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How to Build Machines that Adapt Quickly

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Summary of recent research at https://emtiyaz.github.io/papers/symposium_2022.pdf
Slides used in this presentation can be found at my website

Human Learning at the age of 6 months.

Converged at the age of 12 months

Transfer skills

at the age of 14 months

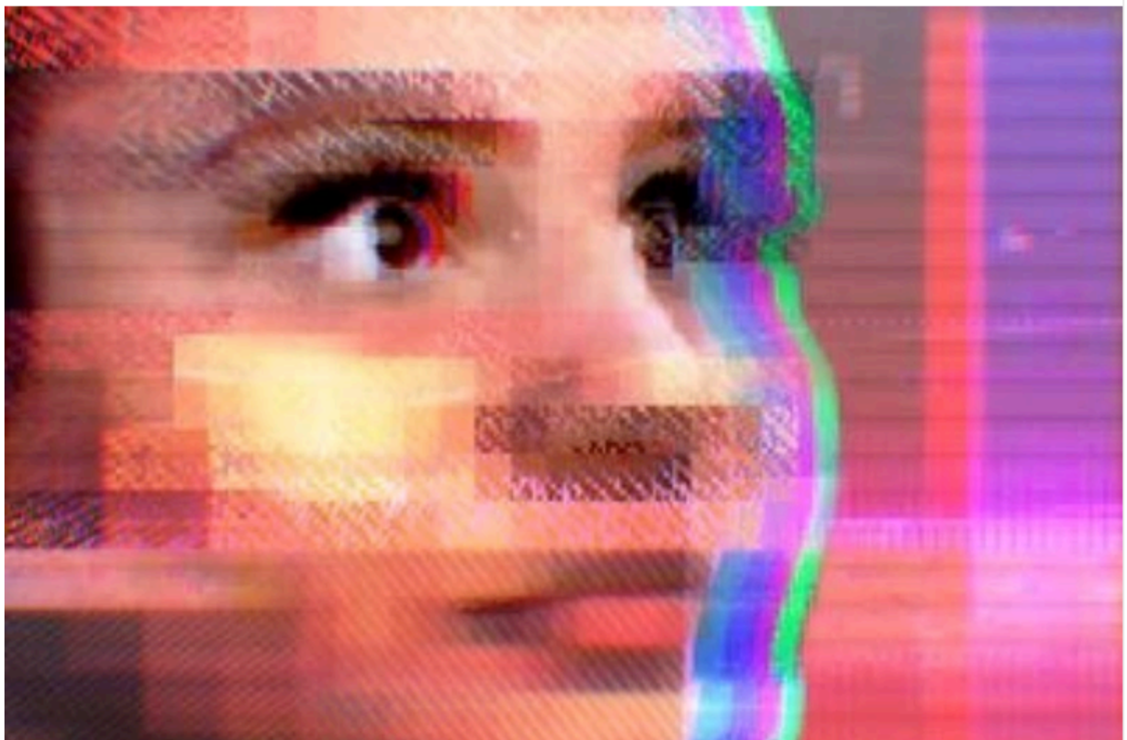
Fail because too slow to adapt

https://www.youtube.com/watch?v=TxobtWAFh8o The video is from 2017

Fail because too quick to adapt

TayTweets: Microsoft AI bot manipulated into being extreme racist upon release

Posted Fri 25 Mar 2016 at 4:38am, updated Fri 25 Mar 2016 at 9:17am



TayTweets is programmed to converse like a teenage girl who has "zero chill", according to Microsoft. *(Twitter: TayTweets)*

https://www.abc.net.au/news/2016-03-25/microsoft-created-ai-bot-becomes-racist/7276266

Adaptation in Machine Learning

- Even a small change may need retraining
- Huge amount of resources are required only few can afford (costly & unsustainable) [1,2, 3]
- Difficult to apply in “dynamic” settings (robotics, medicine, epidemiology, climate science, etc.)
- Our goal is to solve such challenges
- Also to reduce “magic” in deep learning

1. Diethe et al. Continual learning in practice, arXiv, 2019.
2. Paleyes et al. Challenges in deploying machine learning: a survey of case studies, arXiv, 2021.
3. https://www.youtube.com/watch?v=hx7BXih7zx8&t=897s

Towards Quick Adaptation

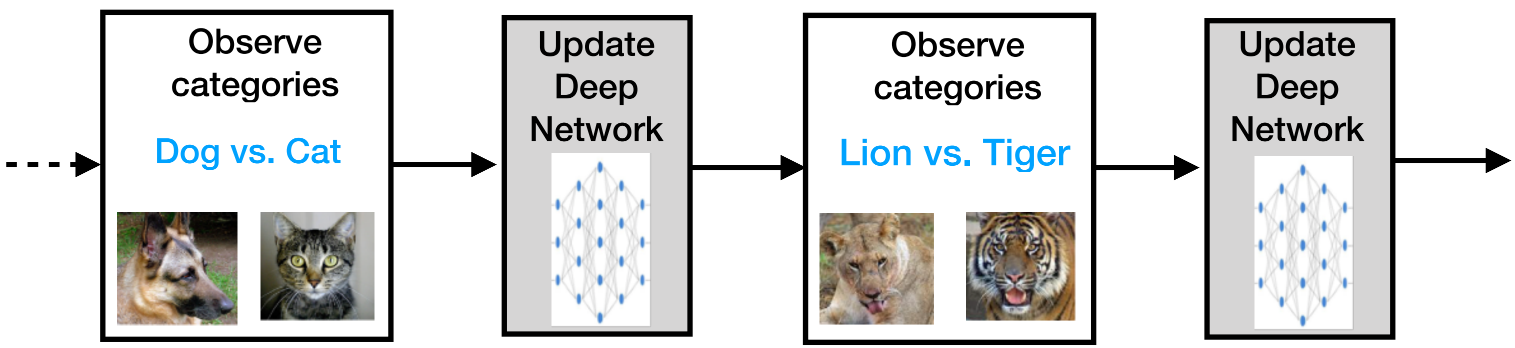
- Better uncertainty [1-4]
  - Bayesian Learning rule (BLR)
- Better regularization [5-7]
  - Knowledge-Adaptation Priors (K-priors)
- Better memory [8]
  - Memory Perturbation Equation (MPE)

1. Khan and Rue, The Bayesian Learning Rule, JMLR (2023).
2. Khan, et al. Fast and scalable Bayesian deep learning by weight-perturbation in Adam, ICML (2018).
3. Osawa et al. Practical Deep Learning with Bayesian Principles, NeurIPS (2019).
4. Lin et al. Handling the positive-definite constraints in the BLR, ICML (2020).
5. Khan and Swaroop. Knowledge-Adaptation Priors, NeurIPS (2021)
6. Pan et al. Continual deep learning by functional regularisation of memorable past, NeurIPS (2020)
7. Daxberger et al. Improving CL by Accurate Gradient Reconstruction of the Past, TMLR (2023).
8. Nickl, Xu, Tailor, Moellenhoff, Khan, The memory-perturbation equation, NeurIPS (2023)

Example: Continual Learning

Standard Deep Learning

Continual Learning: past classes never revisited



Standard training leads to catastrophic forgetting.

Kirkpatrick, James, et al. "Overcoming catastrophic forgetting in neural networks." *Proceedings of the national academy of sciences* 114.13 (2017): 3521-3526.

Bayesian Learning Rule

Better Uncertainty

Weight Regularization

Standard way to is to add a weight-regularizer [1]

$$(\theta - \theta_{\text{old}})^\top F_{\text{old}}(\theta - \theta_{\text{old}})$$

Weight uncertainty

Straightforward improvement in weight-uncertainty is to use variational inference [2-4]

1. Kirkpatrick, James, et al. "Overcoming catastrophic forgetting in neural networks." *PNAS* 2017
2. Khan, et al. "Fast and scalable Bayesian deep learning by weight-perturbation in Adam." *ICML* (2018).
3. Osawa et al. "Practical Deep Learning with Bayesian Principles." NeurIPS (2019).
4. Lin et al. "Handling the positive-definite constraints in the BLR." ICML (2020).

Practical Deep Learning with Bayes

A reliable estimate of Fisher/Hessian/variance

RMSprop

$$
\begin{aligned}
g &\leftarrow \hat{\nabla}\ell(\theta) \\
h &\leftarrow g \cdot g \\
s &\leftarrow (1-\rho)s + \rho h \\
\theta &\leftarrow \theta - \alpha\, g/\sqrt{s}
\end{aligned}
$$

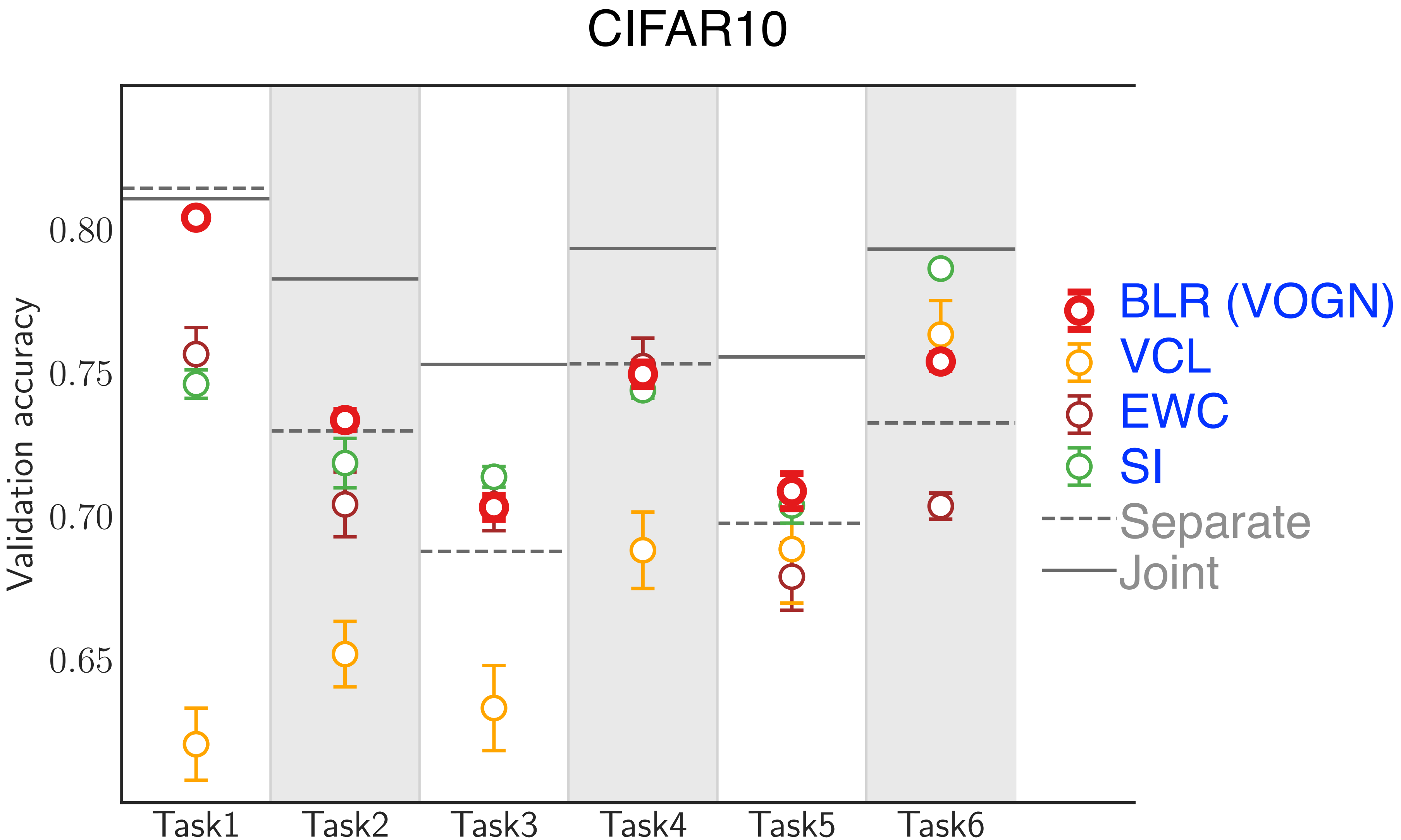
Bayesian Learning Rule [3]

$$
\begin{aligned}
g &\leftarrow \hat{\nabla}\ell(\theta) \\
h &\leftarrow g \cdot \sqrt{s} \cdot \epsilon \\
s &\leftarrow (1-\rho)s + \rho h + \rho^2 h^2/(2s) \\
m &\leftarrow m - \alpha\; g/s \\
\sigma^2 &\leftarrow 1/s, \;\; \theta \leftarrow m + \epsilon \sim \mathcal{N}(0, 1/s)
\end{aligned}
$$

Costs are exactly the same, but the variance quality is much better!!

1. Khan, et al. "Fast and scalable Bayesian deep learning by weight-perturbation in Adam." *ICML* (2018).
2. Osawa et al. “Practical Deep Learning with Bayesian Principles.” NeurIPS (2019).
3. Lin et al. “Handling the positive-definite constraints in the BLR.” ICML (2020).

Improvements over EWC



1. Osawa et al. “Practical Deep Learning with Bayesian Principles.” NeurIPS (2019).

Bayesian learning rule (BLR)

See Table 1 in Khan and Rue, 2021

Learning Algorithm	Posterior Approx.	Natural-Gradient Approx.	Sec.
Optimization Algorithms			
Gradient Descent	Gaussian (fixed cov.)	Delta method	1.3
Newton's method	Gaussian	——"——	1.3
Multimodal optimization (New)	Mixture of Gaussians	——"——	3.2
Deep-Learning Algorithms			
Stochastic Gradient Descent	Gaussian (fixed cov.)	Delta method, stochastic approx.	4.1
RMSprop/Adam	Gaussian (diagonal cov.)	Delta method, stochastic approx., Hessian approx., square-root scaling, slow-moving scale vectors	4.2
Dropout	Mixture of Gaussians	Delta method, stochastic approx., responsibility approx.	4.3
STE	Bernoulli	Delta method, stochastic approx.	4.5
Online Gauss-Newton (OGN) (New)	Gaussian (diagonal cov.)	Gauss-Newton Hessian approx. in Adam & no square-root scaling	4.4
Variational OGN (New)	——"——	Remove delta method from OGN	4.4
BayesBiNN (New)	Bernoulli	Remove delta method from STE	4.5
Approximate Bayesian Inference Algorithms			
Conjugate Bayes	Exp-family	Set learning rate $\rho_t = 1$	5.1
Laplace's method	Gaussian	Delta method	4.4
Expectation-Maximization	Exp-Family + Gaussian	Delta method for the parameters	5.2
Stochastic VI (SVI)	Exp-family (mean-field)	Stochastic approx., local $\rho_t = 1$	5.3
VMP	——"——	$\rho_t = 1$ for all nodes	5.3
Non-Conjugate VMP	——"——	——"——	5.3
Non-Conjugate VI (New)	Mixture of Exp-family	None	5.4

All sorts of algorithms can be derived by using two sets of approximations.

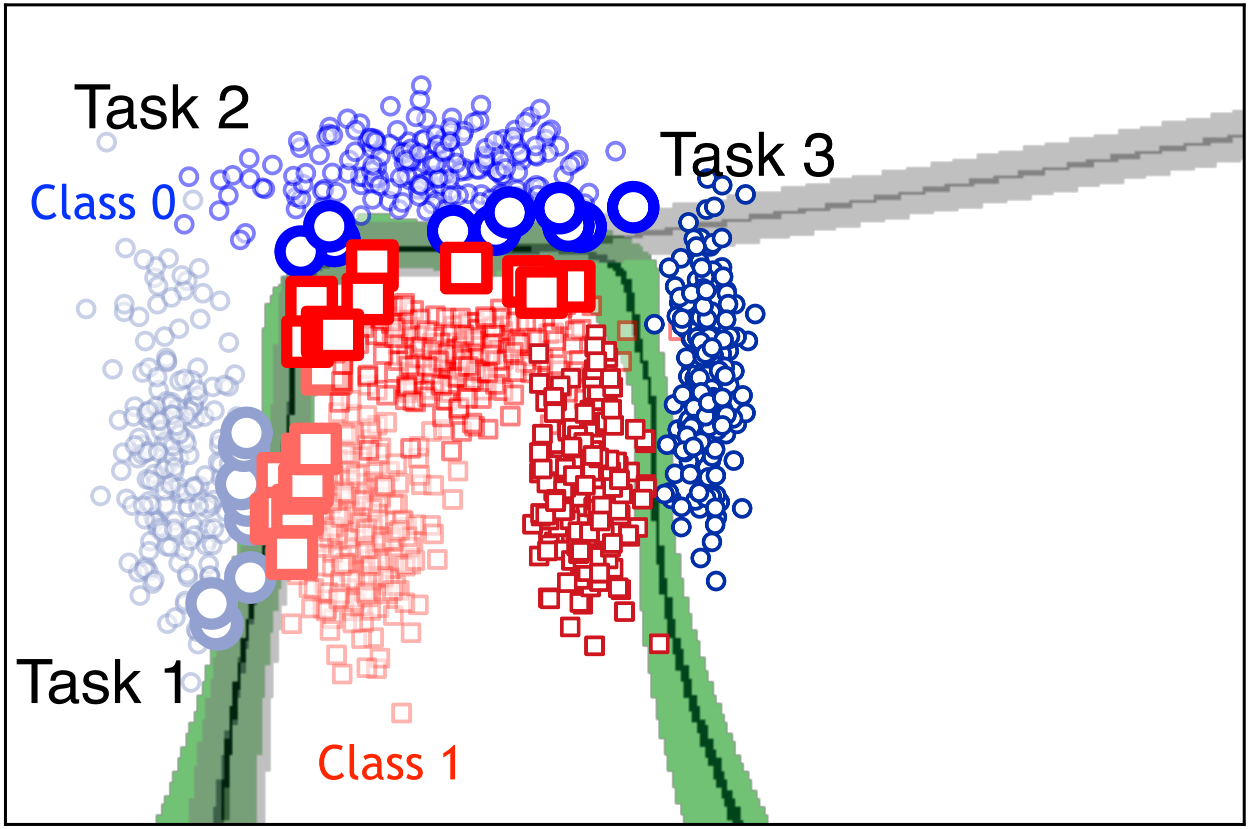
By relaxing the approximations, we get an improvement, for example, uncertainty aware deep learning optimizers

1. Khan and Rue, The Bayesian Learning Rule, arXiv, https://arxiv.org/abs/2107.04562, 2021
2. Khan and Lin. "Conjugate-computation variational inference…." AIstats (2017).

Knowledge-Adaptation Prior

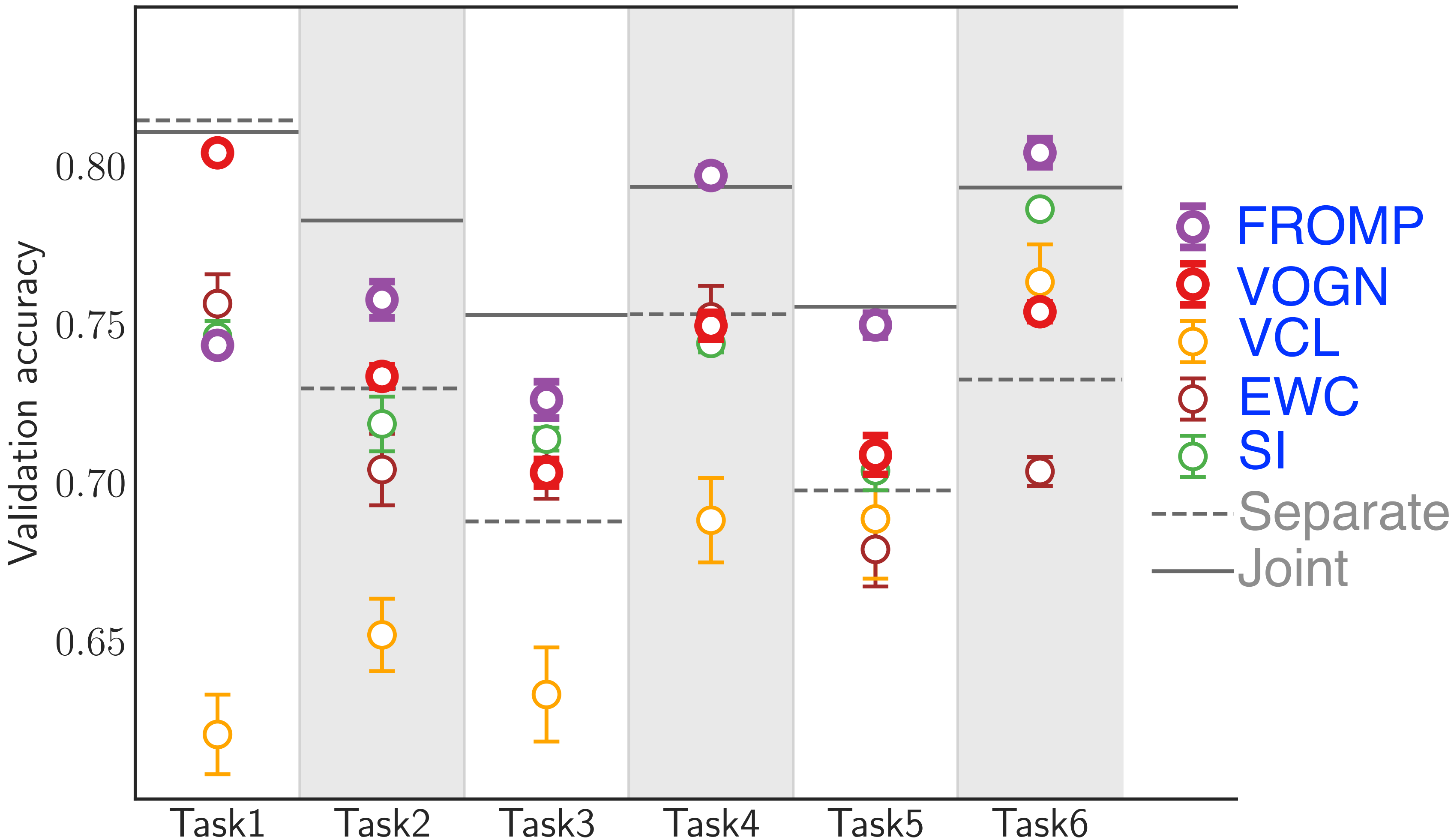
Better Regularization

Function Regularization of Memorable Examples [2]



1. Khan et al. Approximate Inference Turns Deep Networks into Gaussian Process, NeurIPS, 2019
2. Pan et al. Continual Deep Learning by Functional Regularisation of Memorable Past, NeurIPS, 2020

Improvements over EWC and VOGN



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

Functional Regularization of Memorable Past (FROMP)

Weight-regularizer (EWC) [1]

$$(\theta - \theta_{\text{old}})^\top F_{\text{old}}(\theta - \theta_{\text{old}})$$

Weight uncertainty

Functional regularizer (FROMP) [2]

$$[\sigma(\mathbf{f}(\theta)) - \sigma(\mathbf{f}_{old})]^\top K_{old}^{-1}[\sigma(\mathbf{f}(\theta)) - \sigma(\mathbf{f}_{old})]$$

Uncertainty

Predictions

Why does this work?

It is a way to replay past gradients

1. Kirkpatrick, James, et al. "Overcoming catastrophic forgetting in neural networks." *PNAS* 2017
2. Pan et al. Continual Deep Learning by Functional Regularisation of Memorable Past, NeurIPS, 2020

Easy to see in Linear Regression

Weight-space Function-space

$$\arg\min_{\theta} \; \|\theta\|^2 + \|y - X\theta\|^2 \qquad F_{old} = I + X^\top X$$

$$(\theta - \theta_{old})^\top F_{old}(\theta - \theta_{old}) = (\theta - \theta_{old})^\top (I + X^\top X)(\theta - \theta_{old})$$

Entirely in weight-space (EWC) [1]

$$= \|\theta - \theta_{old}\|^2 + \|X\theta - X\theta_{old}\|^2$$

Weight-space Function-space

Knowledge-adaptation prior [3]

$$= (X\theta - X\theta_{old})^\top K^{-1}(X\theta - X\theta_{old})$$

Entirely in function-space (FROMP) [2]

$$= \|\theta\|^2 + \|y - X\theta\|^2 + \text{const.}$$

In linear regression, they are equivalent and are all ways to reconstruct the old problem (or its gradients)

1. Kirkpatrick, James, et al. "Overcoming catastrophic forgetting in neural networks." *PNAS* 2017
2. Pan et al. Continual Deep Learning by Functional Regularisation of Memorable Past, NeurIPS, 2020
3. Khan and Swaroop. Knowledge-Adaptation Priors, NeurIPS, 2021

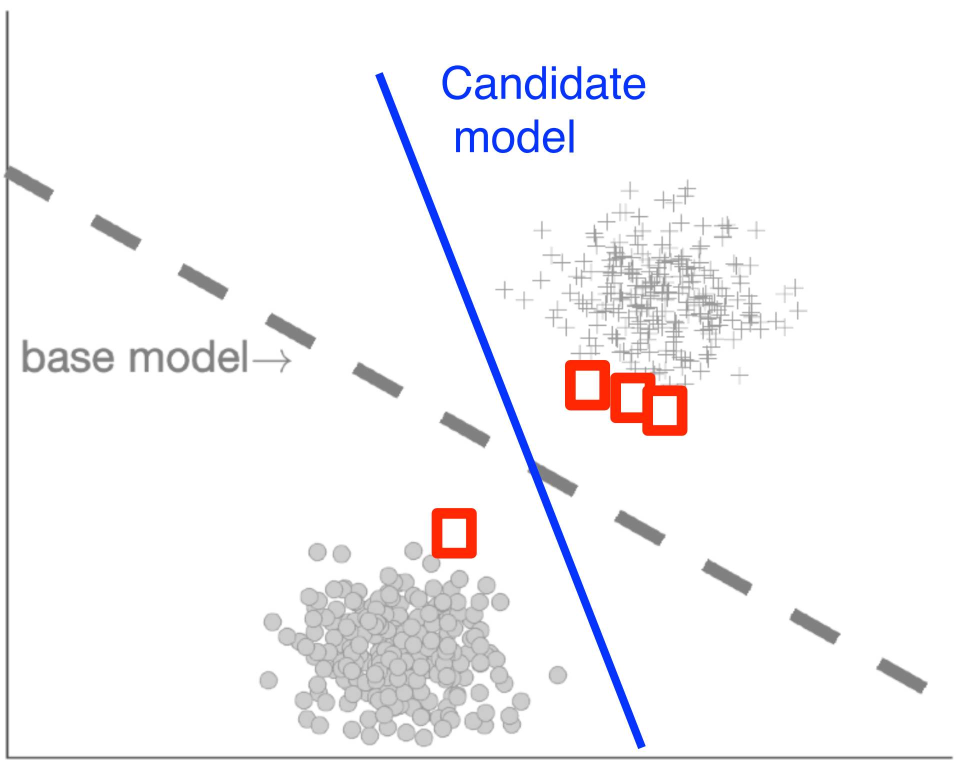
Knowledge-Adaptation Priors

Combine weight and function-space divergences

Weight-space Function-space

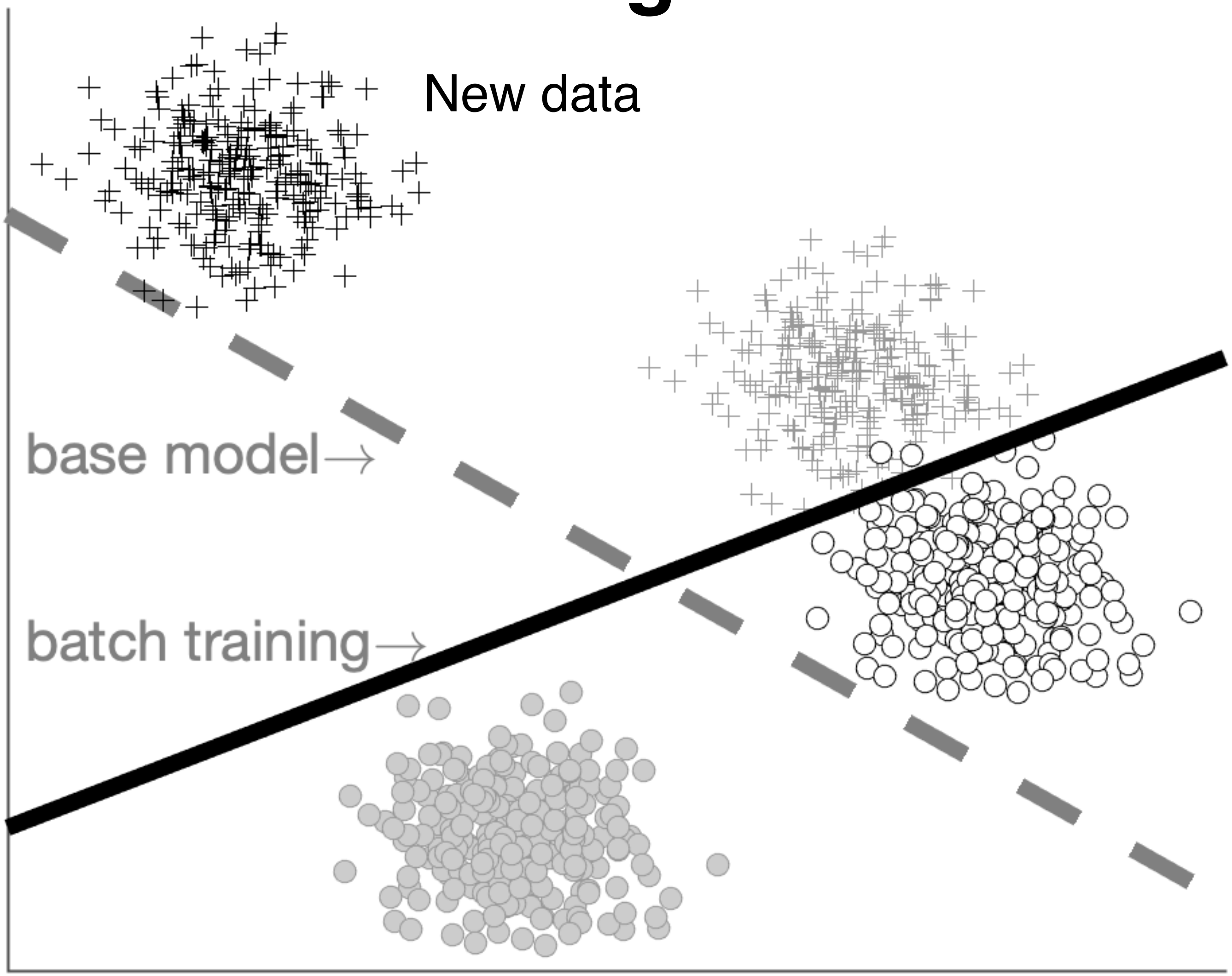
$$\mathcal{K}(\theta) = \tau \mathbb{D}_w(\theta \| \theta_{\text{old}}) + \mathbb{D}_f(\mathbf{f}(\theta) \| \mathbf{f}(\theta_{\text{old}}))$$

$$\begin{bmatrix} f_w^1 \\ f_w^2 \\ f_w^3 \\ f_w^4 \end{bmatrix} \quad \begin{bmatrix} f_{w_*}^1 \\ f_{w_*}^2 \\ f_{w_*}^3 \\ f_{w_*}^4 \end{bmatrix}$$



K-prior is a way to replay past gradients

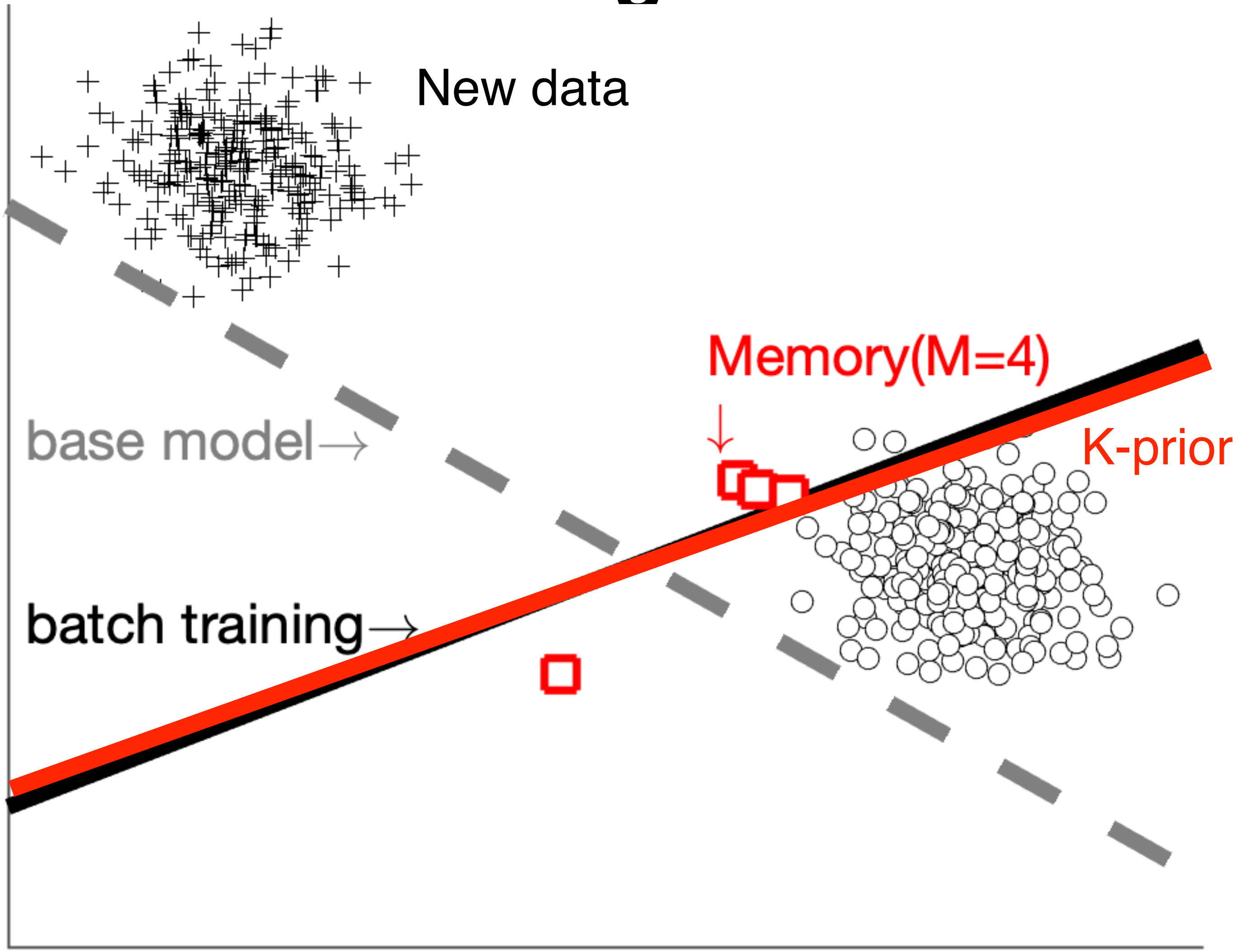
Intuition behind functional regularization



Binary classification with Logistic regression

Each task N=500, each class 250 examples.

Intuition behind functional regularization

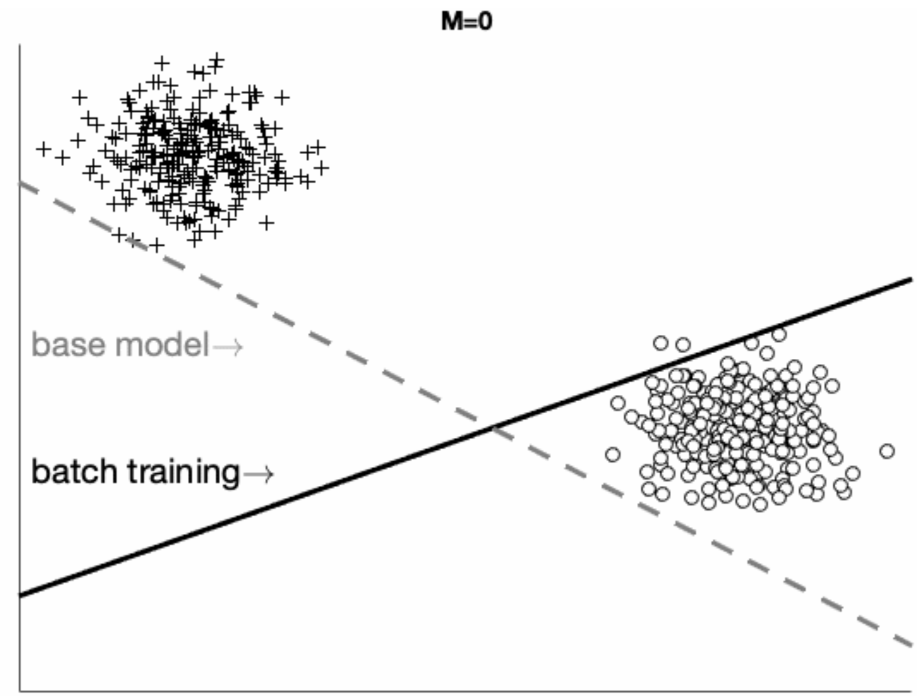


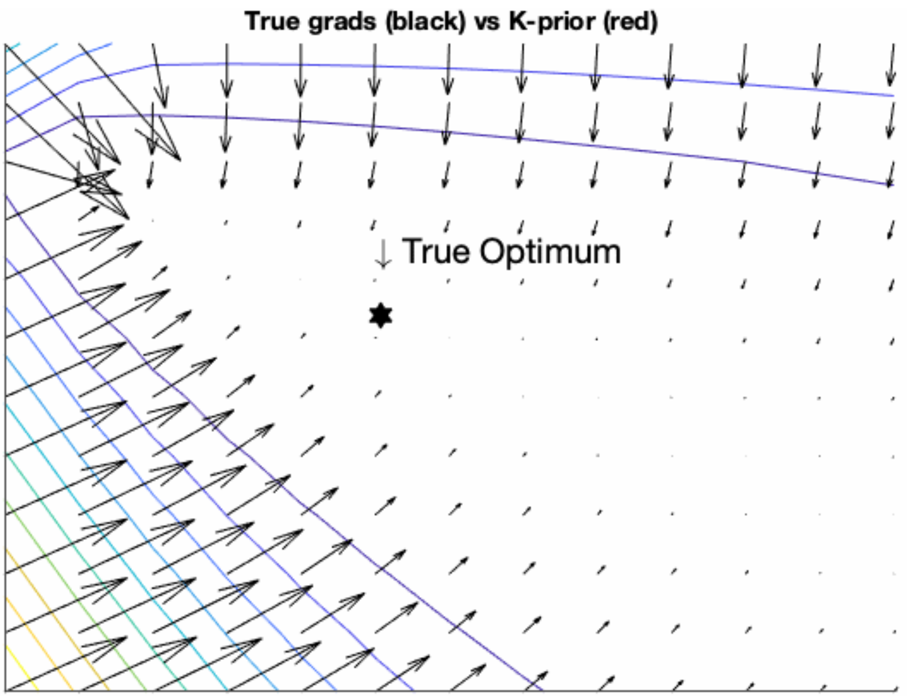
Binary classification with Logistic regression

Each task N=500, each class 250 examples.

A General Principle of Adaptation

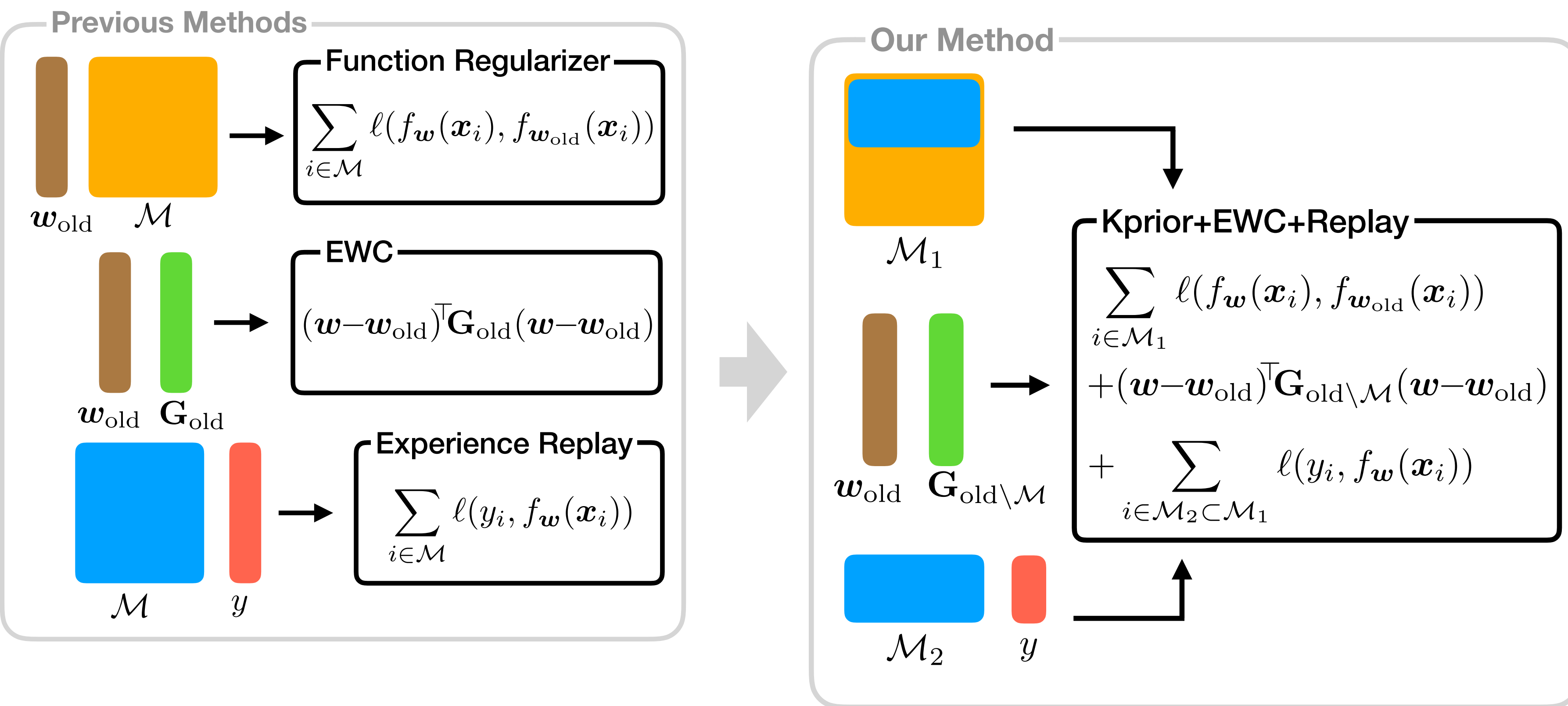
Reconstruct past gradients





1. Khan and Swaroop. Knowledge-Adaptation Priors, NeurIPS, 2021 (https://arxiv.org/abs/2106.08769)

How to combine EWC + FR + Replay



1. Daxberger et al. Improving CL by Accurate Gradient Reconstruction of the Past, TMLR 2023.

Memory-Perturbation Equation

Better Memory

How to Choose Memory?

Minimize the error in the gradients

$$\nabla l_{\text{old}}(\theta) - \nabla K(\theta)$$

$$= \sum_{i \in \mathcal{D} \backslash \mathcal{M}} \nabla f_i(\theta) \left[\sigma(f_i(\theta)) - \sigma(f_i(\theta_{\text{old}}))\right]$$

Feature disagreement
-> prediction variance

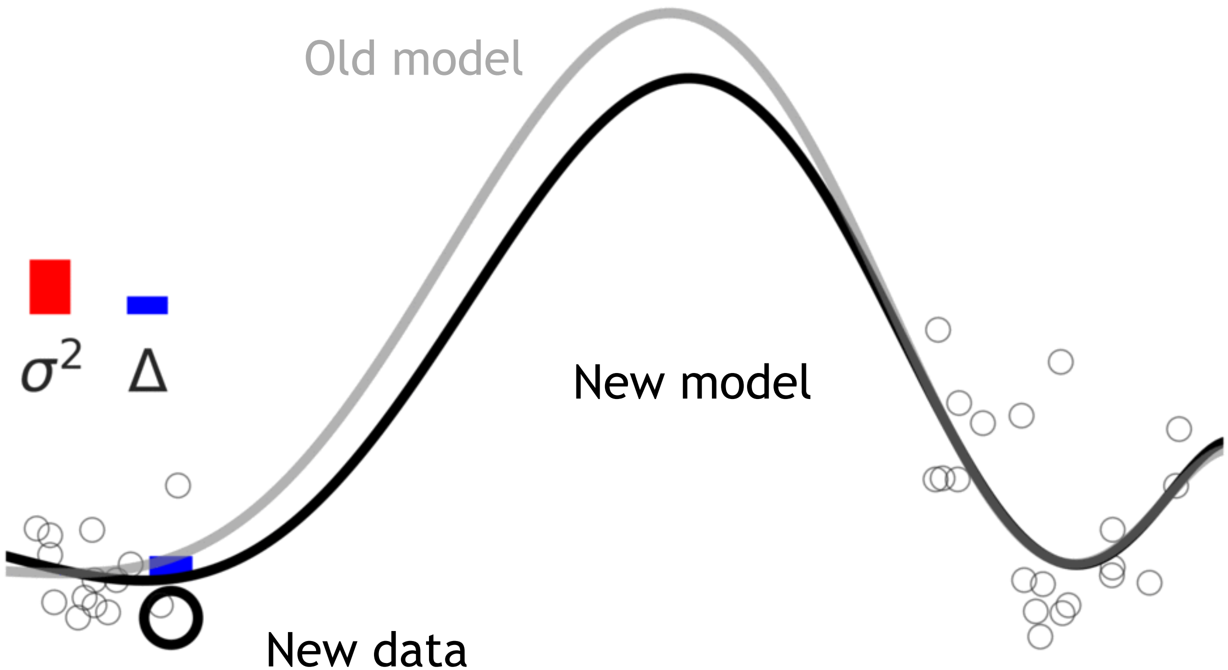
Prediction disagreement
-> prediction error

Past and future should agree. There are some general rules to ensure this, but no magic. In general, we must understand sensitivity of the past to the (expected) future changes.

Memory Perturbation

How sensitive is a model to its training data?

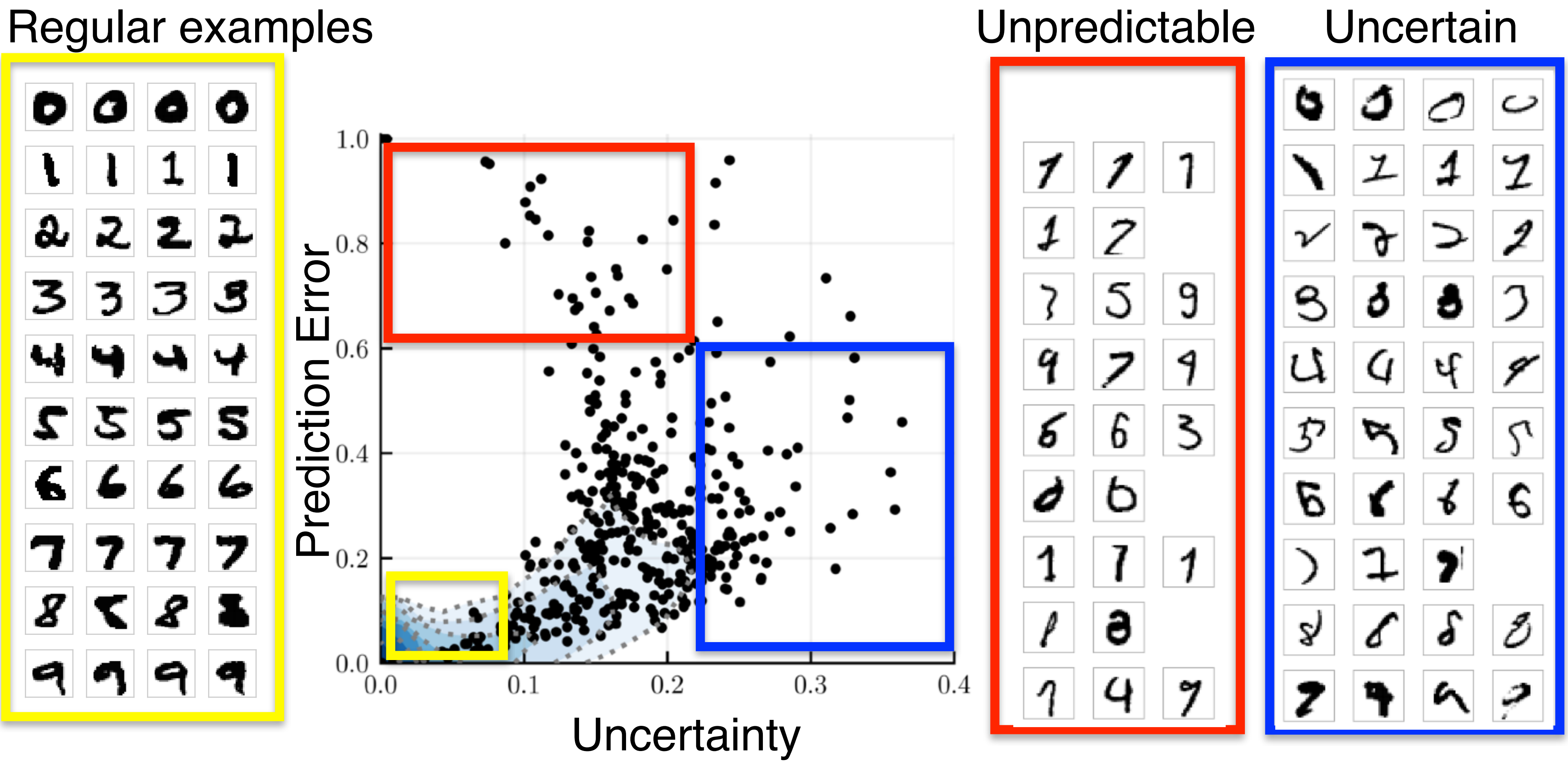
Model-deviation (Δ) = predictError *predictVariance



1. Cook. Detection of Influential Observations in Linear Regression. Technometrics. ASA 1977
2. Nickl, Xu, Tailor, Moellenhoff, Khan, The memory-perturbation equation, NeurIPS, 2023

Memory Maps using the BLR

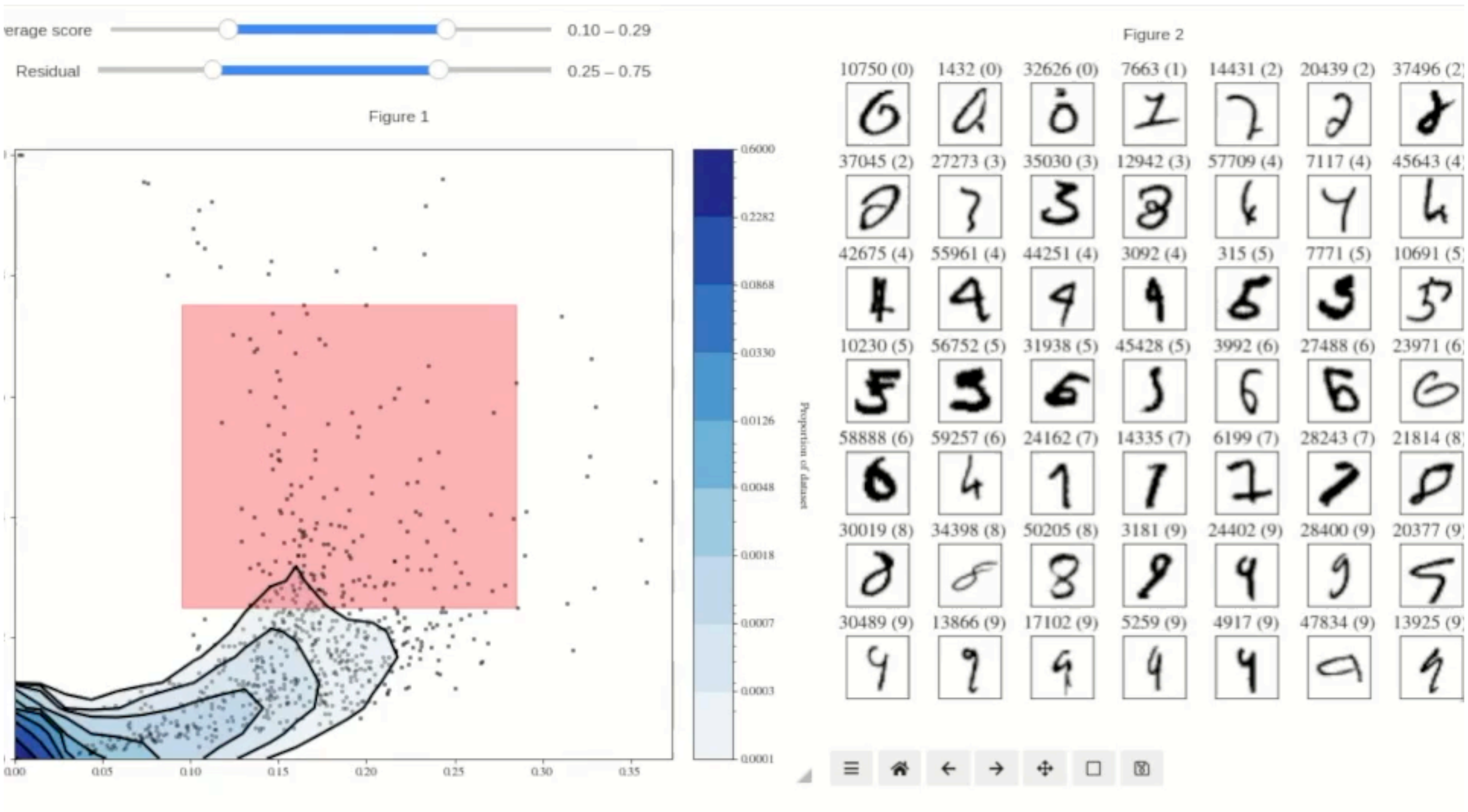
Understand generic ML models and algorithms.



1. Tailor, Chang, Swaroop, Nalisnick, Solin, Khan, Memory maps to understand models (under review)

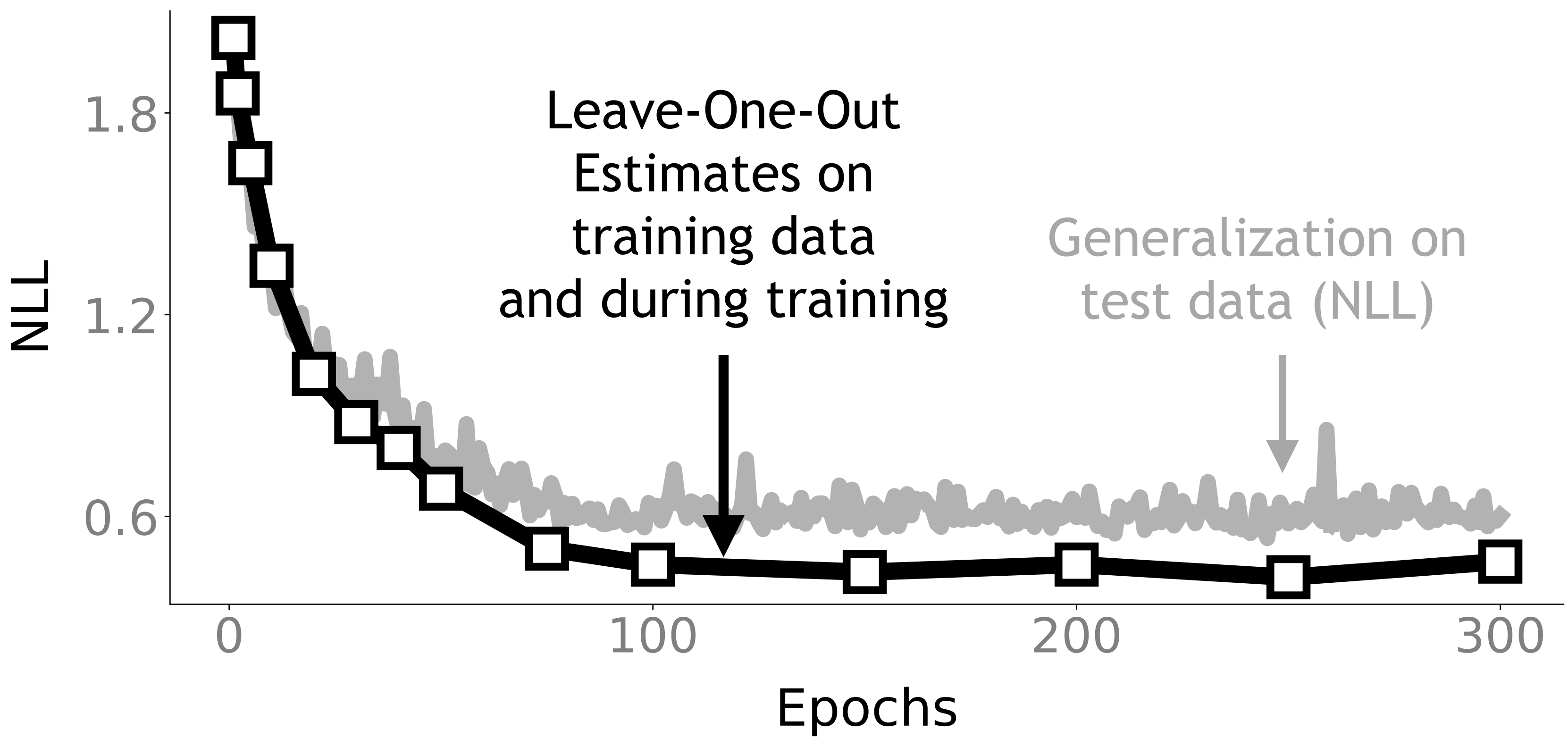
A Tool for Data-Scientists

Understand the memory of a model.



Predict Generalization during Training

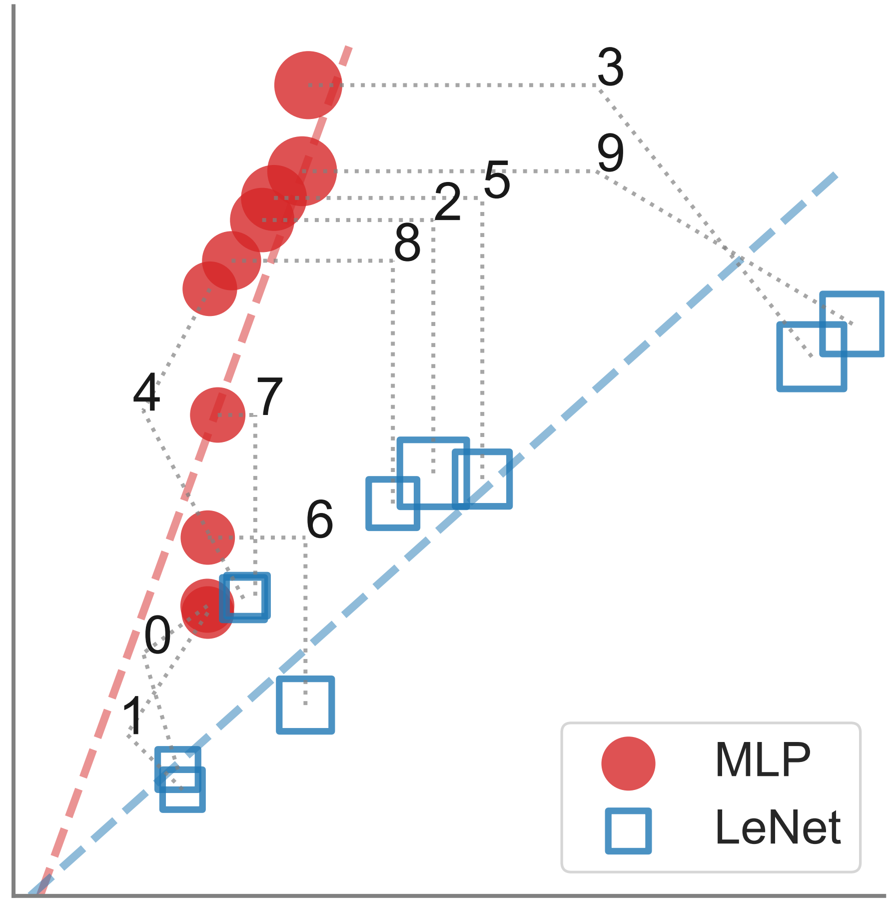
CIFAR10 on ResNet-20 using iBLR [1]. Adam also works but better uncertainty gives better estimates.



1. Lin et al. “Handling the positive-definite constraints in the BLR.” ICML (2020).

Estimating the Effect of Class-Removal

Estimates on training data (no retraining)



Test Performance (NLL) by brute-force retraining

MNIST on LeNet5 using K-FAC Laplace [1]. Adam also works but better uncertainty gives better estimates.

Towards Quick Adaptation

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8. Nickl, Xu, Tailor, Moellenhoff, Khan, The memory-perturbation equation, NeurIPS (2023)

The webpage is available at https://bayesduality.github.io/, and Twitter account @BayesDuality

The Bayes-Duality Project

Toward AI that learns adaptively, robustly, and continuously, like humans

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Many thanks to our group members and collaborators (many not on this slide).

We have open positions and are always looking for new collaborations.