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Feature Grouping as a Stochastic Regularizer for High Dimensional Structured Data

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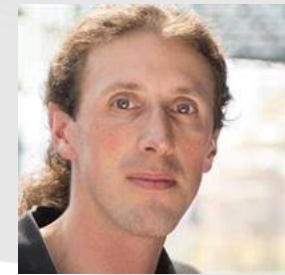
Bertrand Thirion

(INRIA, France)



Gaël Varoquaux

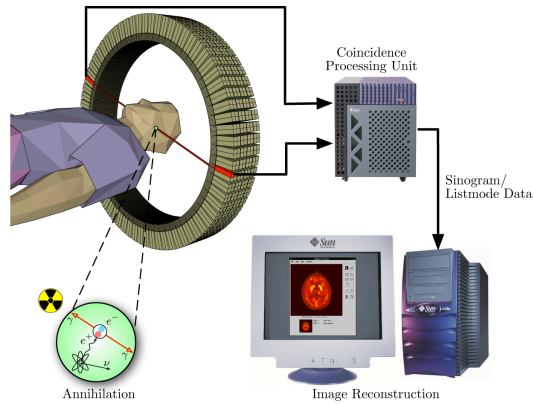
(INRIA, France)



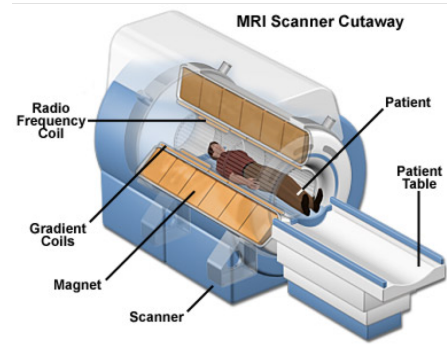
High Dimensional and Small-Sample Data Situations



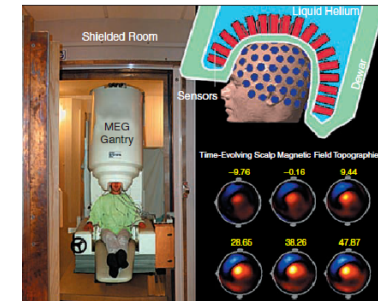
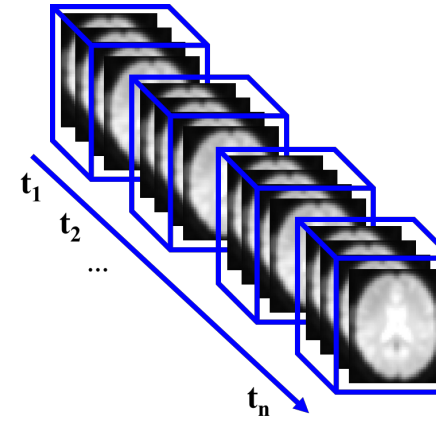
- Brain imaging, Genomics, Seismology, Astronomy, Chemistry, etc.



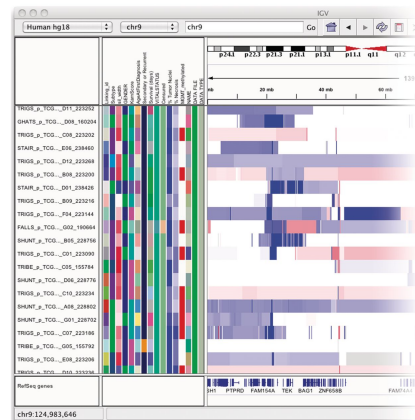
PET acquisition process wikipedia



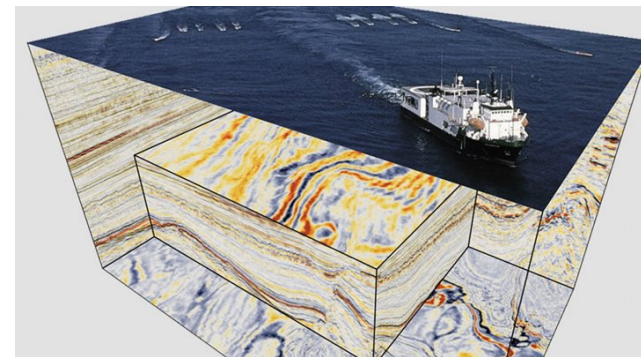
MRI Scanner and rs-fMRI time series acquisition [NVIDIA]



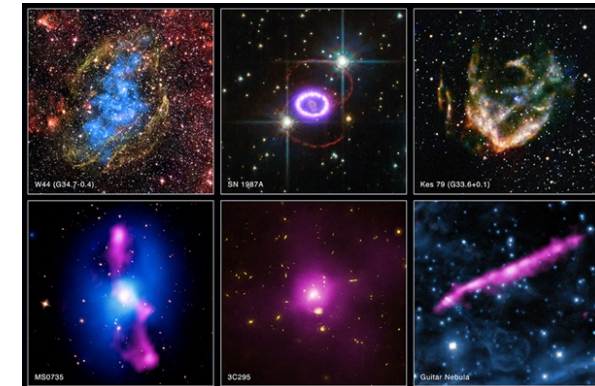
A typical MEG equipment [BML2001]



Genomics
Integrative Genomics Viewer, 2012



Seismology
<https://www.mapnagroup.com>



Astronomy
Astronomy Magazine, 2015

Fitting Complex Models in These Situations



Challenges

1. **Large feature dimension:** due to rich temporal and spatial resolution
2. **Noise in the data:** due to artifacts unrelated to the effect of interest
3. **Small sample size:** due to logistics and cost of data acquisition

Regularization Strategies

- **Early Stopping:** [Yao, 2007]
- **ℓ_1 and ℓ_2 penalties:** [Tibshirami 1996]
- **Pooling Layers in CNNs:** [Hinton 2012]
- **Group LASSO:** [Yuan 2006]
- **Dropout:** [Srivastana 2014]

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- **Group LASSO:** [Yuan 2006]..... **STRUCTURE + SPARSITY**
- **Dropout:** [Srivastana 2014]..... **STOCHASTICITY**

Fitting Complex Models in These Situations



Challenges

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Regularization Strategies

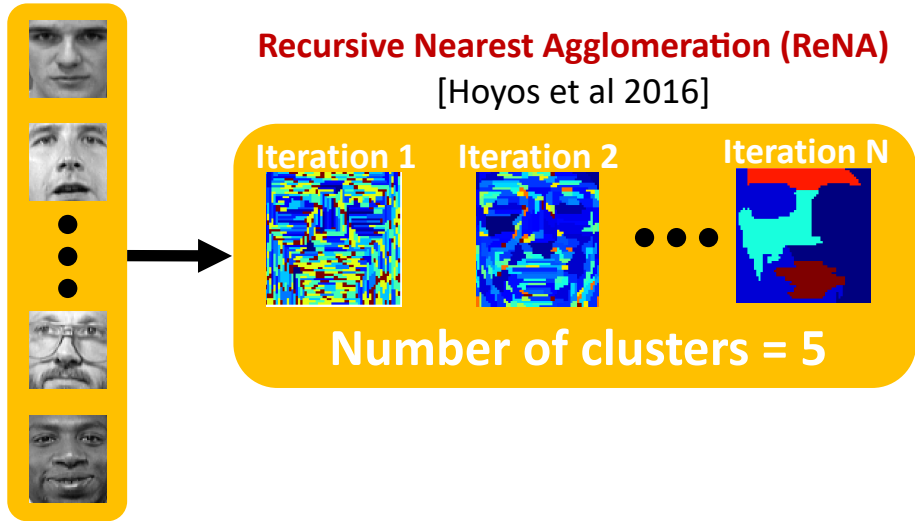
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- **PROPOSED: Use STRUCTURE & STOCHASTICITY**

Feature Grouping to Capture Structure

Algorithm

Training Data



- **ReNA:** a data-driven, graph constrained feature grouping algorithm
- Each feature (pixel) is assigned to a cluster. Clusters are then recursively merged until the desired number of clusters remain.
- Benefits of ReNA: (i) a fast clustering algorithm (ii) leads to good signal approximations.

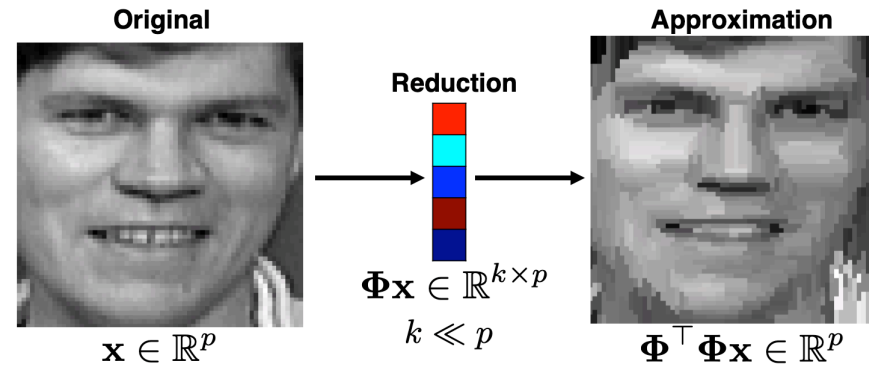
Feature Grouping Matrix $\Phi \in \mathbb{R}^{k \times p}$

$$\Phi = \begin{bmatrix} \alpha_1 \cdots \alpha_1 & 0 \cdots 0 & 0 \cdots 0 & 0 \cdots 0 & 0 \cdots 0 \\ 0 \cdots 0 & \alpha_2 \cdots \alpha_2 & 0 \cdots 0 & 0 \cdots 0 & 0 \cdots 0 \\ 0 \cdots 0 & 0 \cdots 0 & \alpha_3 \cdots \alpha_3 & 0 \cdots 0 & 0 \cdots 0 \\ 0 \cdots 0 & 0 \cdots 0 & 0 \cdots 0 & \alpha_4 \cdots \alpha_4 & 0 \cdots 0 \\ 0 \cdots 0 & 0 \cdots 0 & 0 \cdots 0 & 0 \cdots 0 & \alpha_5 \cdots \alpha_5 \end{bmatrix}$$

Each row captures a different structure



Reduction and Low-rank Approximation



Proposed Approach

Consider fully connected neural network with H layers

Algorithm 1 Training of a Neural Network with Feature Grouping as a Stochastic Regularizer

Require: Learning Rate η

Require: Initial Parameters for H layers

$$\Theta \triangleq \{\mathbf{W}_0, \mathbf{b}_0, \mathbf{W}_1, \mathbf{b}_1, \dots, \mathbf{W}_H, \mathbf{b}_H\}$$

Ensure: Generate a bank of feature grouping matrices where each is generated by randomly sampling r samples from the training data set with replacement

$$\Phi = \{\Phi^{(1)}, \Phi^{(2)}, \dots, \Phi^{(b)}\}$$

1: **while** stopping criteria not met **do**

2: Sample a minibatch of m samples from the training set $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$ with corresponding labels $y^{(i)}$

3: Sample Φ from the bank Φ .

4: Define $\Xi \triangleq \{\hat{\mathbf{W}}_0, \mathbf{b}_0, \mathbf{W}_1, \mathbf{b}_1, \dots, \mathbf{W}_H, \mathbf{b}_H\}$ where $\hat{\mathbf{W}}_0 \triangleq \mathbf{W}_0 \Phi^T$.

5: Compute gradient estimate:

$$\mathbf{g} \leftarrow \frac{1}{m} \nabla_{\Xi} \sum_i \mathcal{L}(f(\Phi \mathbf{x}^{(i)}; \Xi), y^{(i)})$$

6: Apply updates:

- $\mathbf{W}_0 \leftarrow \mathbf{W}_0 - \eta \mathbf{g}_{\mathbf{w}_0} \Phi$
where $\mathbf{g}_{\mathbf{w}_0} \triangleq \frac{1}{m} \nabla_{\hat{\mathbf{W}}_0} \sum_i \mathcal{L}(f(\Phi \mathbf{x}^{(i)}; \Xi), y^{(i)})$

- $\mathbf{b}_j \leftarrow \mathbf{b}_j - \eta \mathbf{g}_{\mathbf{b}_j}$
where $\mathbf{g}_{\mathbf{b}_j} \triangleq \frac{1}{m} \nabla_{\mathbf{b}_j} \sum_i \mathcal{L}(f(\Phi \mathbf{x}^{(i)}; \Xi), y^{(i)})$
for $j \in \{0, \dots, H\}$

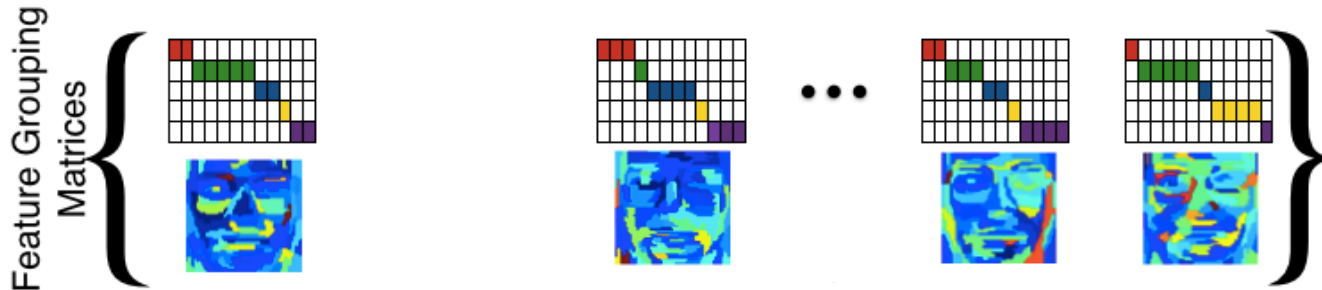
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7: **end while**



Proposed Approach

Pre-compute a bank of feature grouping matrices



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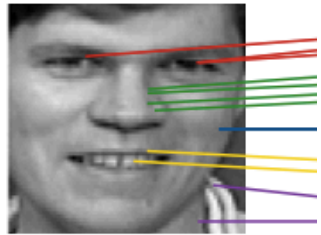
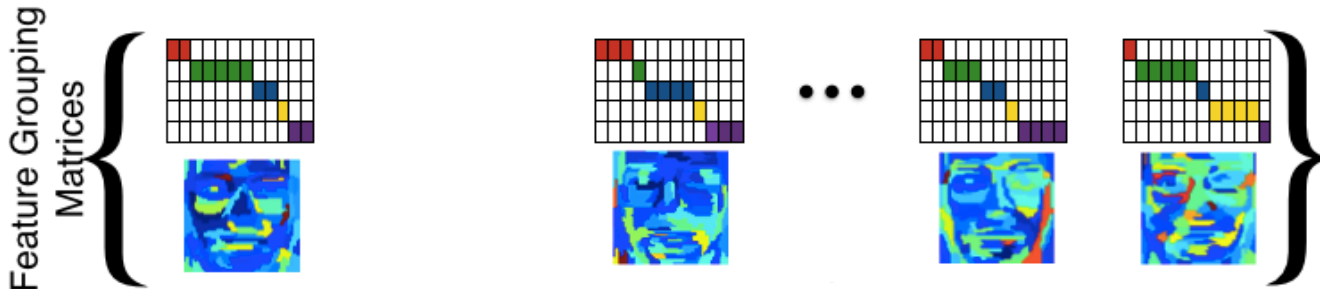
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- 7: **end while**



Proposed Approach

Sample from the training set



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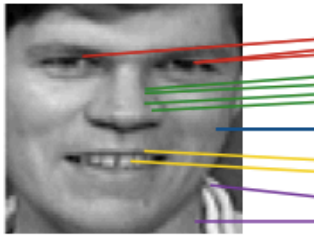
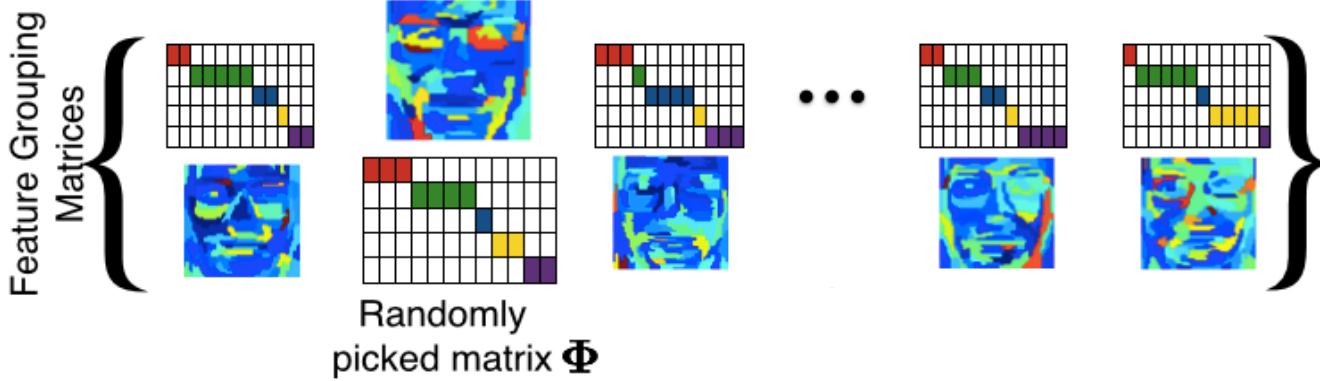
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7: **end while**



Proposed Approach

Sample Φ from the bank of feature grouping matrices



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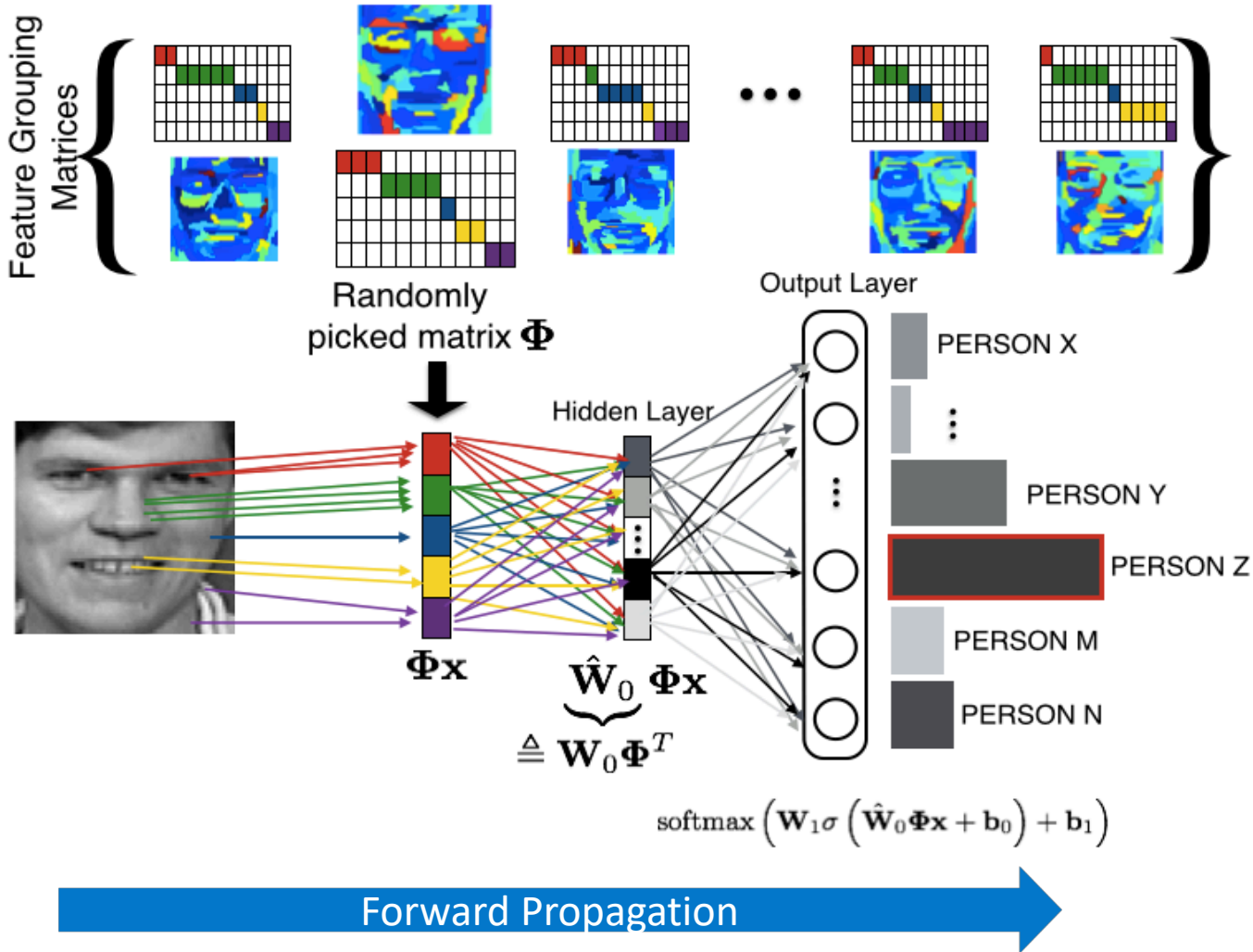
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7: **end while**



Proposed Approach

Re-define parameter space and project input onto lower dimensional space



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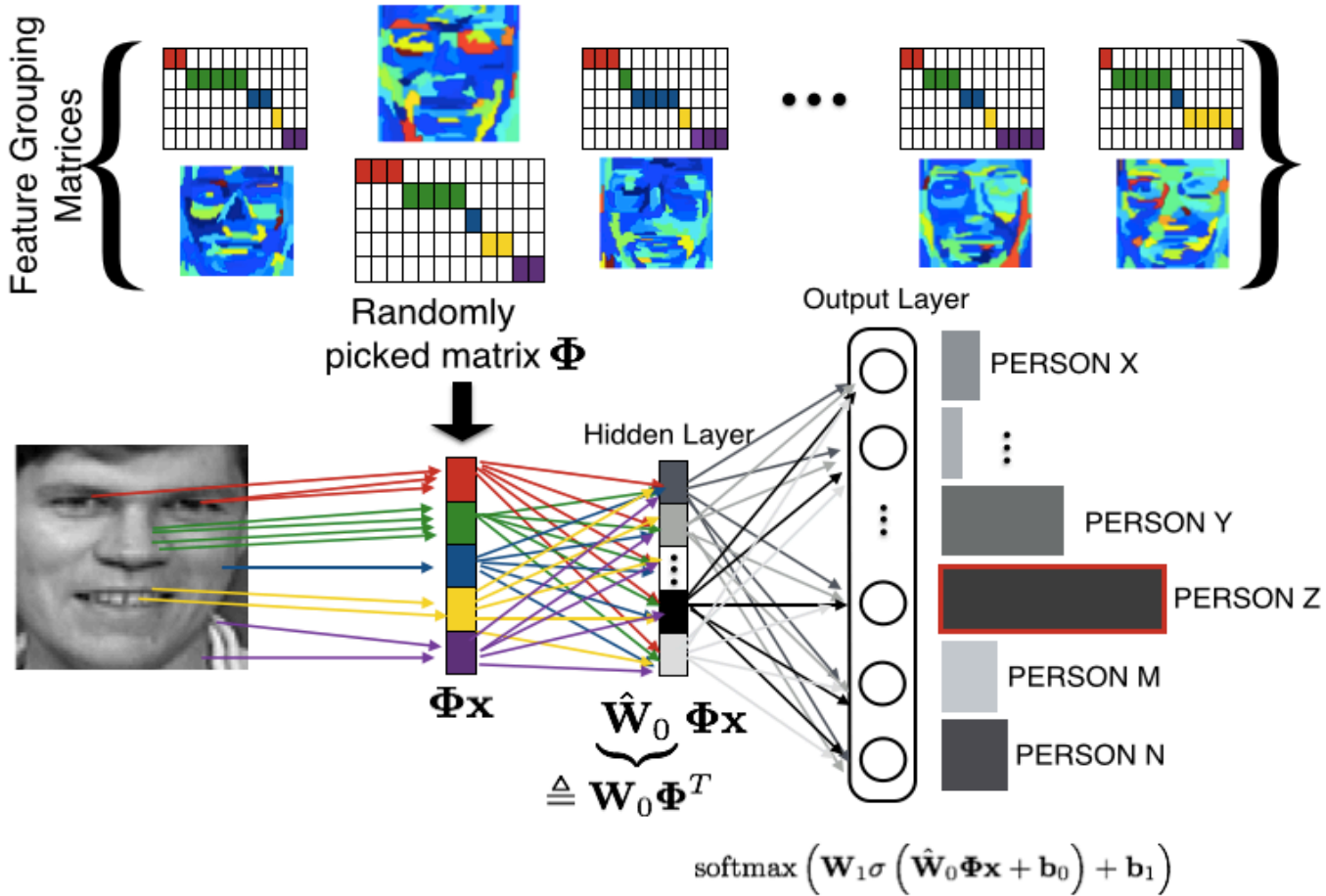
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7: **end while**



Proposed Approach

Apply back propagation



← Back Propagation



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for $j \in \{1, \dots, H\}$

7: **end while**

Proposed Approach

Update parameters

To update \mathbf{W}_0 , project gradients back to the original space.

Other terms are updated in a standard way.

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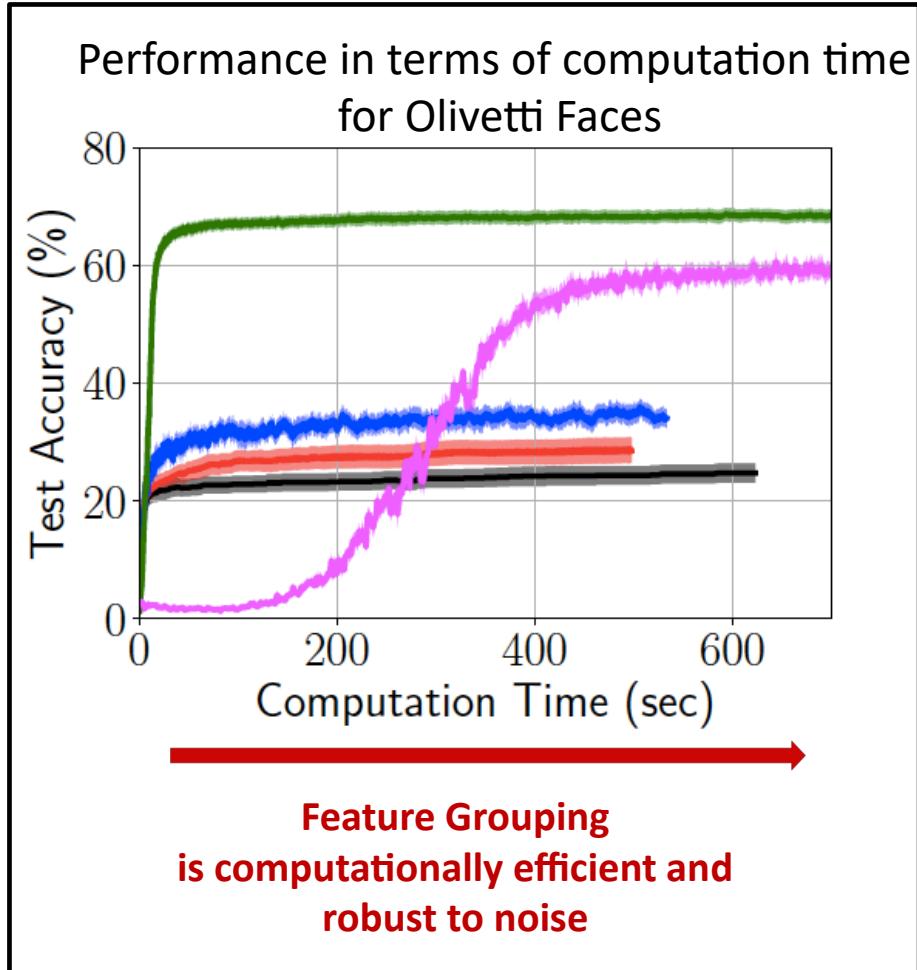
7: **end while**



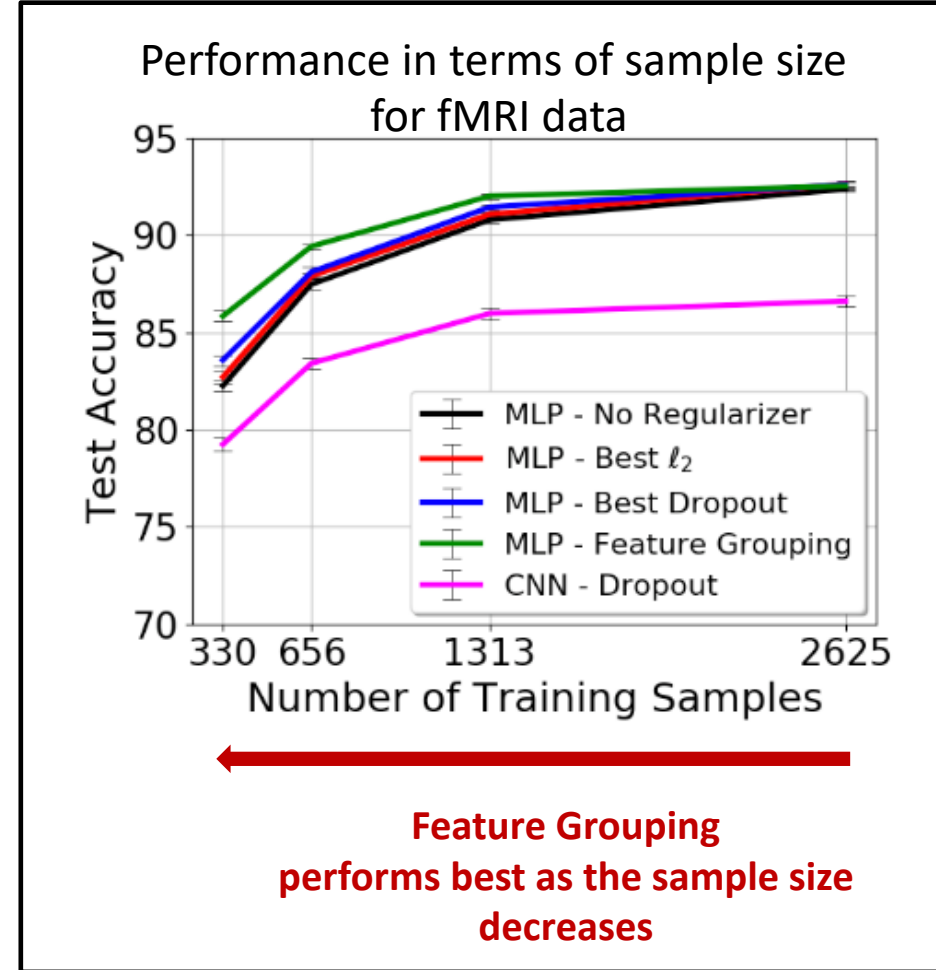
Experimental Results



Noisy Settings



Small-sample Settings





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