^*)) = \int \underbrace{p(f_H(x^*, f_L^*(x^*))|y_H, x_H, x^*)}_{\text{Local posterior from fidelity } H} \underbrace{p(f_L^*(x^*))}_{\text{Predictive from fidelity } L} df_L^*$$