DNN2GP: From Deep Networks to Gaussian Processes

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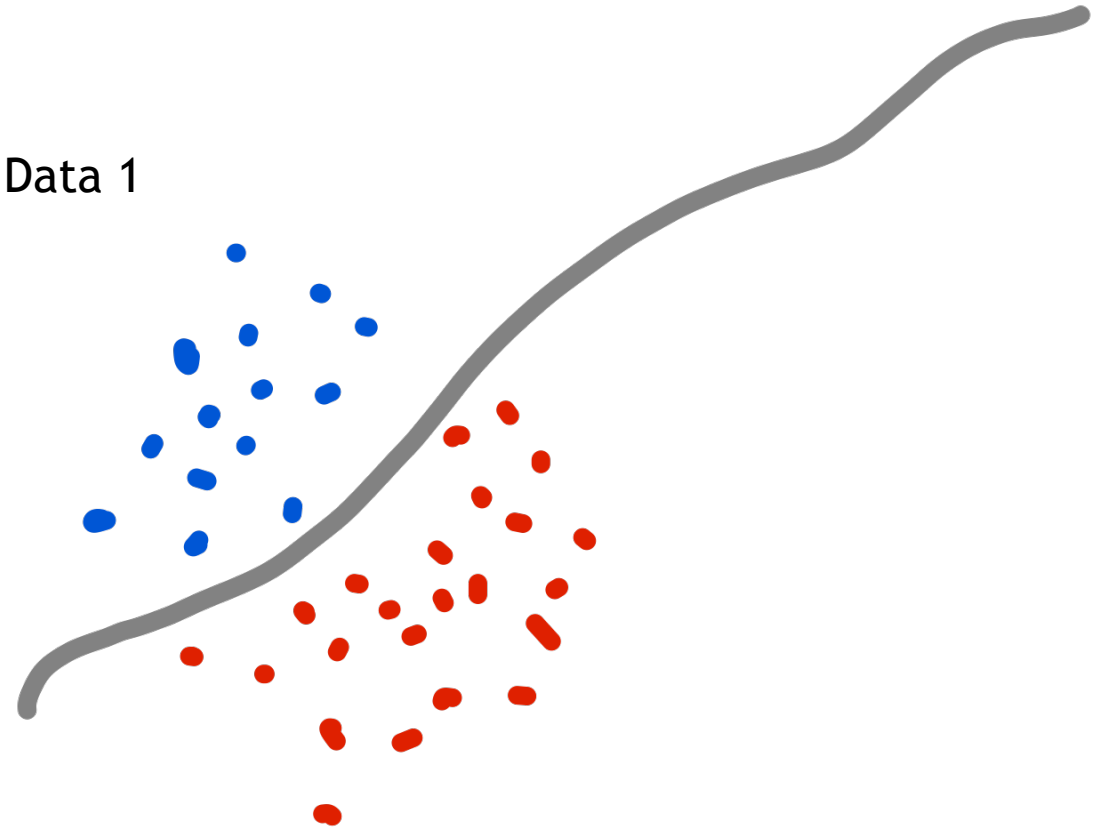
RIKEN Center for AI Project, Tokyo
http://emtiyaz.github.io

Motivation: Life-Long Learning



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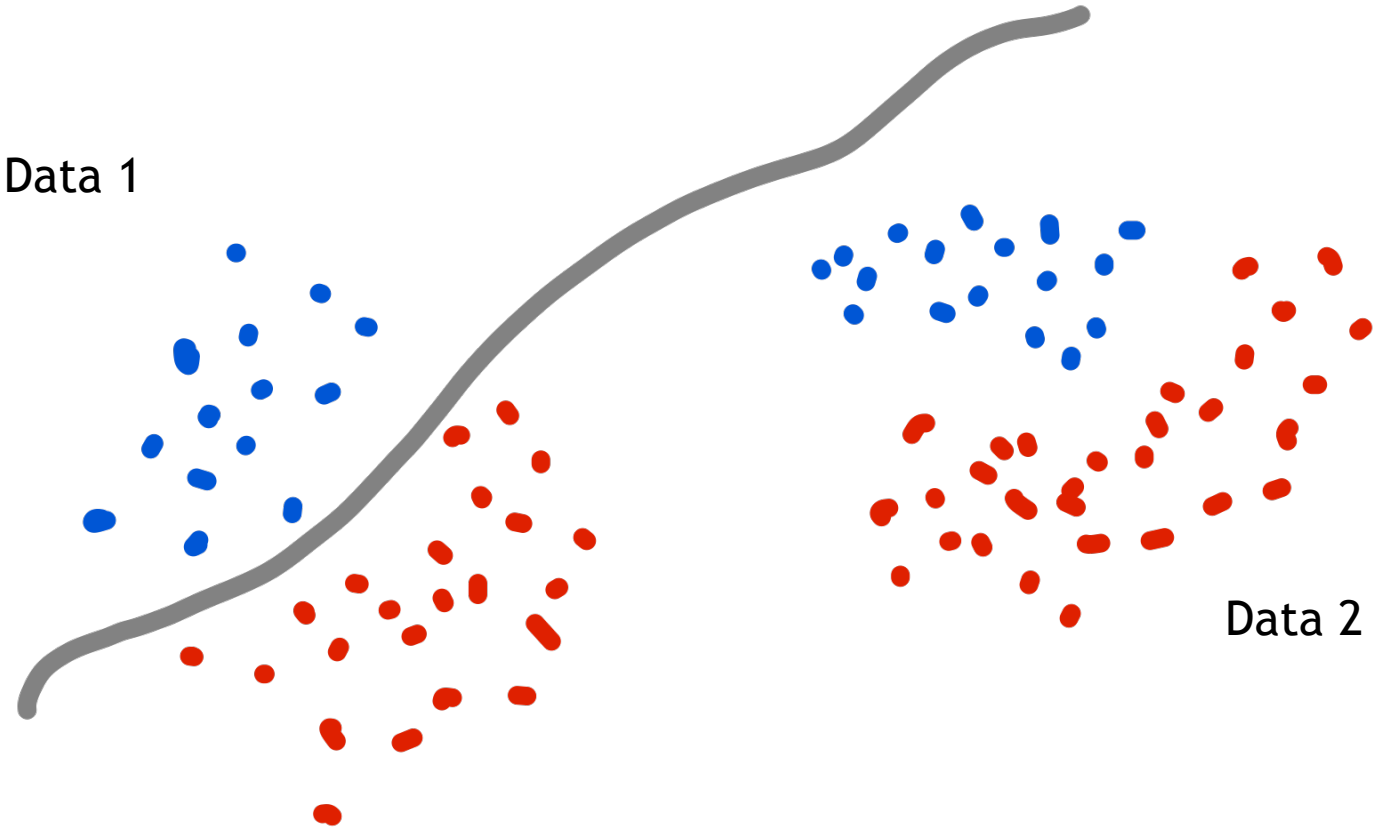

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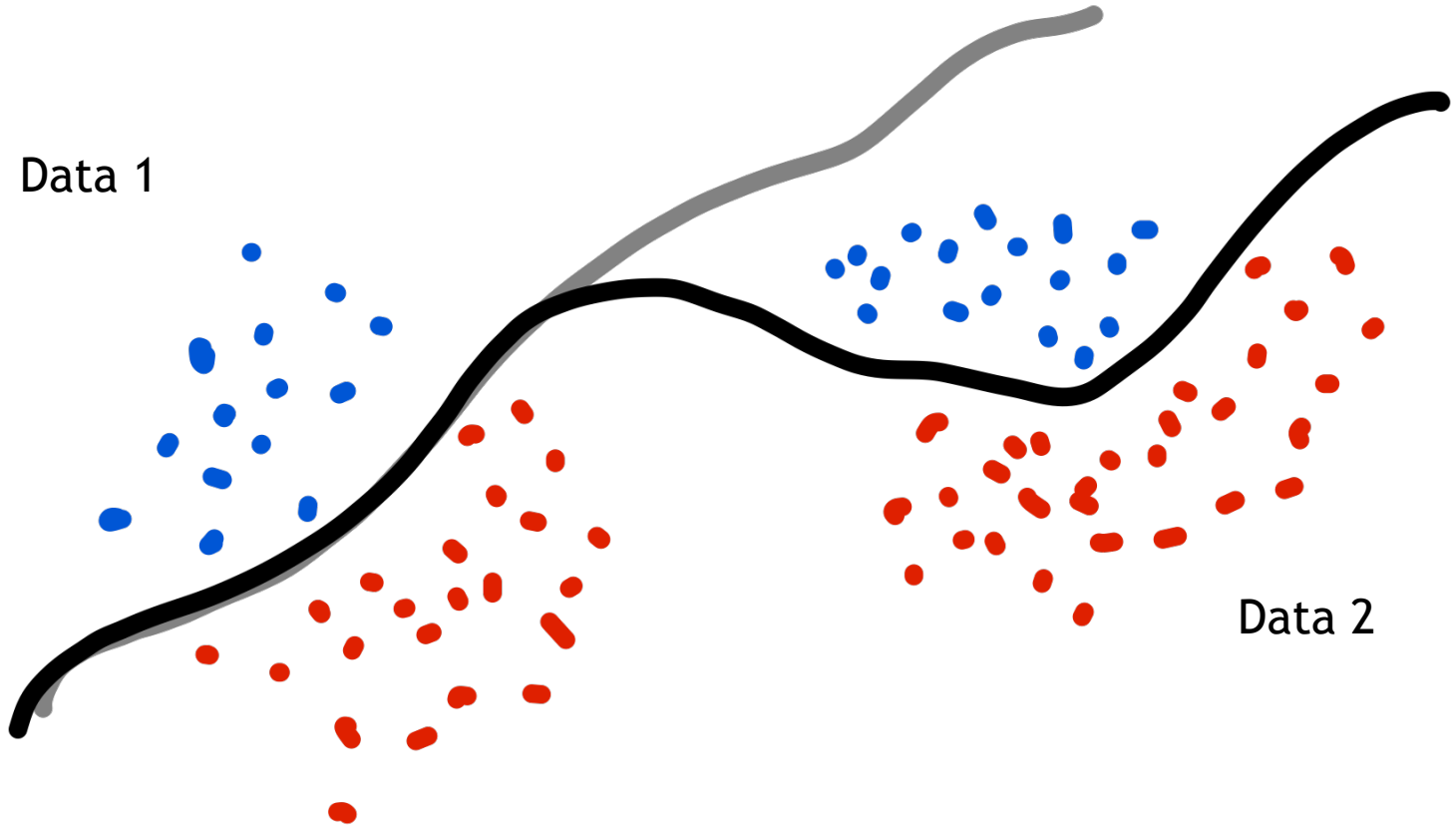

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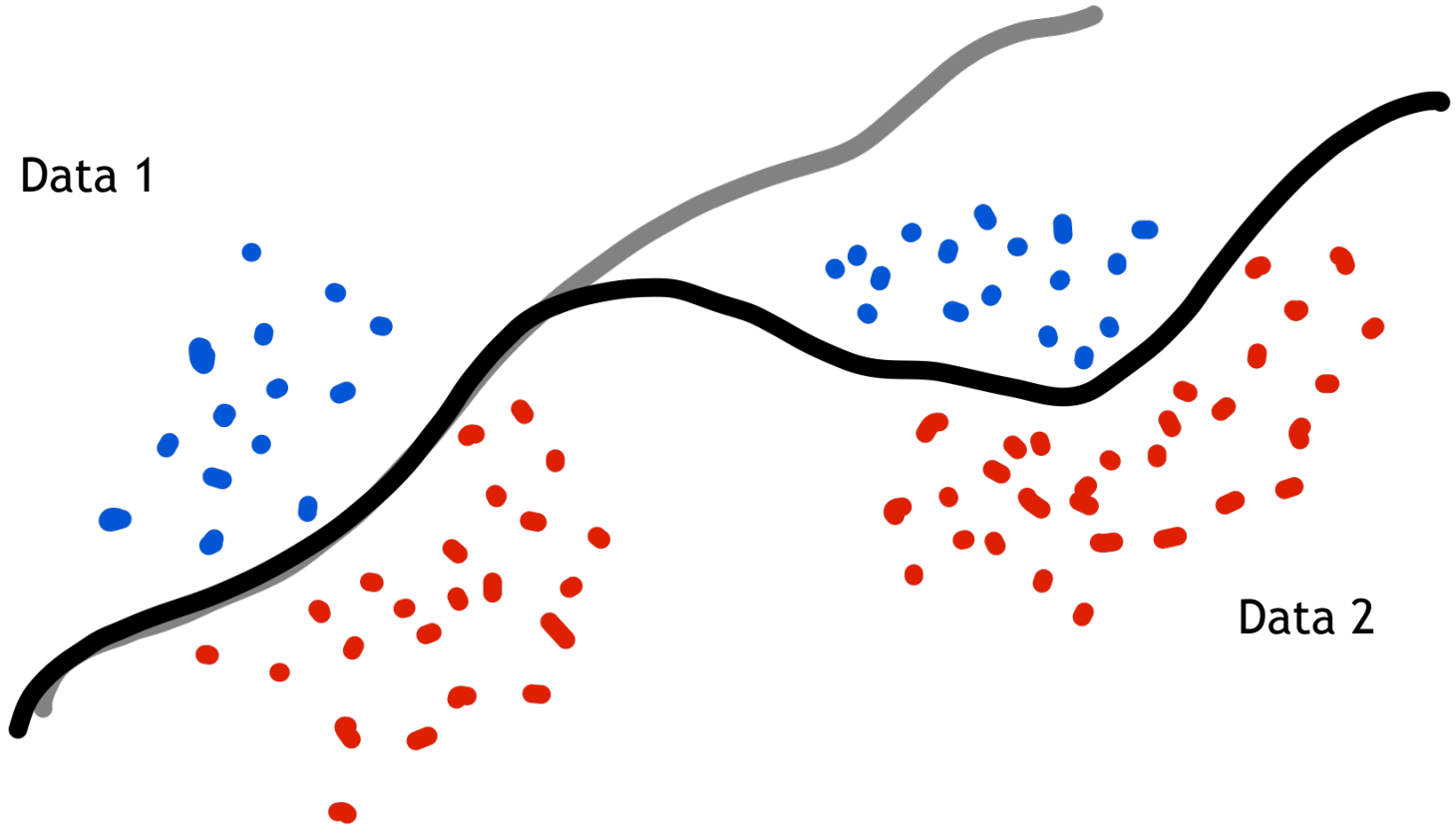

Change the network weights to match the network output (function) at Data 1 while classifying Data 2

Weight-Space vs Function-Space

Weight/parameter space

- Finite dimensional
- Easy to train
  - e.g., SGD is scalable
- Difficult to regularize
  - Actual value of the weights do not matter
  - Complex relationship between network outputs and weights

Function/data space

- Infinite dimensional
- Difficult to train
  - e.g. GP reg is not
- Easy to regularize
  - Properties of the network outputs are easier to specify and interpret.

This Talk

- Connections between the weight and function spaces.
  - Cheap algorithms to train in the weight space while regularizing in the function space.
- Background
  - Linear models and GPs
  - Neural Nets and GPs (requires infinite-width nets)
- DNN2GP
  - Convert trained finite-widths nets to GPs
  - Convert the iterates of DL algorithms to GPs
- Applications to Continual Learning

Linear model and GPs

Gaussian prior on weights induces GP prior on functions

Chapter 2 in Rasmussen and Williams, Gaussian processes for Machine Learning, 2006

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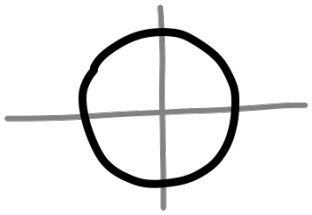
$$w \sim N(0, I)$$



$$\text{function} \quad f(x) = \phi(x)^T w \quad \text{feature}, \ \text{weights}$$

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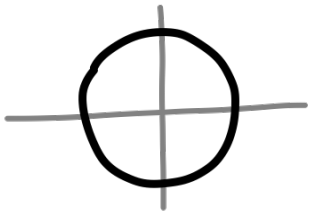
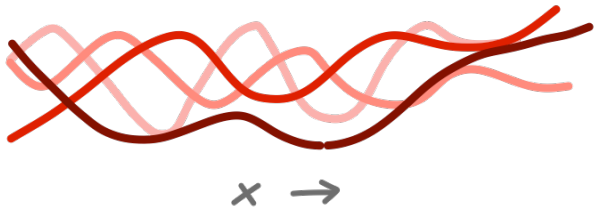


function $f(x) = \phi(x)^T w$ feature weights

$f(x) \sim GP(0, \phi(x)^T \phi(x'))$

mean kernel



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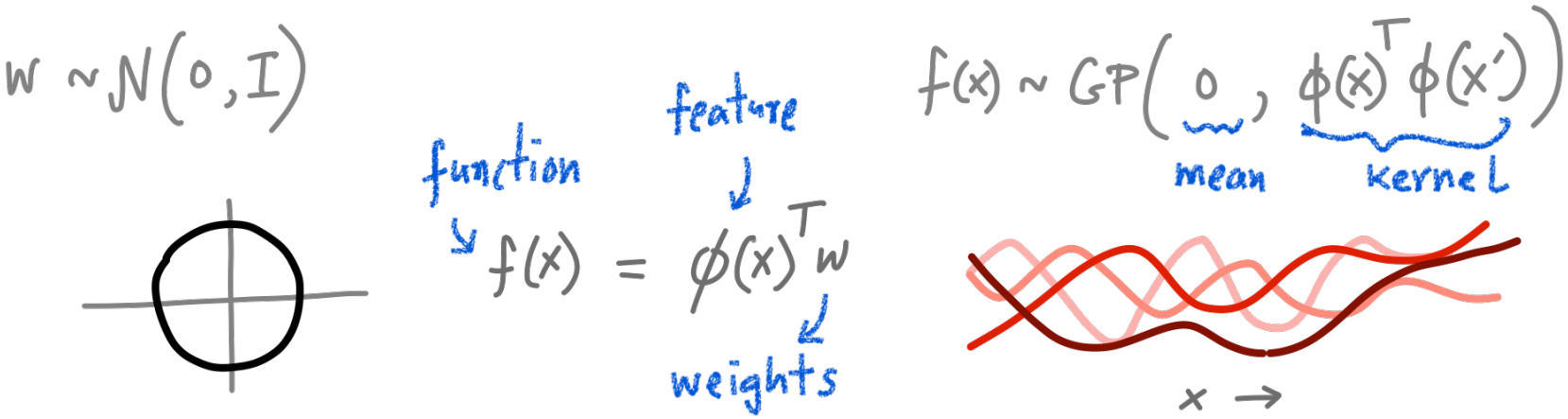

Gaussian posterior on w induces a GP posterior on f

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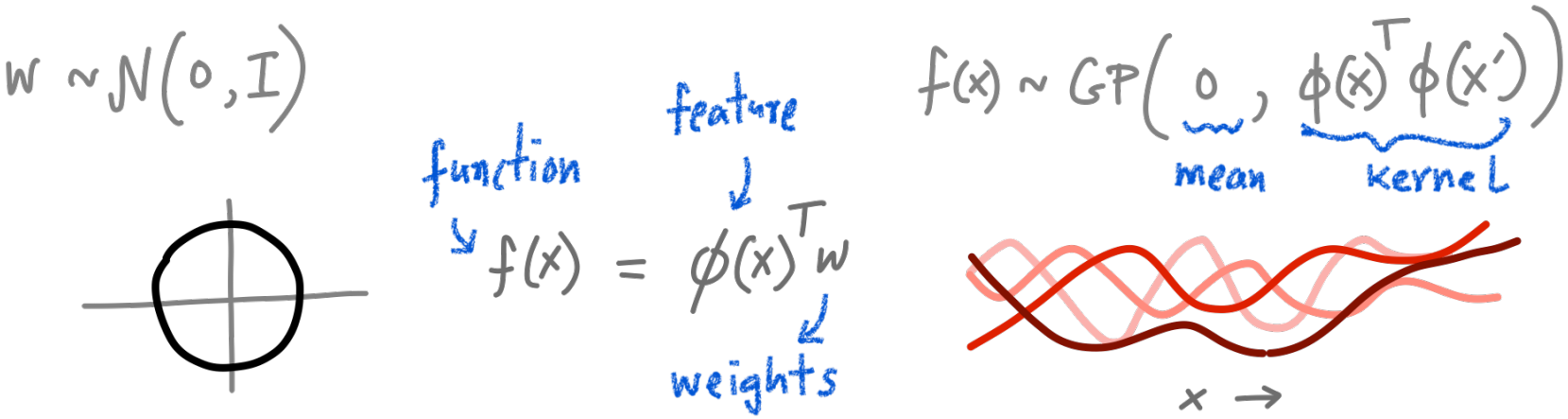

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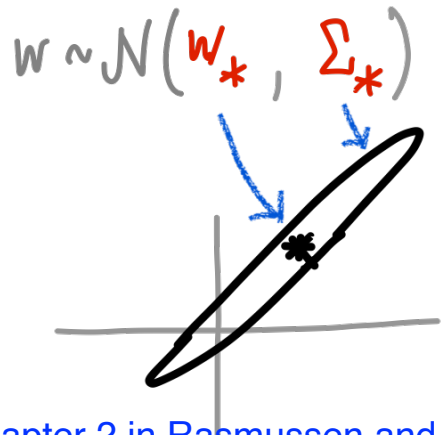

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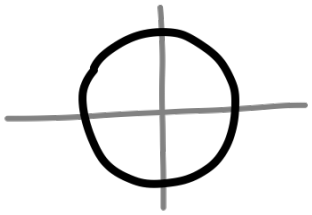
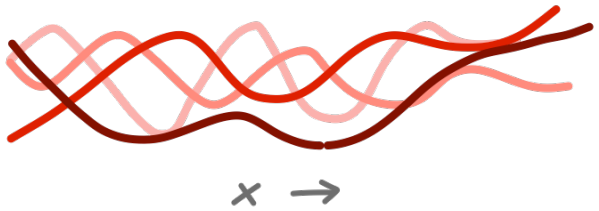


$$\text{function} \quad f(x) = \phi(x)^T w \quad \text{feature} \quad \text{weights}$$

$$f(x) \sim GP\left(\underbrace{0}_{\text{mean}}, \underbrace{\phi(x)^T \phi(x')}_{\text{kernel}}\right)$$



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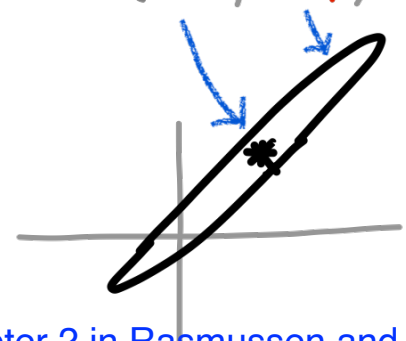
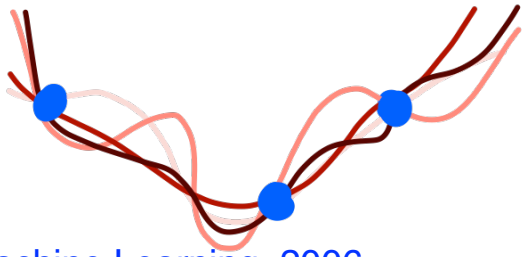


$$f(x) \sim GP\left(\phi(x)^T w_*, \phi(x)^T \Sigma_* \phi(x')\right)$$



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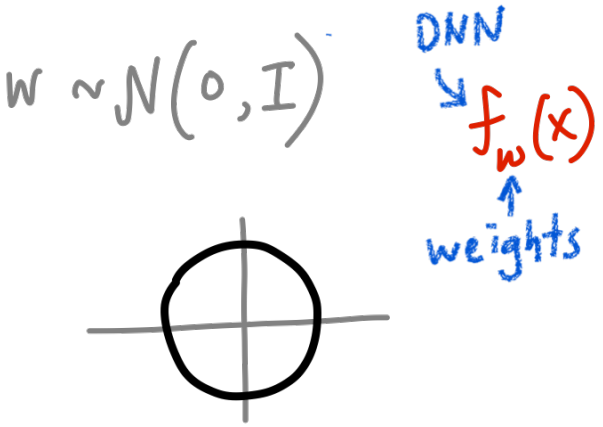

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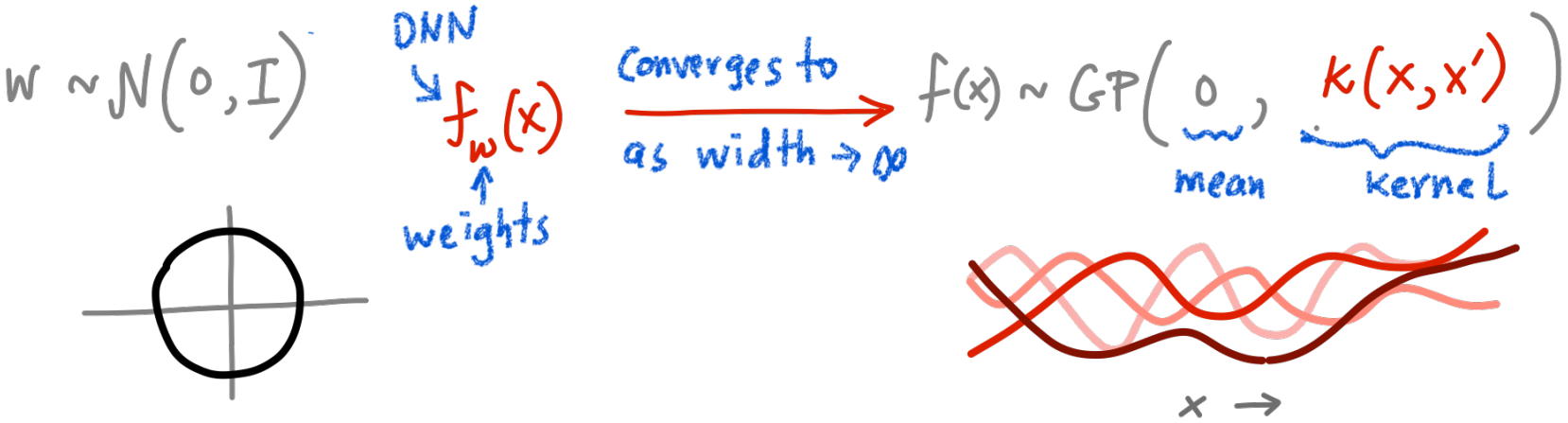

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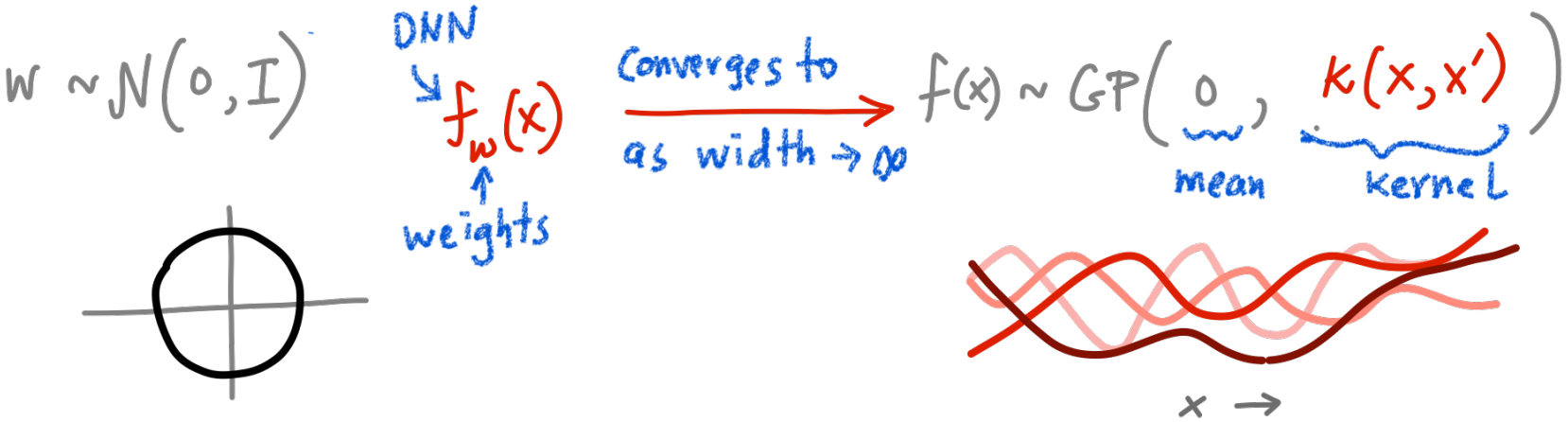

Q: Does this hold at finite width? And for posteriors?

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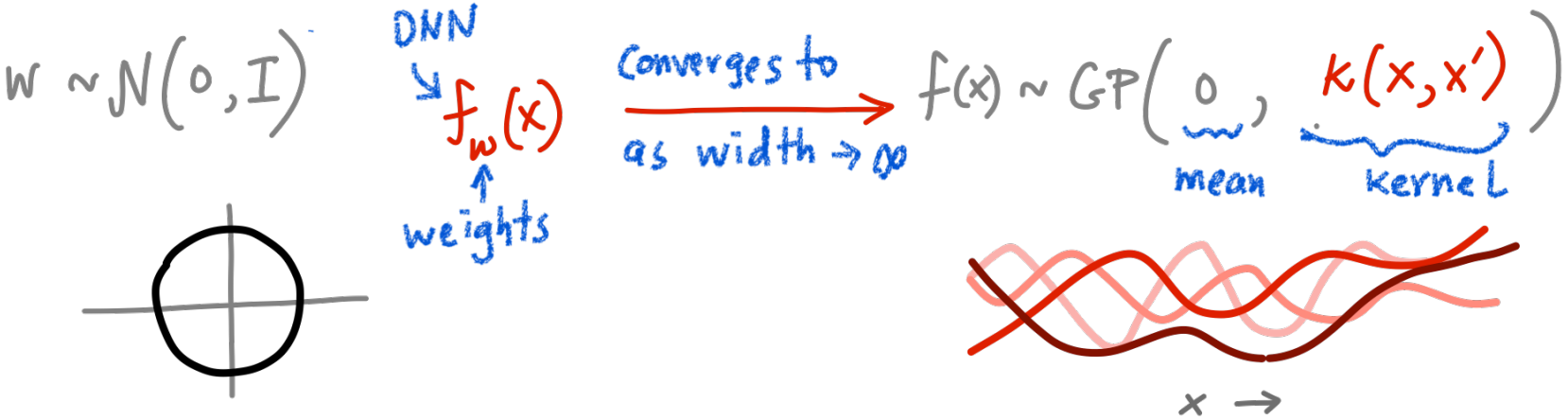

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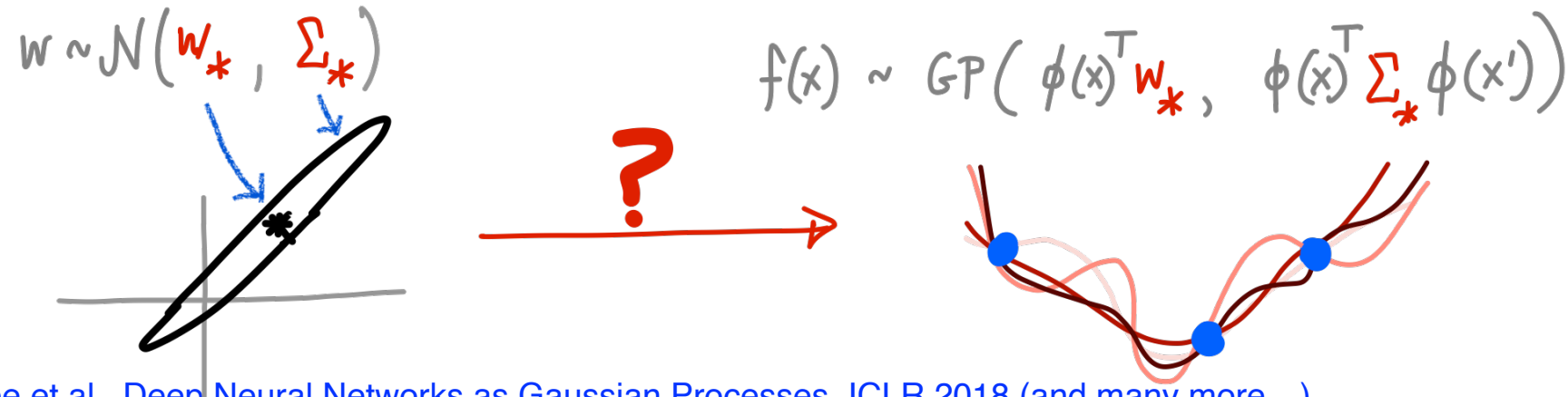

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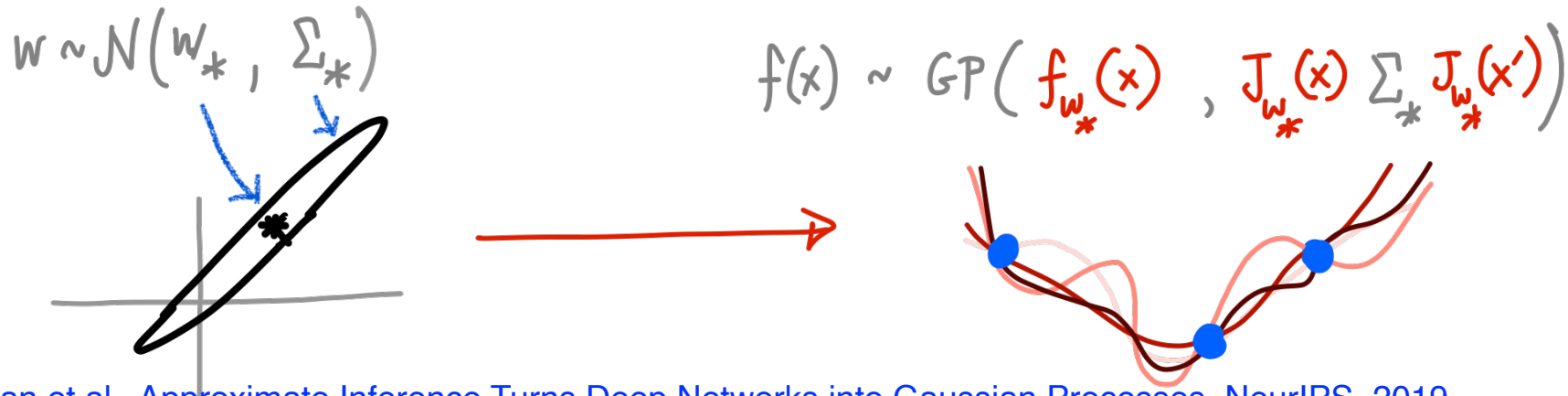
DNN2GP for regression

Using DNN2GP, we can convert a trained network into GP



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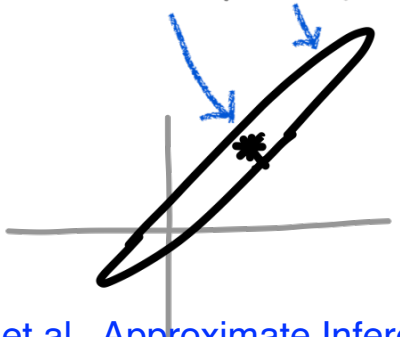
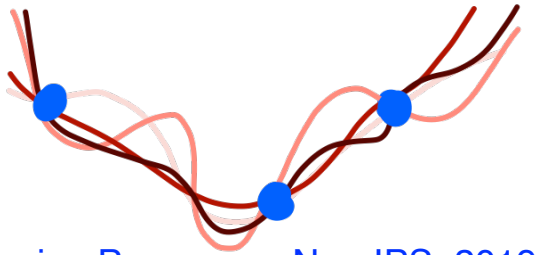
Using DNN2GP, we can convert a trained network into GP

$$w_* = \arg\min_w \sum_{i=1}^{N} \underbrace{\left(y_i - f_w(x_i)\right)^2}_{\text{squared loss}} + \underbrace{\delta\, w^T w}_{L_2 \text{ prior}}$$

$$w \sim \mathcal{N}(w_*, \Sigma_*)$$

$$f(x) \sim GP\left(f_{w_*}(x),\ J_{w_*}(x)\, \Sigma_*\, J_{w_*}(x')\right)$$





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$$\Sigma_*^{-1} = \sum_{i=1}^{N} \nabla_w f_{w_*}(x_i)\, \underbrace{\nabla_w f_{w_*}(x_i)^T}_{J_{w_*}(x_i)^T \leftarrow \text{Jacobian}} + \delta I \quad \leftarrow \text{Gauss-Newton Curvature}$$

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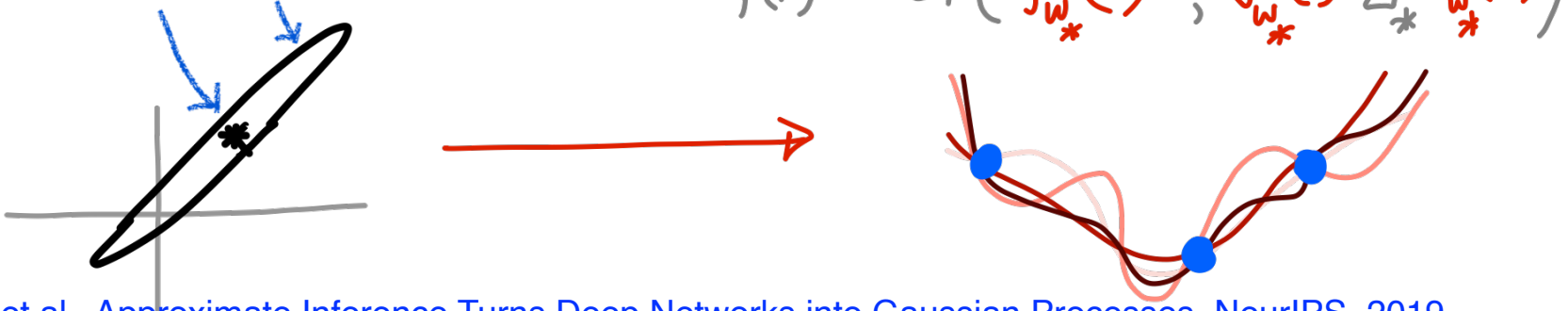

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DNN2GP Generalization

This generalizes to twice differentiable loss and priors

$$w_* = \arg\min_w \sum_{i=1}^{N} \underbrace{\ell(y_i, \sigma(f_w(x_i)))}_{\text{Diff. loss}} + \underbrace{\delta R(w)}_{\text{Convex prior}}$$

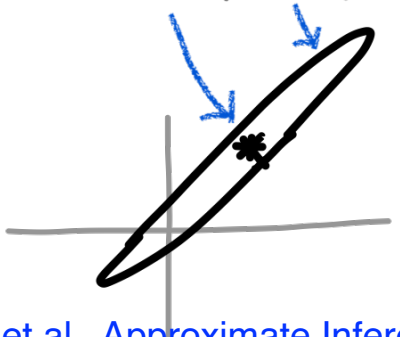
(Link function: σ)

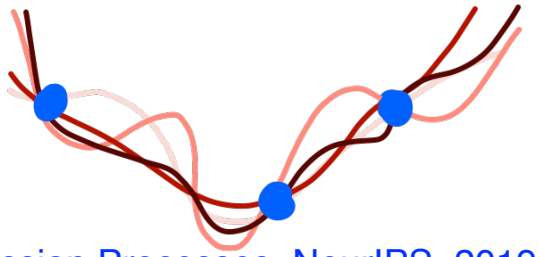
$$\Sigma_*^{-1} = \sum_{i=1}^{N} \nabla_w f_{w_*}(x_i) \underbrace{\nabla^2_{ff} \ell(\,)}_{\Lambda_{w_*}(x)} \nabla_w f_{w_*}(x_i)^T + \delta \nabla^2_{ww} R(w)$$

← Generalized Gauss-Newton Curvature

$$w \sim \mathcal{N}(w_*, \Sigma_*)$$

$$f(x) \sim \mathrm{GP}\left(\sigma\left(f_{w_*}(x)\right), \lambda^{(x)}_{w_*} J_{w_*}(x)\, \Sigma_*\, J_{w_*}(x') \lambda^{(x)}_{w_*}\right)$$





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Deep Learning as GP inference

Iterations of algorithms too can be written as GP inference

$$w_{t+1} \leftarrow w_t - \rho \underbrace{(S_t + \delta I)^{-1}}_{\Sigma_t} \left[\sum_{i \in M} g_i\right] \leftarrow \text{minibatch gradient}$$

$$\text{Scale matrix} \rightarrow S_{t+1} \leftarrow (1-\beta) S_t + \sum_{i \in M} J_{w_t}(x_i) J_{w_t}(x_i)^T \leftarrow \text{minibatch GN curvature}$$

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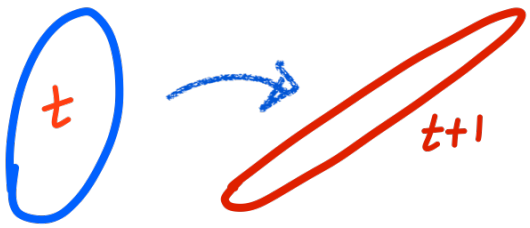
$\mathcal{N}(w_t, \Sigma_t)$

$\mathcal{N}(w_{t+1}, \Sigma_{t+1})$



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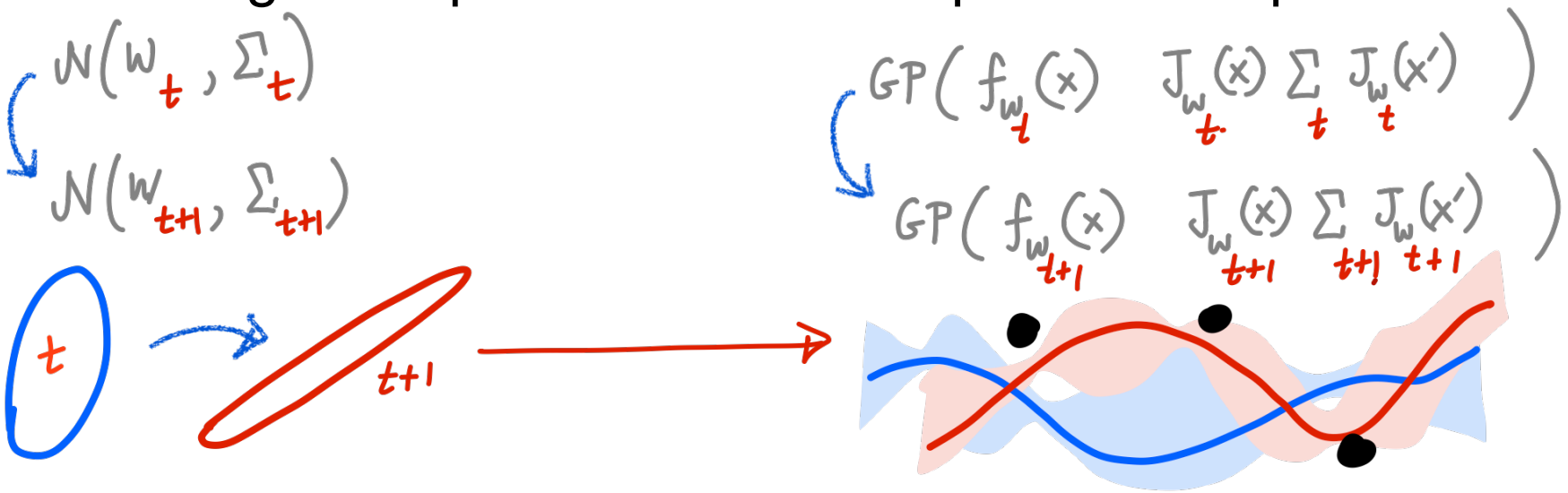

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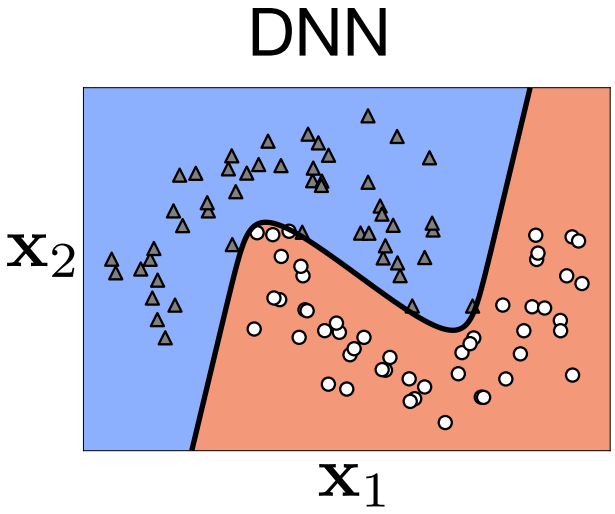
Outline of the derivation



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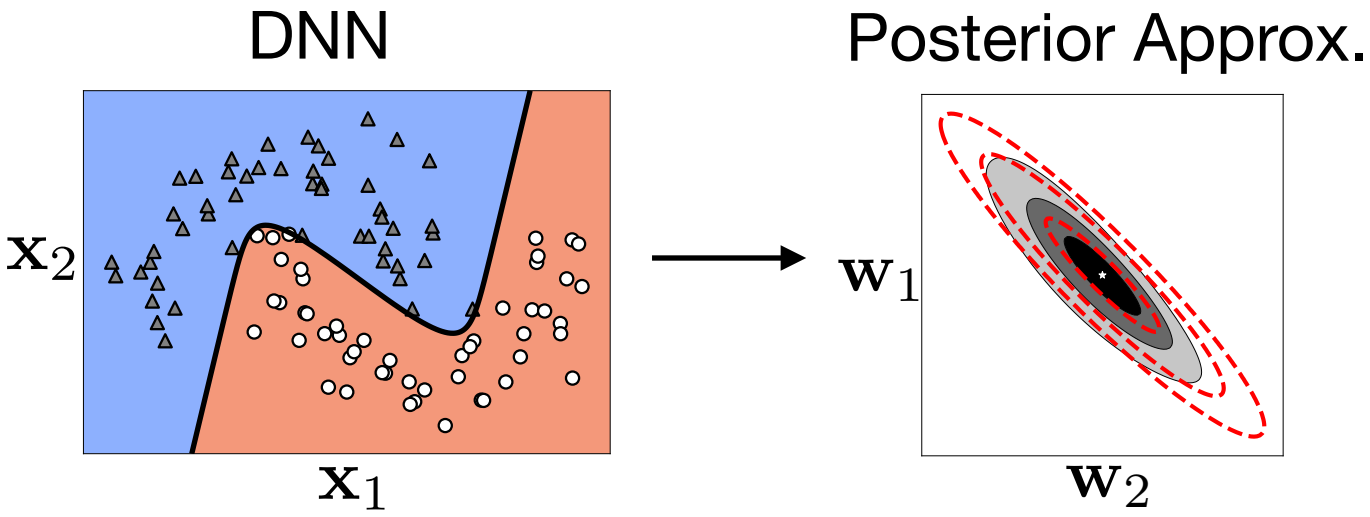

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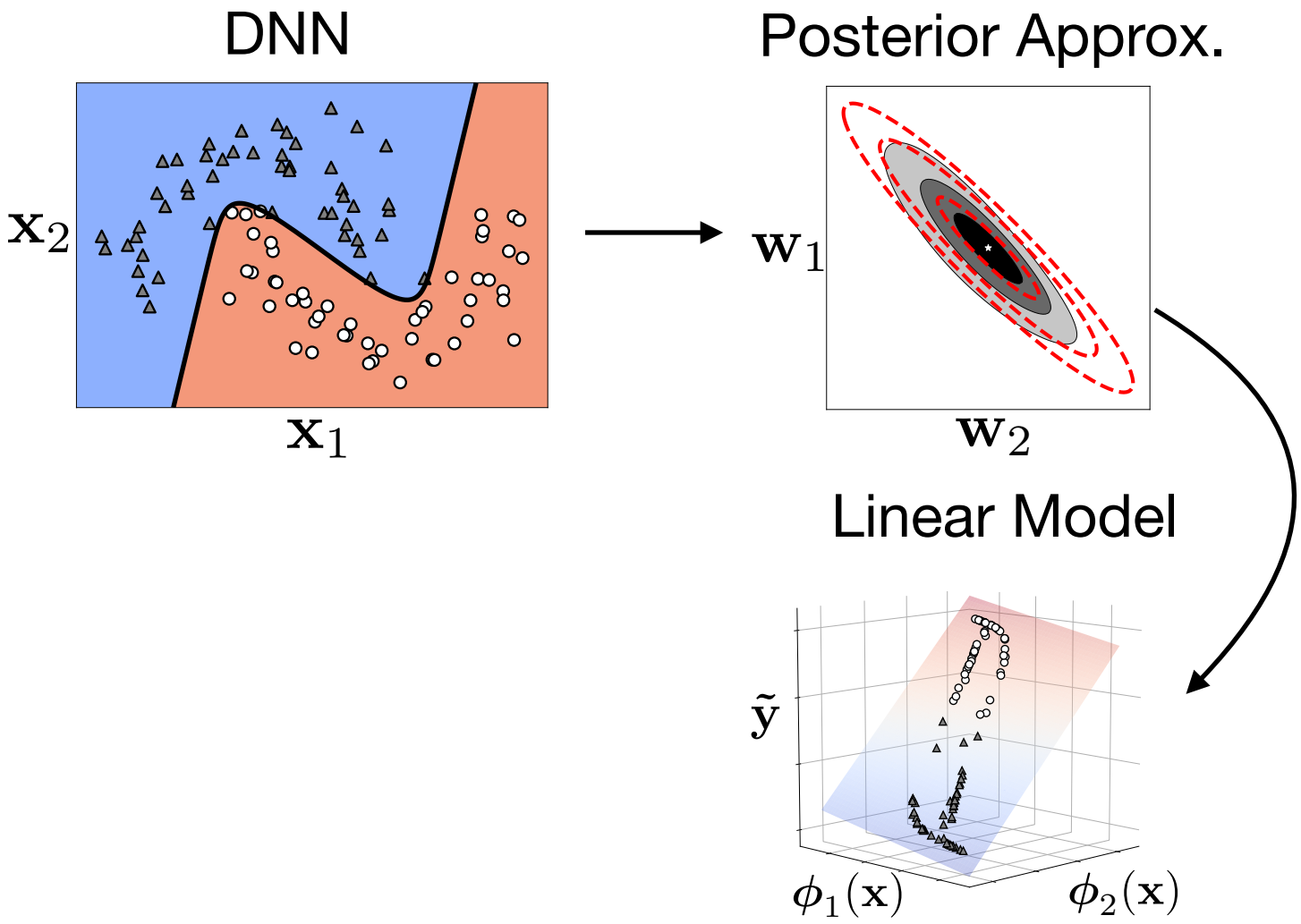

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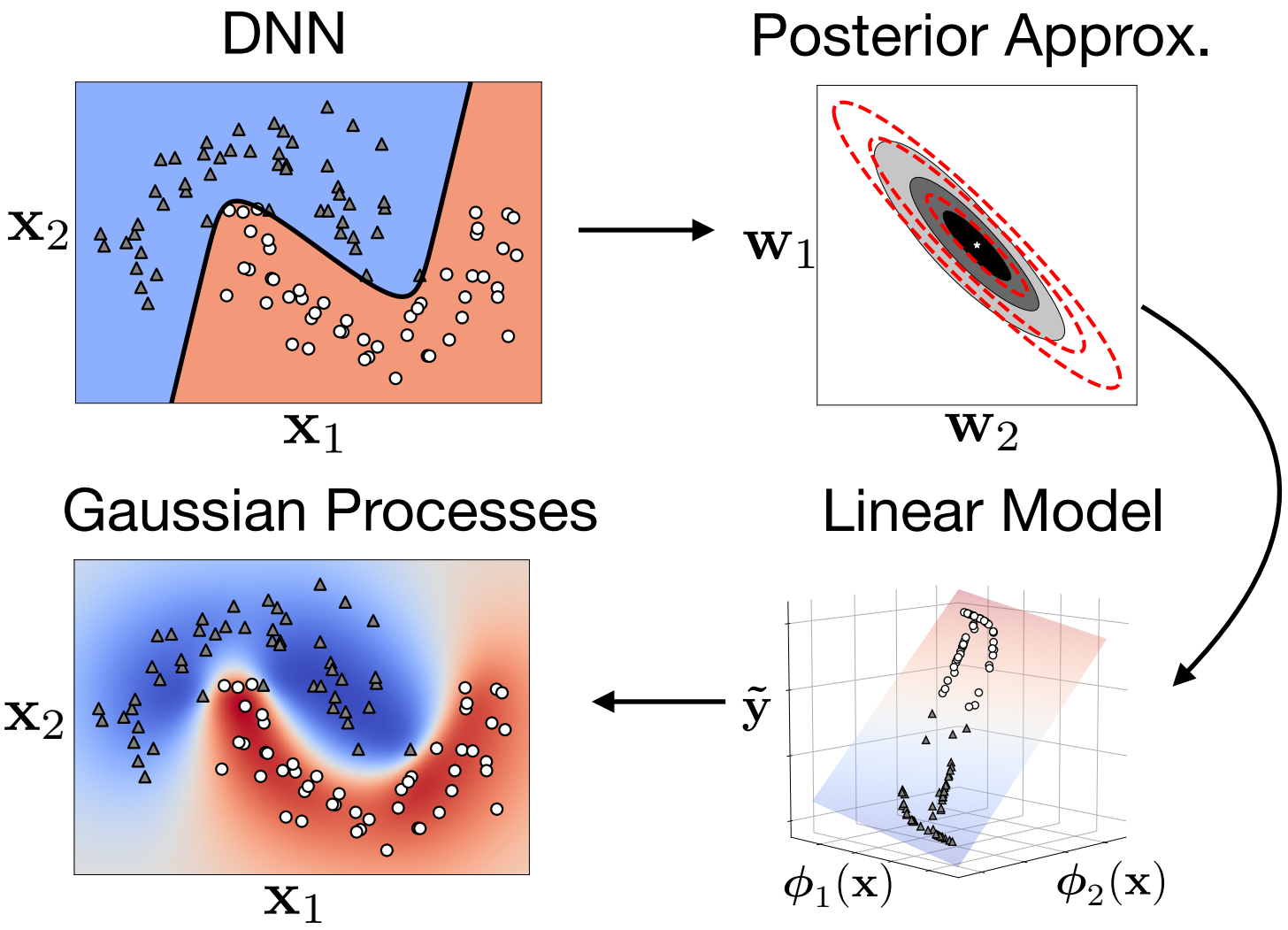

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Application to Continual Learning

Standard Deep Learning

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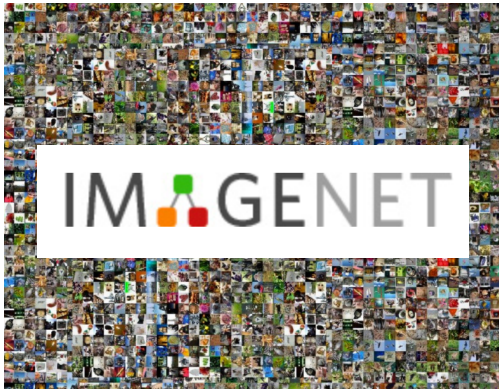
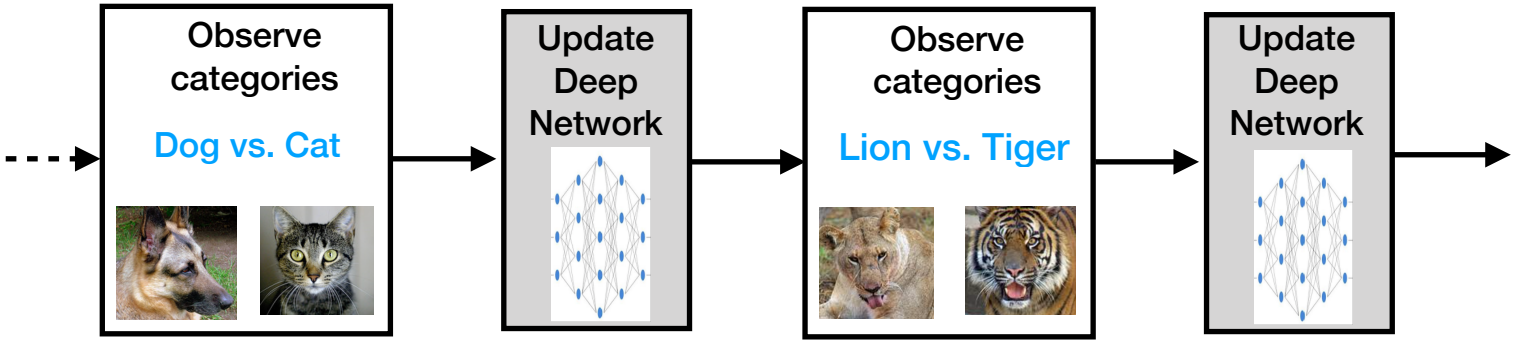


Continual Learning: past classes never revisited



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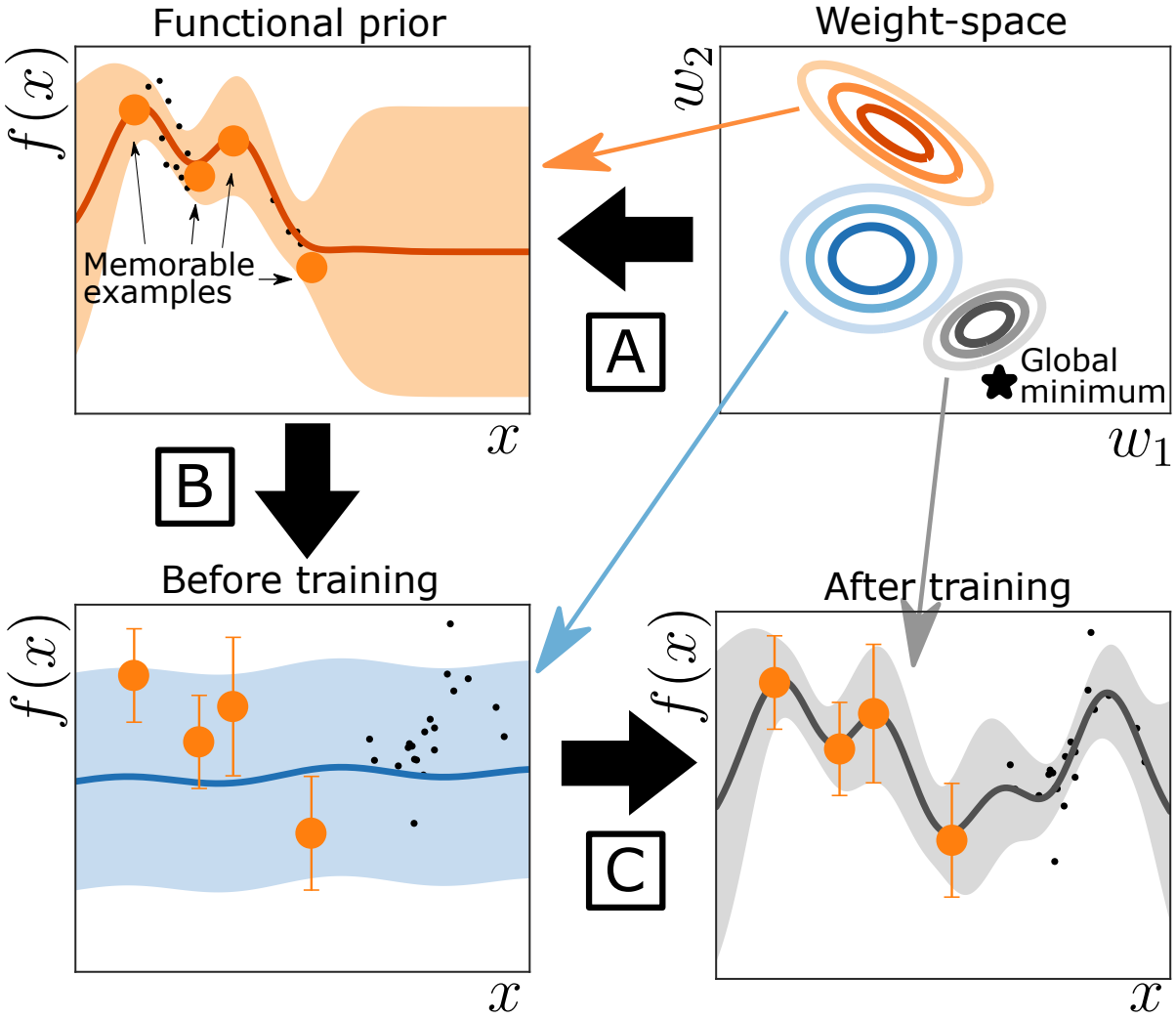
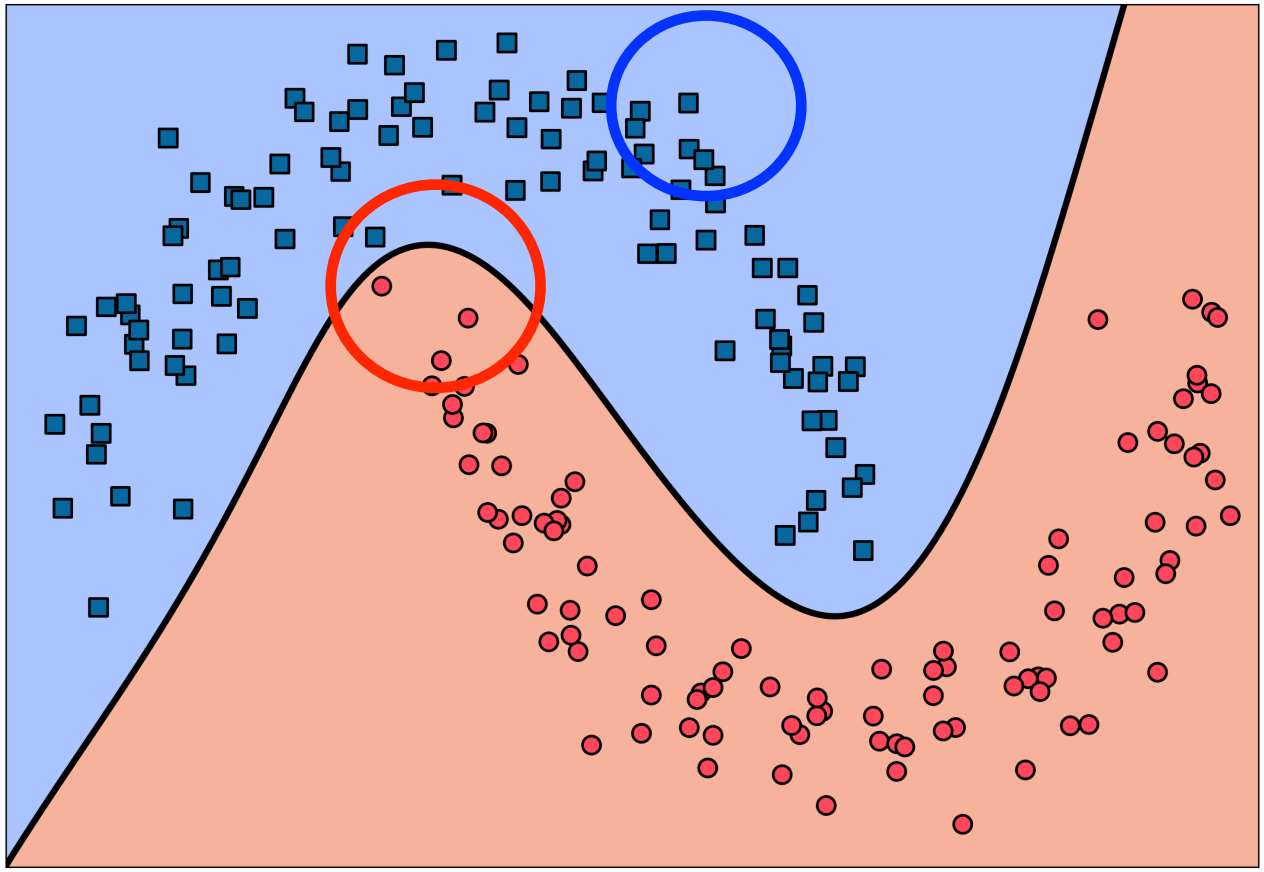
FROMP in Three Steps



Pan et al. Continual Deep Learning by Functional Regularisation of Memorable Past, ArXiv 2020

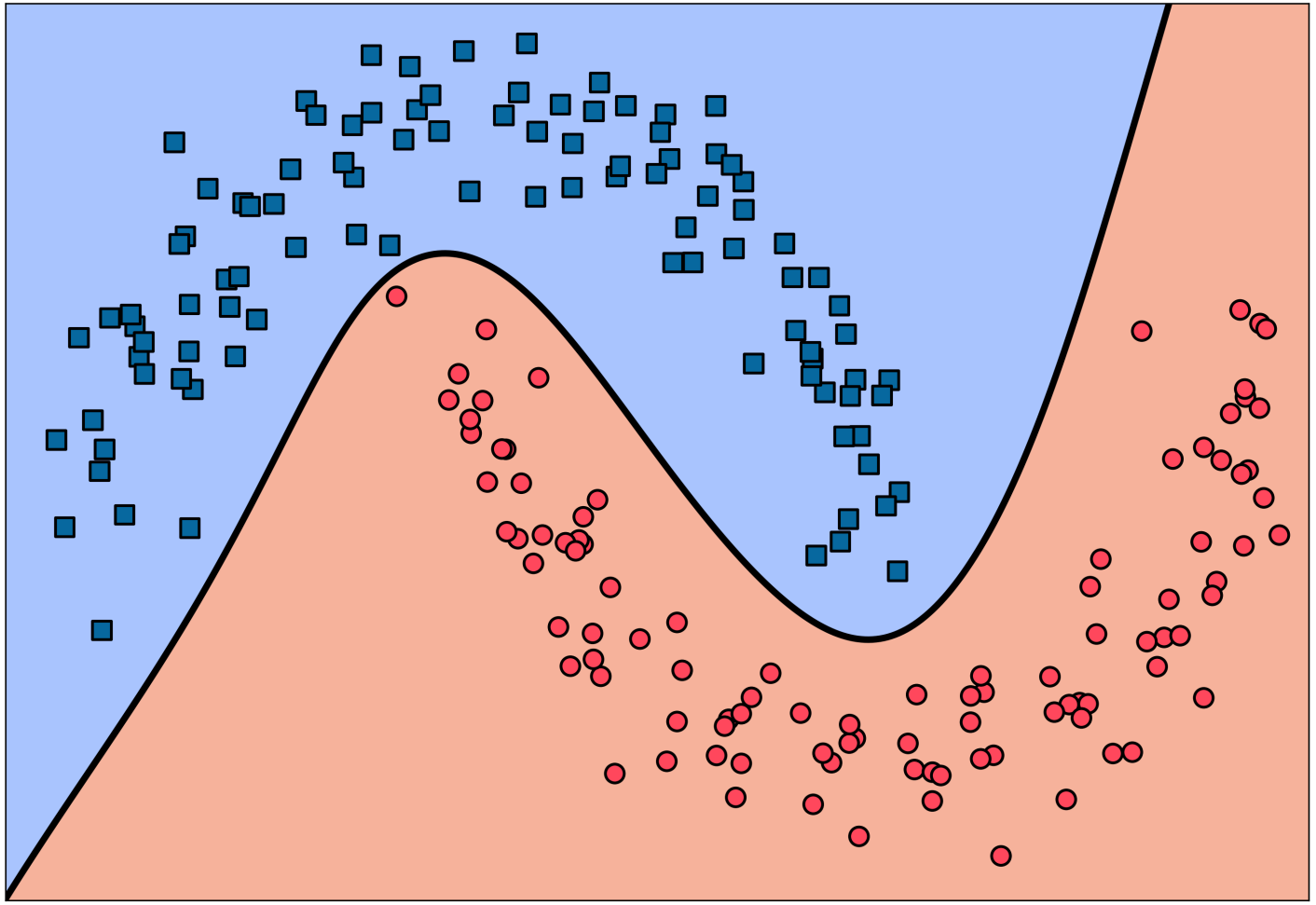
Memorable Past

Which examples are most relevant for the classifier? Red circle vs Blue circle.



Model view vs Data view

DNN2GP provides a measure of relevance



Model view

(By Roman Bachmann)

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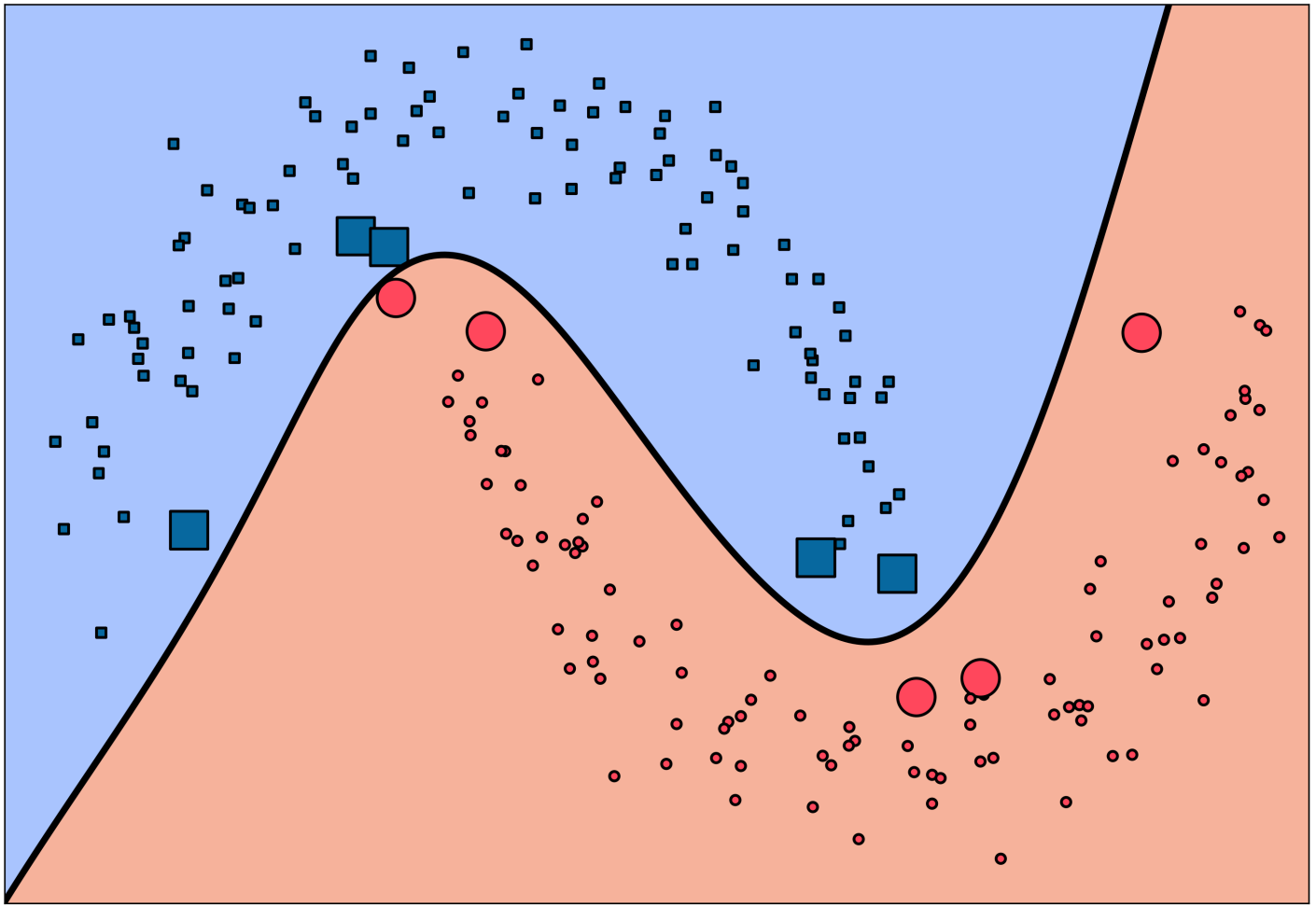

Data view

(By Roman Bachmann)

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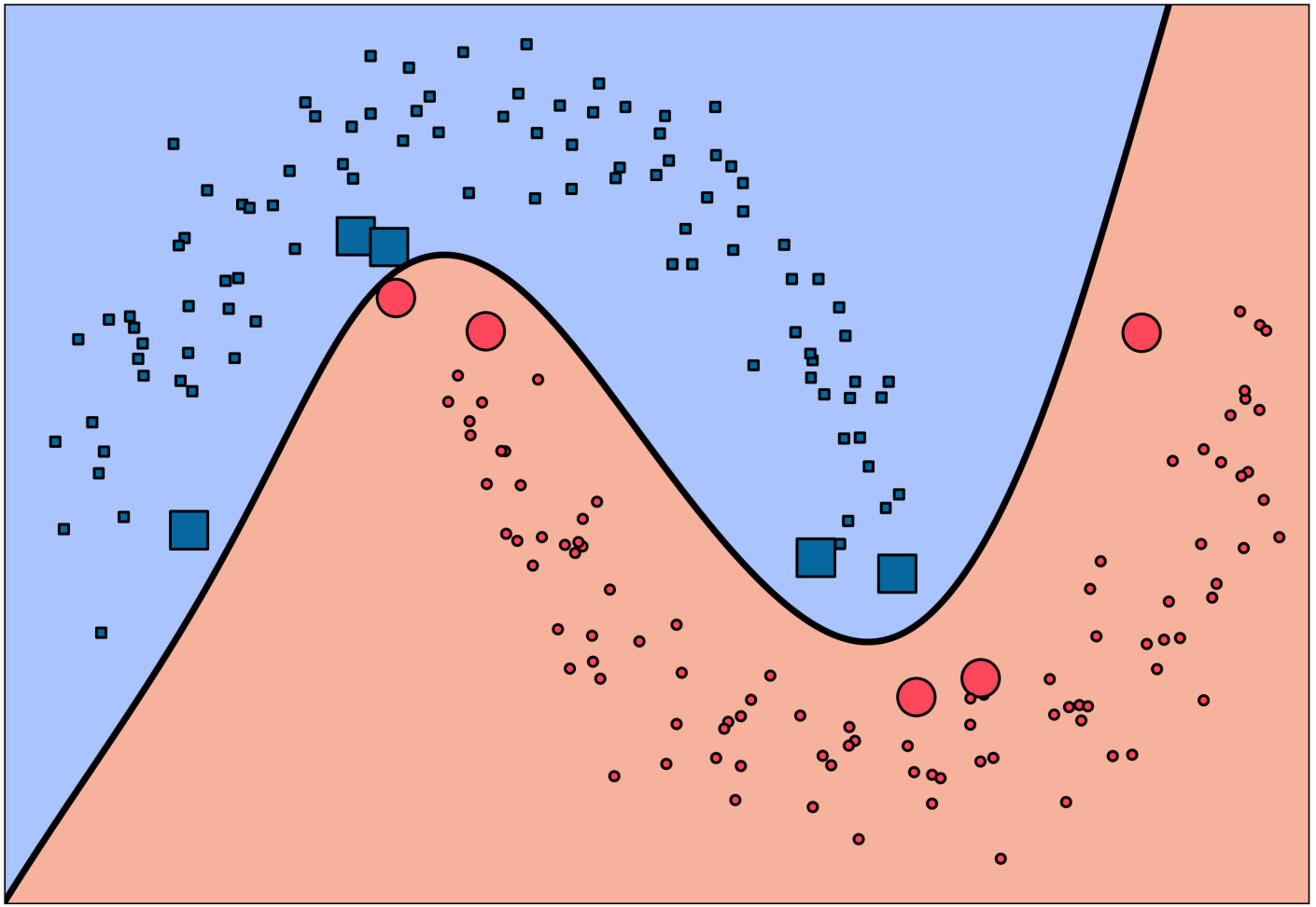


Data view

Sort

$\pi_i(x)$

$= \nabla^2_{ff} \ell(y_i, f_0(x_i))$

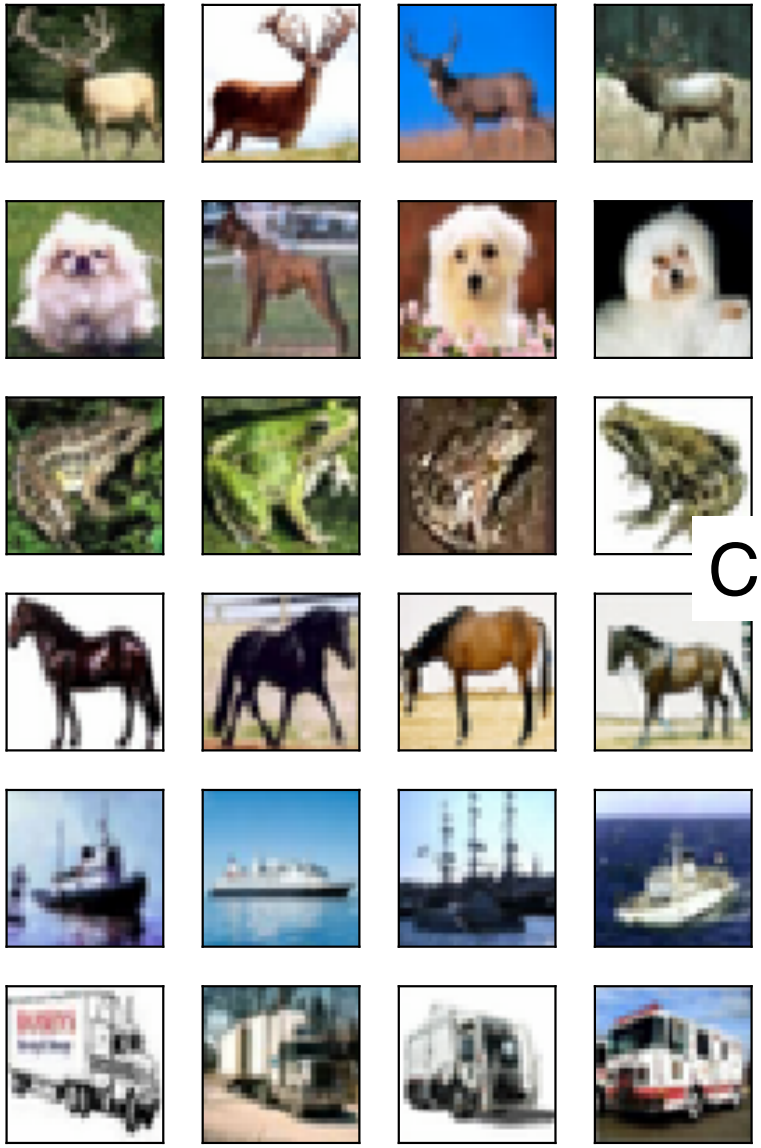
(By Roman Bachmann)

Least Relevant

MNIST

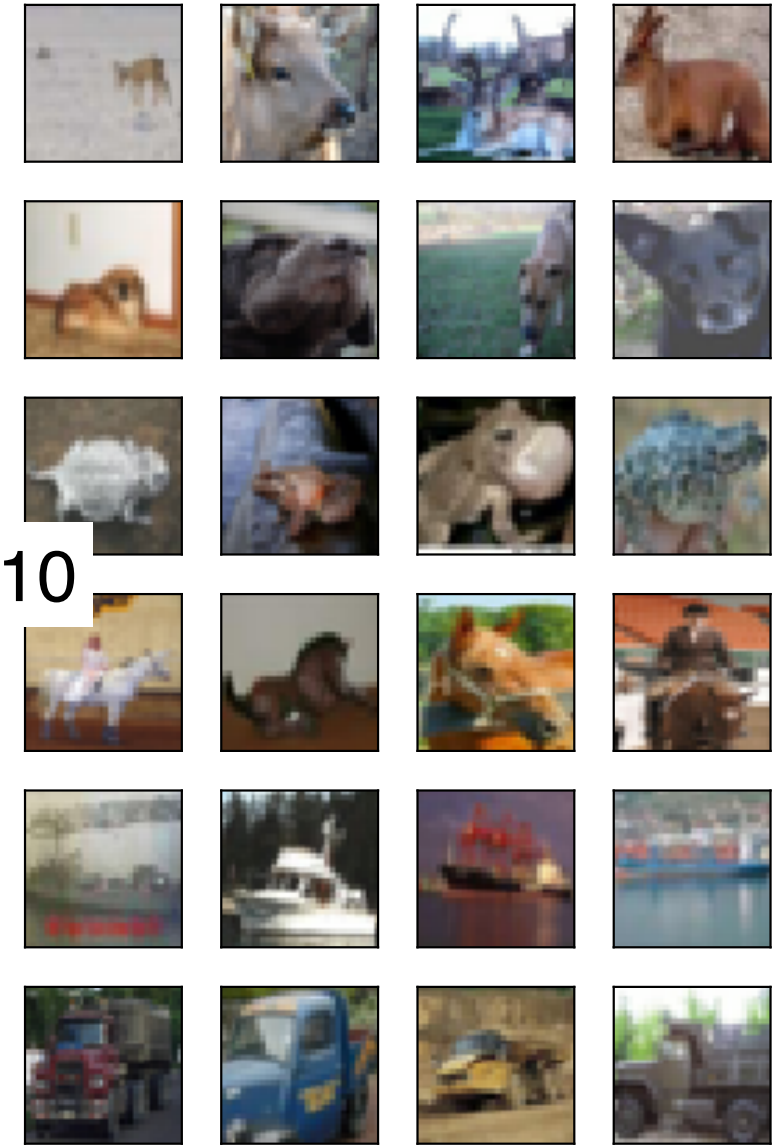
Most Relevant

Least Relevant



CIFAR-10

Most Relevant



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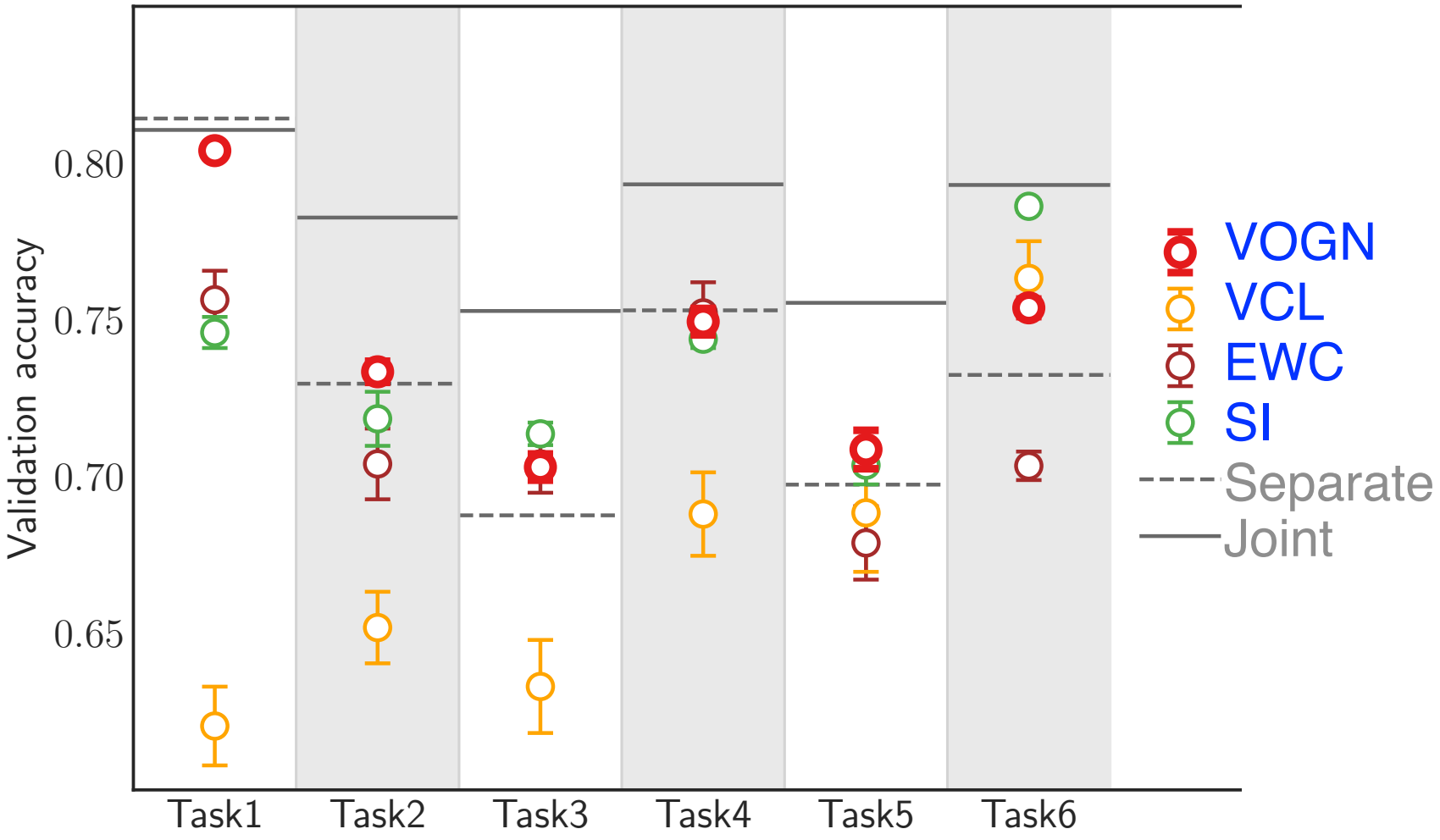
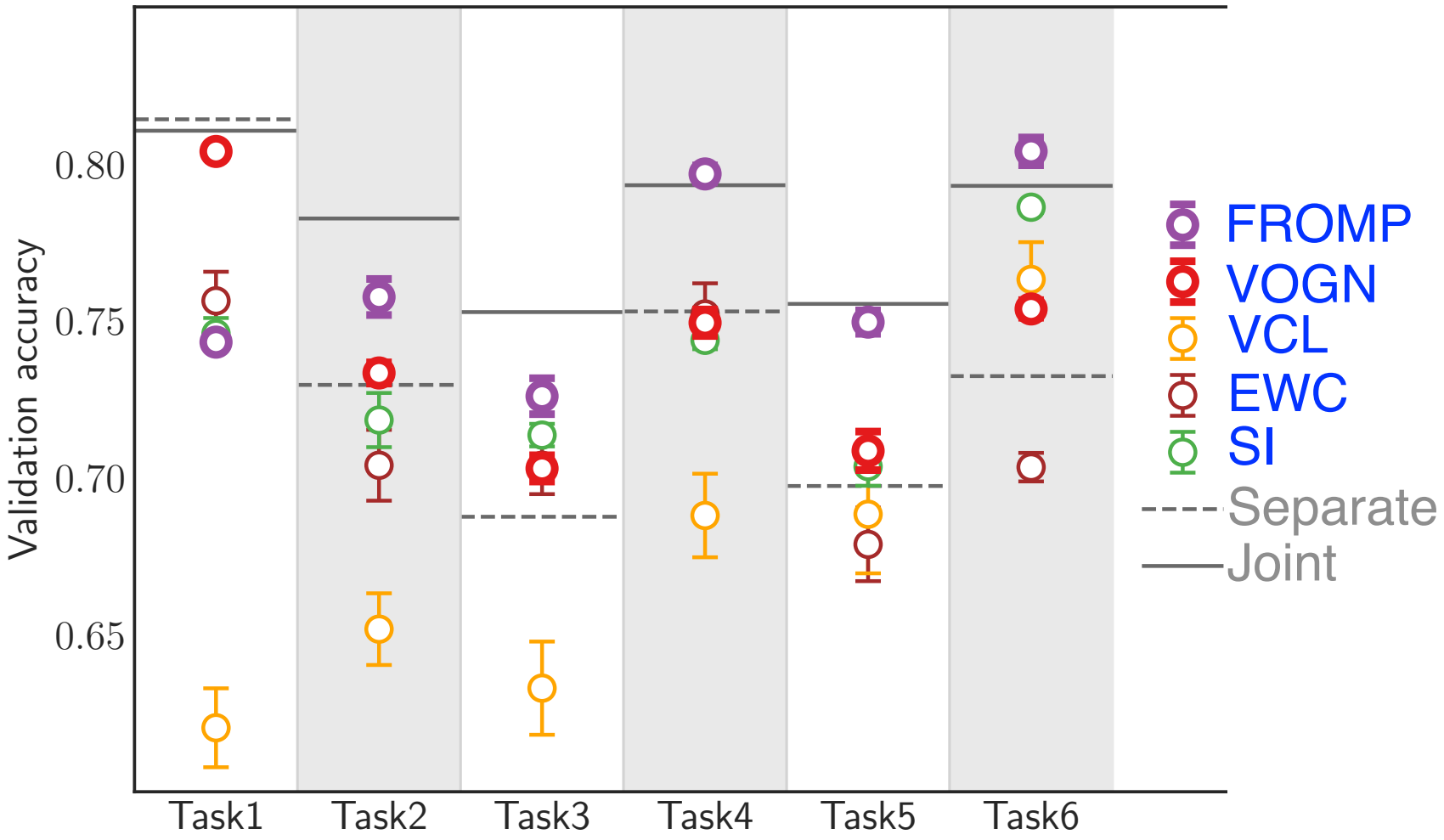


FROMP improves over EWC!

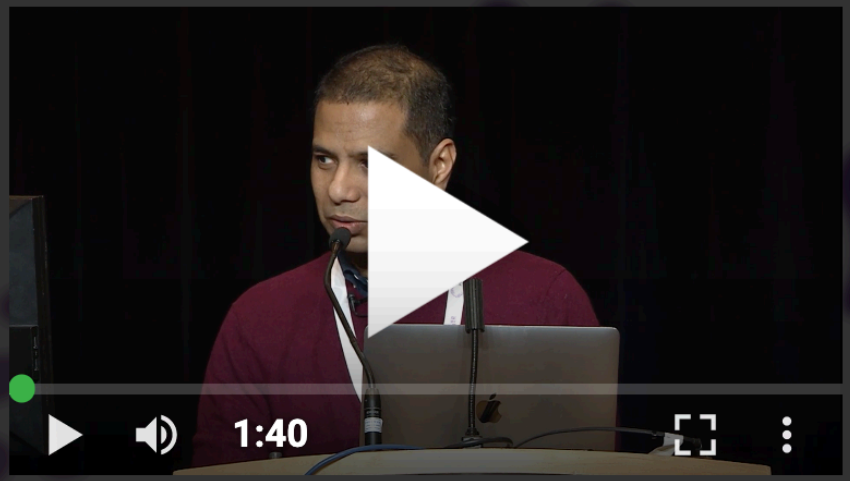


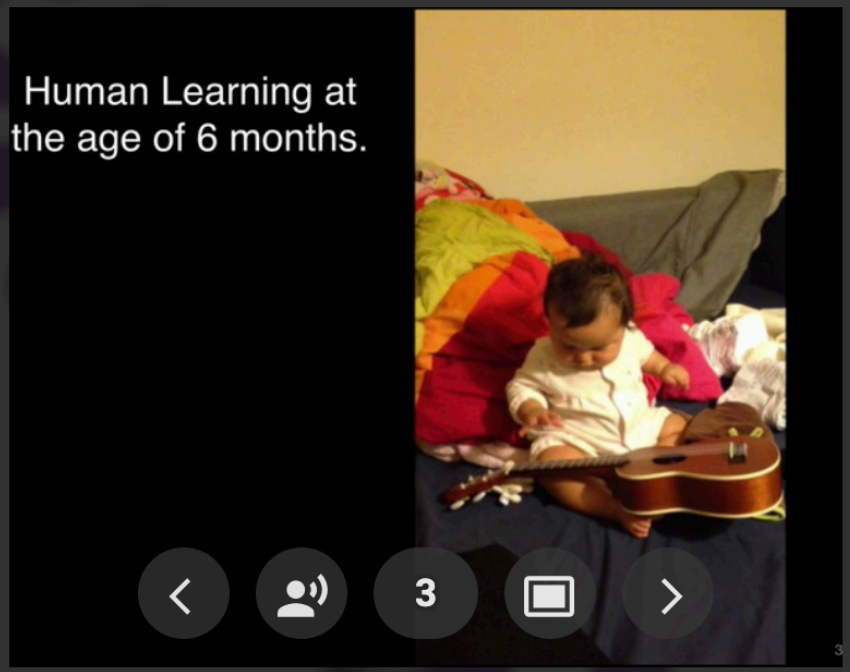
Pan et al. Continual Deep Learning by Functional Regularisation of Memorable Past, ArXiv 2020

(Some) Regularization-based Continual Learning Methods

- Elastic-weight consolidation (EWC) [1]
  - Based on a diagonal Laplace approximation
  - [2] considers structured Laplace
- Synaptic Intelligence (SI) [3]
- Variational Continual learning (VCL) [4]
  - Based on variational inference
- With better approximations, we expect accuracy to improve, but unfortunately we don't see this!

1. Kirkpatrick, James, et al. "Overcoming catastrophic forgetting in neural networks." *PNAS* (2017).
2. Ritter et al. "Online structured laplace … for overcoming catastrophic forgetting." *NeurIPs*. 2018.
3. Zenke et al. "Continual learning through synaptic intelligence." *ICML,* 2017.
4. Nguyen et al. "Variational continual learning." *arXiv preprint arXiv:1710.10628* (2017).





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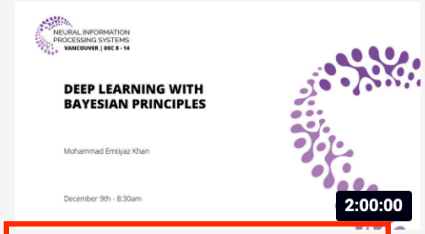

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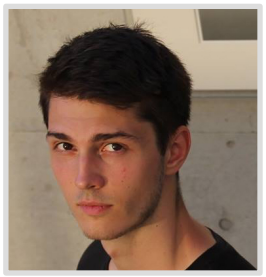

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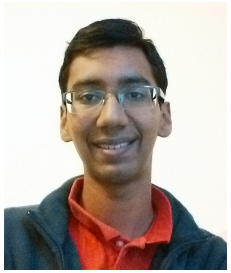

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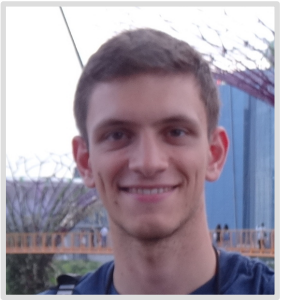

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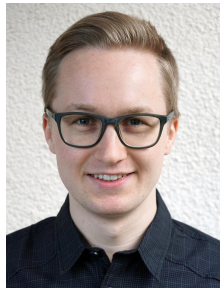

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