

Neural networks regularization through representation learning

✧ **PhD defense** ✧

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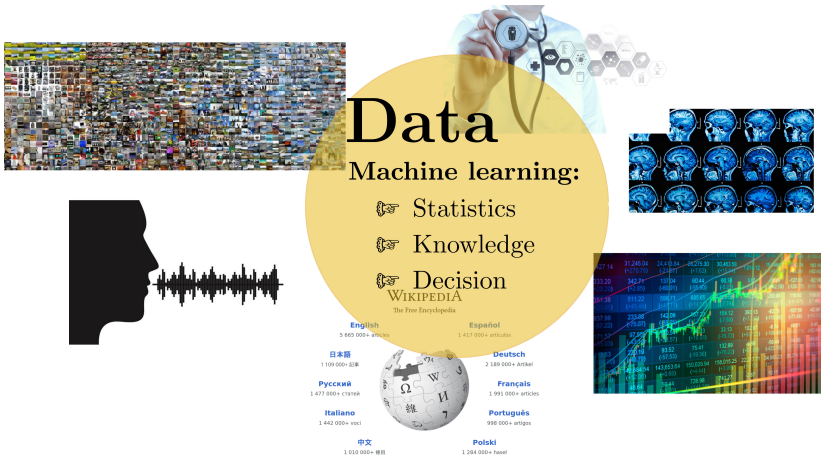
Jul. 06, 2018

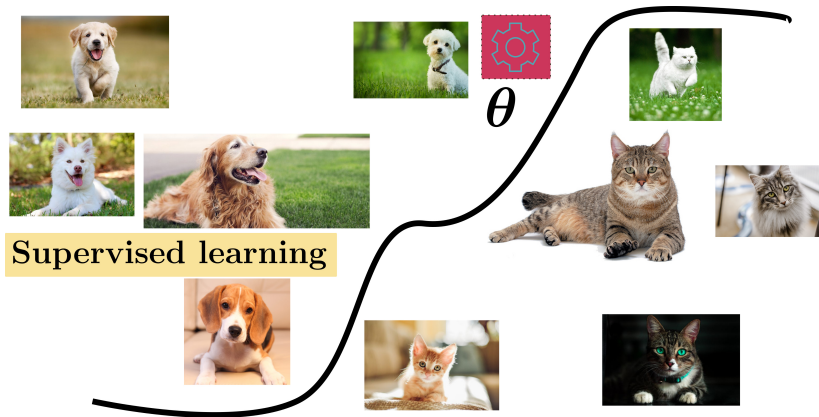


Introduction: Learning from data

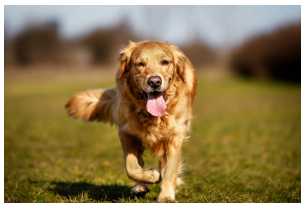
Introduction: Learning from data



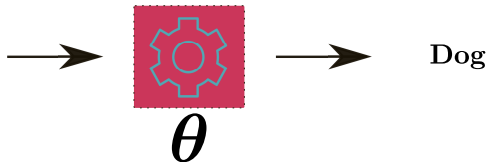


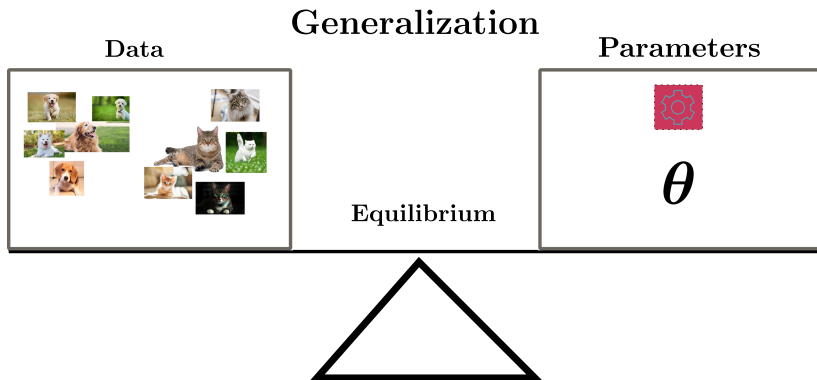


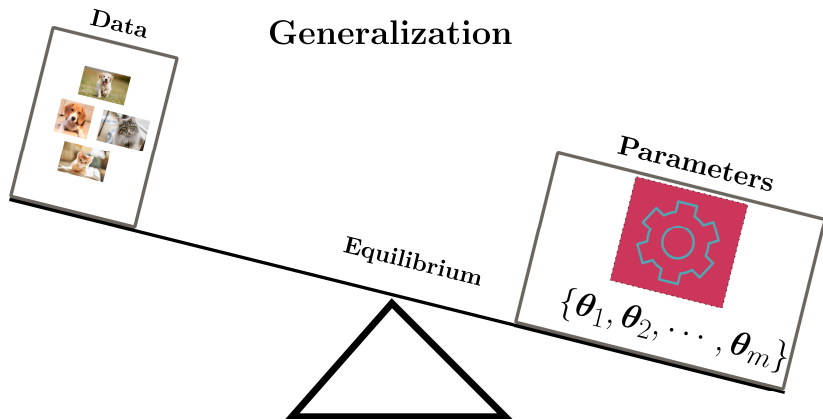
Prediction: Generalization

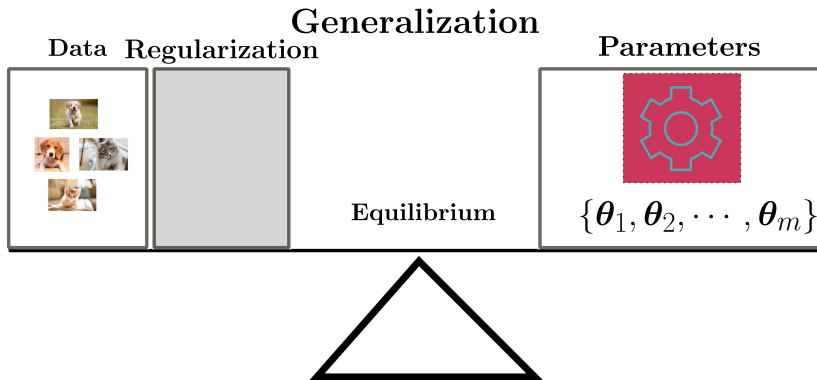


What is this?

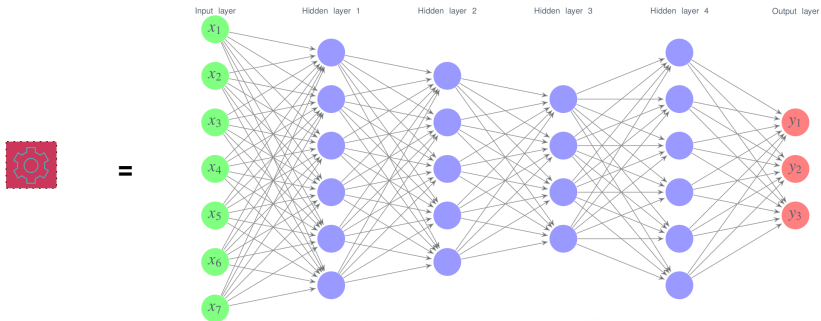


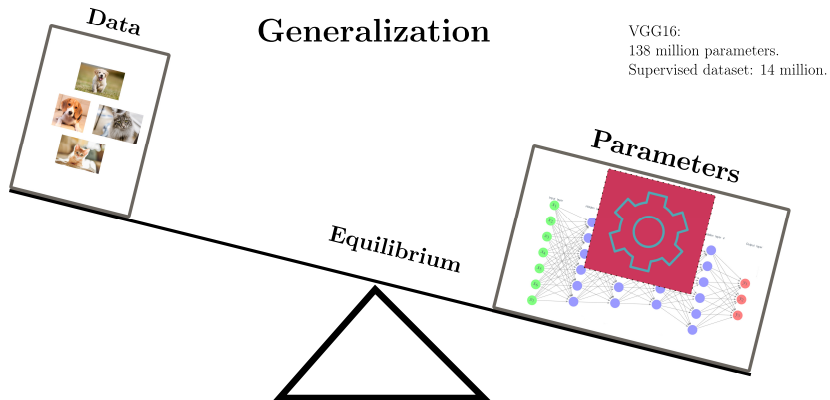


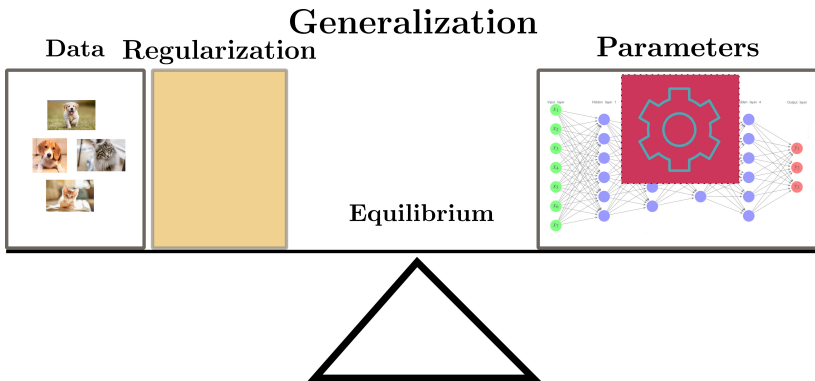




Introduction: Learning from data







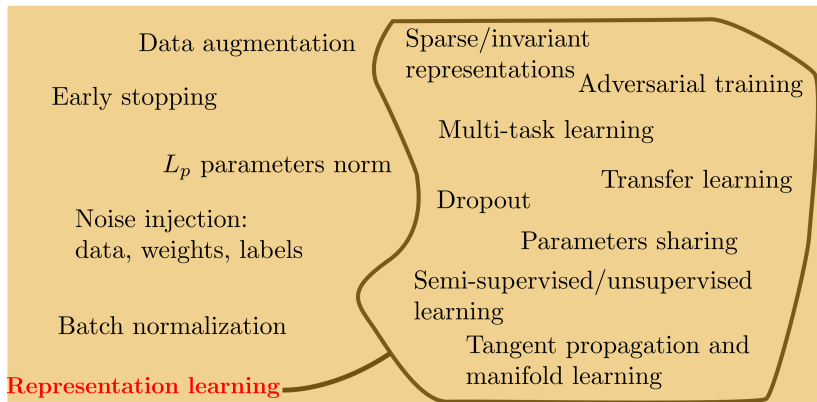
Neural networks regularization

Data augmentation
Early stopping
 L_p parameters norm
Noise injection:
data, weights, labels
Batch normalization

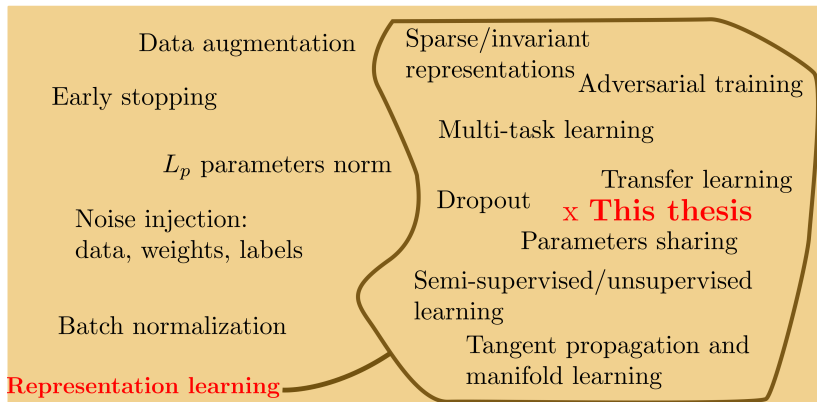
Sparse/invariant
representations
Adversarial training
Multi-task learning
Dropout
Parameters sharing
Semi-supervised/unsupervised
learning
Tangent propagation and
manifold learning

Transfer learning

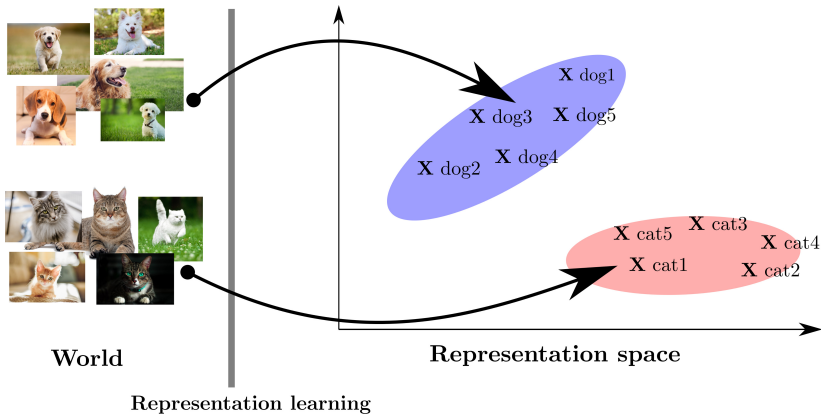
Neural networks regularization



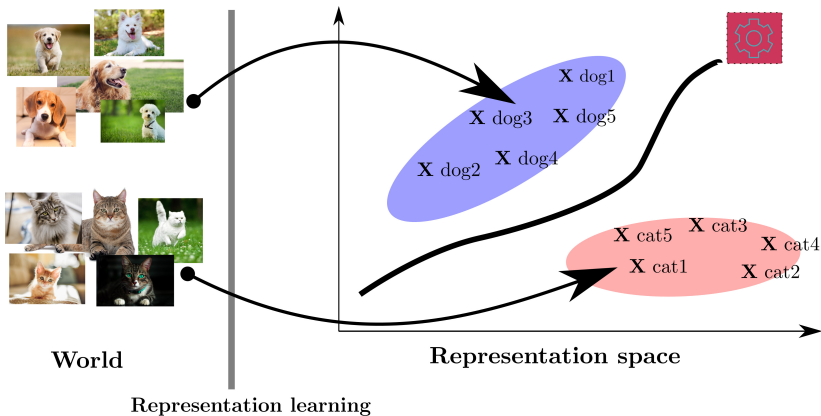
Neural networks regularization



Introduction: Learning from data



Introduction: Learning from data



PhD contributions

Contribution 1

☞ Unsupervised learning: Structured output prediction.



Contribution 2

☞ Prior knowledge: Classification.



Contribution 3 (medical application)

☞ Transfer learning: Regression.



Unsupervised learning for structured output predictions

➡ Traditional Machine Learning Problems $f : \mathcal{X} \rightarrow \mathcal{Y}$

➡ Inputs $\mathcal{X} \in \mathbb{R}^d$

➡ Outputs $\mathcal{Y} \in \mathbb{R}$ for the task: classification, regression, ...

➡ Machine Learning for *Structured Output* Problems $f : \mathcal{X} \rightarrow \mathcal{Y}$

➡ Inputs $\mathcal{X} \in \mathbb{R}^d$

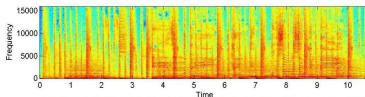
➡ Outputs $\mathcal{Y} \in \mathbb{R}^{d'}$, $d' > 1$, a structured object: **dependencies** among its components.

C. Lampert slides.

Structured output problems: Data and structure

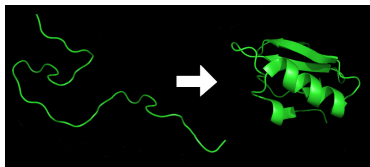
$$\text{Data} = \text{representation (values)} + \text{structure (dependencies)}$$

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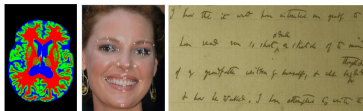


Text: part-of-speech tagging, translation

speech \leftrightarrow text



Protein folding



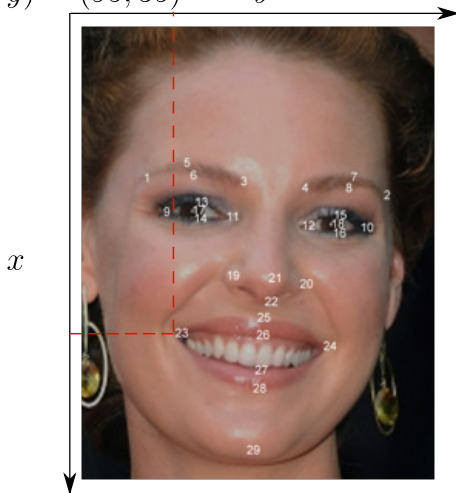
Image

Structured data

Structured output problems: Data and structure

Data = *representation* (values) + *structure* (dependencies)

Point 23: $(x, y) = (95, 35)$ y



Geometric
structured
data.

☞ Approaches that Deal with Structured Output Data:

- ☞ Kernel based methods: Kernel Density Estimation (KDE).
- ☞ Discriminative methods: Structure output SVM.
- ☞ Graphical methods: HMM, CRF, MRF,

⚠ Drawbacks:

- ⚠ Perform one single data transformation.
- ⚠ Most of them have difficulties to deal with *high dimensional* data.

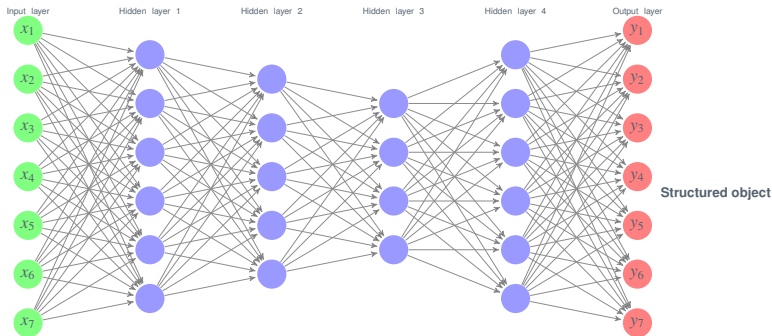
☞ Ideal approach:

- ☞ High dimension data.
- ☞ Multiple data transformations (complex mapping functions).

☞ **Neural networks!**

Structured output problems: Feedforward neural networks issue

High dimensional output:



- 👉 High dimension data. 😊
- 👉 Multiple data transformations (complex mapping functions). 😊
- ⚠️ No support to structured output. 😞
- ⚠️ Overfitting, output average structure. 😞

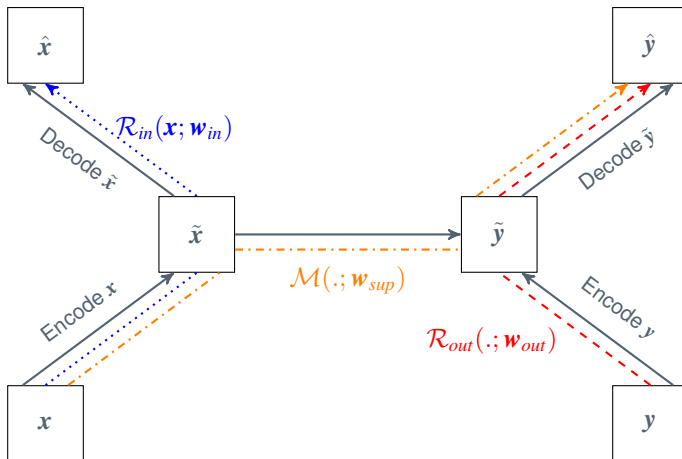
👉 Regularization through unsupervised learning.

Key idea:

Use **unsupervised** learning to **Learn/discover** the hidden **structure** of the output data.

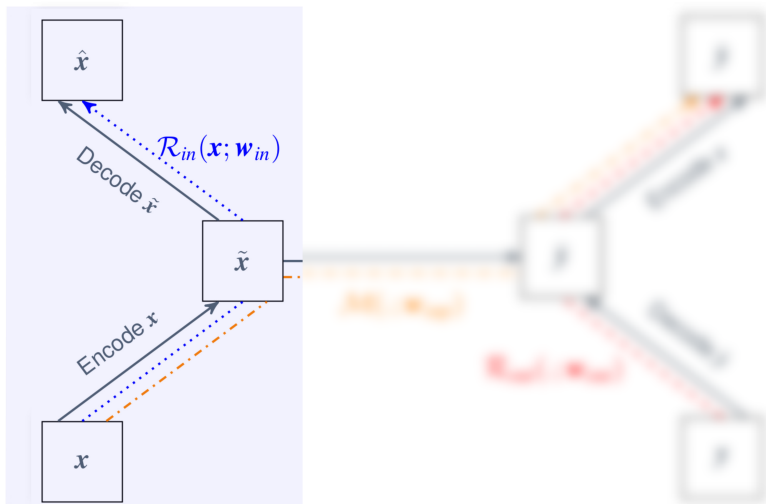
Structured output problems: Feedforward neural networks issue

> Unsupervised learning regularization > Proposed approach



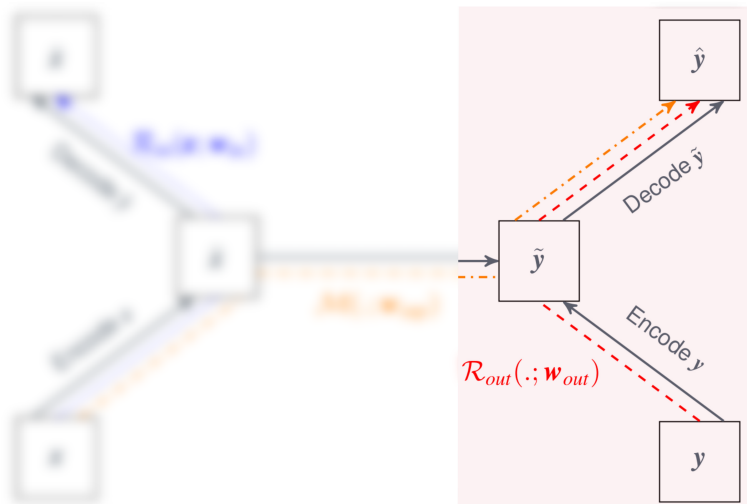
Structured output problems: Feedforward neural networks issue

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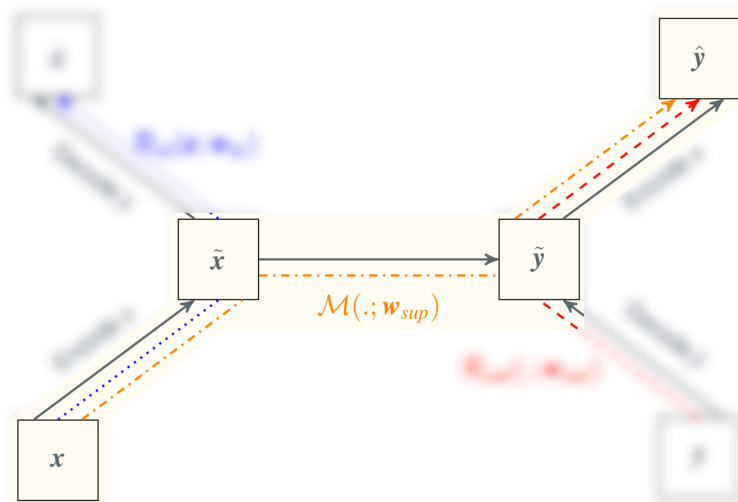
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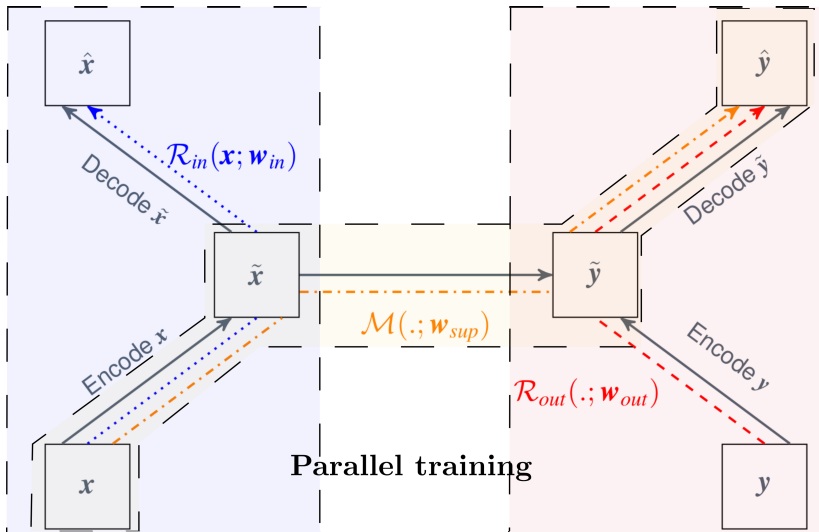
Structured output problems: Feedforward neural networks issue

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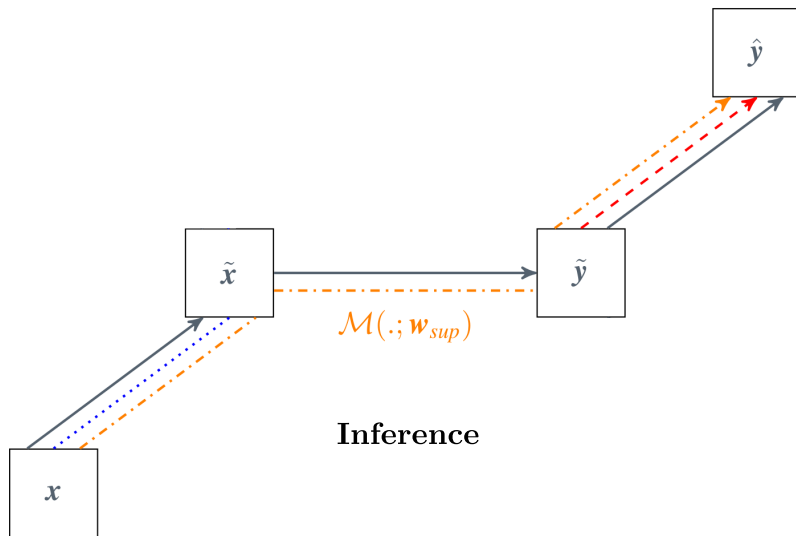
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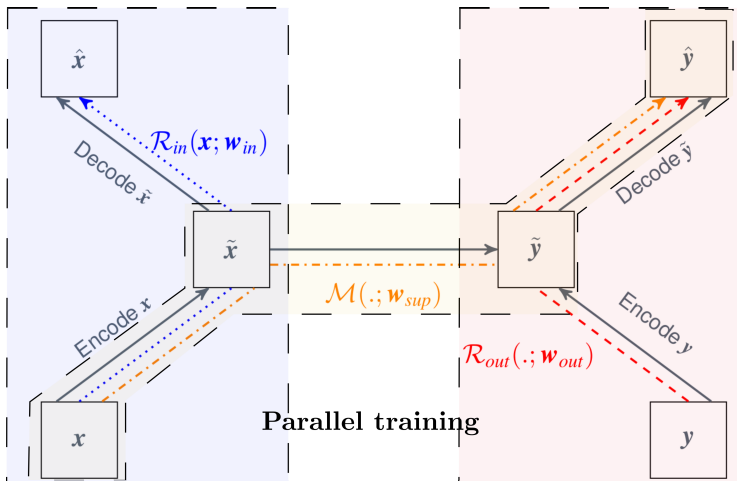
Structured output problems: Feedforward neural networks issue

> Unsupervised learning regularization > Proposed approach



Tasks combination:

$$J(\mathbb{D}; \mathbf{w}) = \lambda_{sup}(t) \cdot J_s(\mathbb{S}; \mathbf{w}_{sup}) + \lambda_{in}(t) \cdot J_{in}(\mathbb{F}; \mathbf{w}_{in}) + \lambda_{out}(t) \cdot J_{out}(\mathbb{L}; \mathbf{w}_{out}) .$$



Tasks combination:

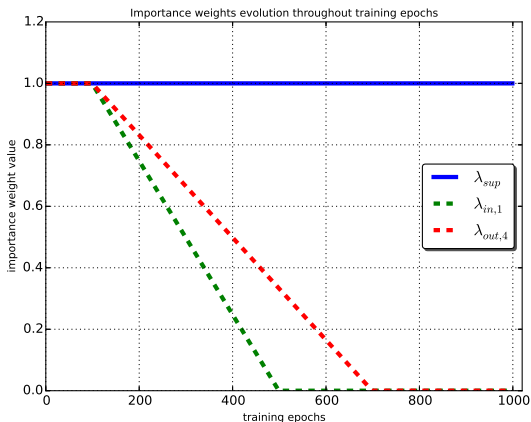
$$J(\mathbb{D}; \mathbf{w}) = \lambda_{sup}(t) \cdot J_s(\mathbb{S}; \mathbf{w}_{sup}) + \lambda_{in}(t) \cdot J_{in}(\mathbb{F}; \mathbf{w}_{in}) + \lambda_{out}(t) \cdot J_{out}(\mathbb{L}; \mathbf{w}_{out}) .$$

The framework training for one epoch

- 1: \mathbb{D} is a *shuffled* training set. \mathbb{B} a mini-batch.
 - 2: **for** \mathbb{B} in \mathbb{D} **do**
 - 3: $\mathbb{B}_S \leftarrow$ examples of \mathbb{B} that contain both (\mathbf{x}, \mathbf{y}) .
 - 4: $\mathbb{B}_F \leftarrow$ all the \mathbf{x} samples of \mathbb{B} .
 - 5: $\mathbb{B}_L \leftarrow$ all the \mathbf{y} samples of \mathbb{B} .
 - 6: Make a gradient step toward $\lambda_{in} \cdot J_{in}$ using \mathbb{B}_F . # Update \mathbf{w}_{in}
 - 7: Make a gradient step toward $\lambda_{out} \cdot J_{out}$ using \mathbb{B}_L . # Update \mathbf{w}_{out}
 - 8: Make a gradient step toward $\lambda_{sup} \cdot J_s$ using \mathbb{B}_S . # Update \mathbf{w}_{sup}
 - 9: **end for**
 - 10: Update λ_{sup} , λ_{in} and λ_{out} .
-

Tasks combination:

$$J(\mathbb{D}; \mathbf{w}) = \lambda_{sup}(t) \cdot J_s(\mathbb{S}; \mathbf{w}_{sup}) + \lambda_{in}(t) \cdot J_{in}(\mathbb{F}; \mathbf{w}_{in}) + \lambda_{out}(t) \cdot J_{out}(\mathbb{L}; \mathbf{w}_{out}) .$$



Linear adaptation of the importance weights during training. [Belharbi et al. 2016]

Task: Facial landmark detection. Localize 68 points (x,y).



Datasets: LFPW (1035 images), HELEN (2330 images).

Experimental results: Numerical quantification

AUC and **CDF_{0.1}** performance over LFPW test dataset with and without data augmentation. [Zhang,2014]

CDF_{0.1} \approx 95% cascaded networks + multiple supervised datasets.

	No augmentation		with augmentation	
	AUC	CDF _{0.1}	AUC	CDF _{0.1}
Mean shape	68.78%	30.80%	77.81%	22.33%
MLP	76.34%	46.87%	-	-
MLP + in	77.13%	54.46%	80.78%	67.85%
MLP + out	80.93%	66.51%	81.77%	67.85%
MLP + in + out	81.51%	69.64%	82.48%	71.87%

AUC and **CDF_{0.1}** performance over HELEN test dataset with and without data augmentation. [Zhang,2014]

CDF_{0.1} \approx 95% cascaded networks + multiple supervised datasets.

	No augmentation		With augmentation	
	AUC	CDF _{0.1}	AUC	CDF _{0.1}
Mean shape	64.60%	23.63%	64.76%	23.23%
MLP	76.26%	52.72%	-	-
MLP + in	77.08%	54.84%	79.25%	63.33%
MLP + out	79.63%	66.60%	80.48%	65.15%
MLP + in + out	80.40%	66.66%	81.27%	71.51%

Structured output problems: Feedforward neural networks issue

> Unsupervised learning regularization > Proposed approach > Experiments



LFPW test set. Red segments: ground truth \longleftrightarrow prediction. Top row: MLP. Bottom row: MLP+in+out.

Structured output problems: Feedforward neural networks issue

> Unsupervised learning regularization > Proposed approach > Conclusion

Conclusion:

- ✚ Generic regularization scheme for structured output problems based on transfer learning.
- ✚ Exploit input/output unlabeled data.
- ✚ Speedup convergence and improve generalization.
- ✚ Code at github:

<https://github.com/sbelharbi/structured-output-ae>

Perspectives:

- ✚ Adapt the importance weight according to the train/validation error.
⇒ Toward automatic schedules.
- ✚ Use generative models to learn the output structure (VAEs, GANs).

Publications:

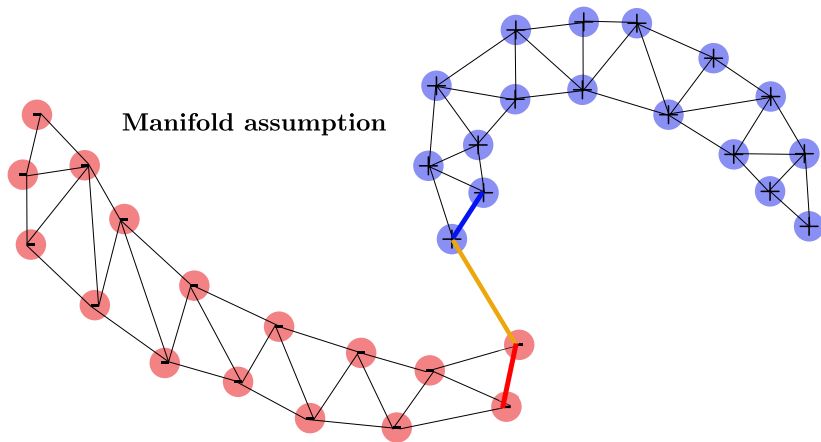
- ✚ S. Belharbi, R. Héroult, C. Chatelain and S. Adam. **Deep Neural Networks Regularization for Structured Output Prediction**, Neurocomputing, vol. 281C, pp. 169-177, 2018.
- ✚ S. Belharbi, R. Héroult, C. Chatelain, S. Adam. **Deep Multi-Task Learning with evolving weights**. European Symposium on Artificial Neural Networks, Computational Intelligence and Machine Learning (ESANN) (talk). 2016.
- ✚ S. Belharbi, C. Chatelain, R. Héroult, S. Adam. **Learning Structured Output Dependencies using Deep Neural Networks**. Deep Learning workshop, International Conference on Machine Learning (ICML), 2015.



Prior knowledge for classification

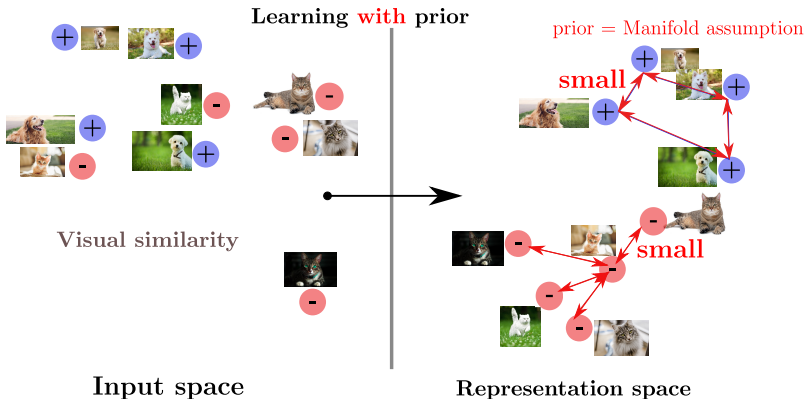
Learning representations in a neural network for classification:

Intuition & motivation



Learning representations in a neural network for classification:

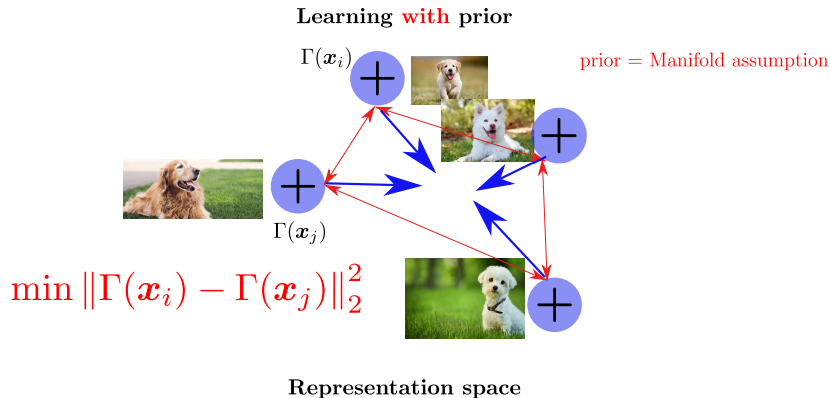
Intuition & motivation



- 👉 Our goal:
Learn **invariant representations** within each class (class-wise).
- 👉 Related to:
Linear discriminant analysis (Fisher criterion)^[Sugiyama, 07], metric learning (Siamese networks).

Learning representations in a neural network for classification:

Intuition & motivation



Learning representations in a neural network for classification:

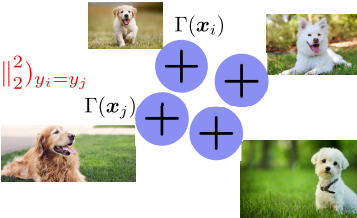
Intuition & motivation

Learning **with** prior

prior = Manifold assumption

$$\min \bar{\sum} (\|\Gamma(\mathbf{x}_i) - \Gamma(\mathbf{x}_j)\|_2^2)_{y_i=y_j}$$

Regularization



Representation space

Training objective:

$$J(\mathbb{D}; \theta) = \underbrace{\sum_{(x,y) \in \mathbb{D}} \mathcal{C}_{sup}(\mathcal{M}(x_i), y_i)}_{\text{standard classification loss } J_{sup}} + \lambda \underbrace{\sum_{(x,y) \in \mathbb{D}} (\|\Gamma(\mathbf{x}_i), \Gamma(\mathbf{x}_j)\|_2^2)_{y_i=y_j}}_{\text{invariance loss } J_I}.$$

Learning representations in a neural network for classification:

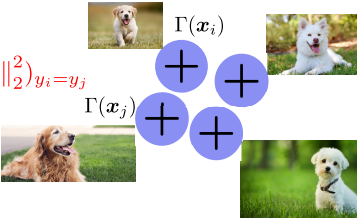
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Learning representations in a neural network for classification:

Proposed approach > Formulation

Training objective:

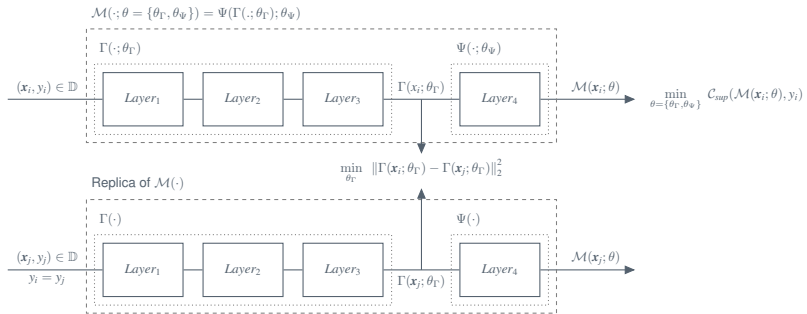
$$J(\mathbb{D}; \theta) = \underbrace{\sum_{(\mathbf{x}, y) \in \mathbb{D}} \mathcal{C}_{sup}(\mathcal{M}(\mathbf{x}_i), y_i)}_{\text{standard classification loss } J_{sup}} + \lambda \underbrace{\sum_{(\mathbf{x}, y) \in \mathbb{D}} (\|\Gamma(\mathbf{x}_i) - \Gamma(\mathbf{x}_j)\|_2^2)_{y_i=y_j}}_{\text{invariance loss } J_r} .$$

Training strategy

- 1: \mathbb{D} is a training set.
 - 2: \mathbb{B}_s a mini-batch. \mathbb{B}_r a mini-batch of all the possible pairs in \mathbb{B}_s .
 - 3: OP_s an optimizer of the supervised term. OP_r an optimizer of the dissimilarity term.
 - 4: max_epochs: maximum epochs. λ is a regularization weight.
 - 5: **for** $i = 1$ **to** max_epoch **do**
 - 6: Shuffle \mathbb{D} . Then, split it into mini-batches.
 - 7: **for** $(\mathbb{B}_s, \mathbb{B}_r)$ in \mathbb{D} **do**
 - 8: Make a gradient step toward J_{sup} using \mathbb{B}_s and OP_s .
 - 9: Make a gradient step toward J_r using \mathbb{B}_r and OP_r .
 - 10: **end for**
 - 11: **end for**
-

Learning representations in a neural network for classification:

Proposed approach > Formulation



Constraining the intermediate learned representations to be similar over a decomposed network $\mathcal{M}(\cdot)$ during the *training phase*.

Benchmarks: 10 classes.



Samples from training set of each benchmark. Top row: **mnist-std** benchmark. Middle row: **mnist-noise** benchmark. Bottom row: **mnist-img** benchmark (MNIST + CIFAR 10).

👉 Study the effect of the size of train set: *1k*, *3k*, *5k*, *50k* and *100k*.

Models: two each one has 4 layers.

👉 **Multilayer perceptron (*mlp*)**: 1200 – 1200 – 200.

👉 **LeNet convolutional network (*lenet*)**: $(20, 5 \times 5)$, $(50, 5 \times 5)$, 500.

Reference to layers (from input to output): h_1, h_2, h_3, h_4 .

Empirical results:

👉 Apply the regularization at the last hidden layer (h_3).

Results on **mnist-noise** and **mnist-img** using *lenet*:

Model/train data size	1k	3k	5k	100k
	Test error			
	<i>mnist-std</i>			
<i>lenet</i>	7.27 ± 0.033	4.02 ± 0.073	2.90 ± 0.058	-
<i>lenet</i> + <i>reg.</i>	5.05 ± 0.115	2.85 ± 0.082	2.37 ± 0.105	-
	<i>mnist-noise</i>			
<i>lenet</i>	10.72 ± 0.116	6.39 ± 0.032	5.11 ± 0.012	2.011 ± 0.018
<i>lenet</i> + <i>reg.</i>	7.74 ± 0.148	4.62 ± 0.059	3.98 ± 0.167	1.64 ± 0.116
	<i>mnist-img</i>			
<i>lenet</i>	15.34 ± 0.124	8.66 ± 0.024	6.46 ± 0.033	2.55 ± 0.007
<i>lenet</i> + <i>reg.</i>	11.18 ± 0.290	6.61 ± 0.212	5.65 ± 0.310	2.21 ± 0.032

Mean \pm standard deviation error over validation and test set of the benchmarks *mnist-noise* and *mnist-img* using *lenet* model (regularization applied over the layer h_3).
(**bold font indicates lowest error.**)

Conclusion:

- 👉 Our proposal helps improving the network generalization (small train set).
 - 👉 Toward more explicit constraints/priors.
-

Publications:

- 👉 S. Belharbi, C. Chatelain, R. Hérault and S. Adam. ***Neural Networks Regularization Through Class-wise Invariant Representation Learning***, Under modification.
arxiv.org/abs/1709.01867, 2018.

Transfer learning for medical domain

✿ Medical application ✿

Problem setup: L3 slice localization in CT scans

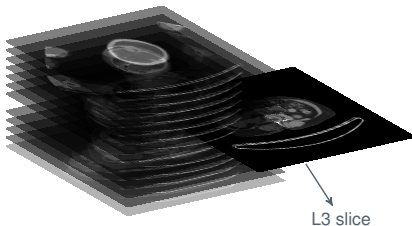
Context: Collaboration with Henri-Becquerel center at Rouen (cancer).

Main goal: Estimate the sarcopenia¹ level from a computerized tomography (CT) scan based only on the third lumbar vertebra (L3).

☞ A CT scan is stack of N slices (2D images). ☞ N is variable.

☞ In a CT scan, a specific slice is selected to represent the L3.

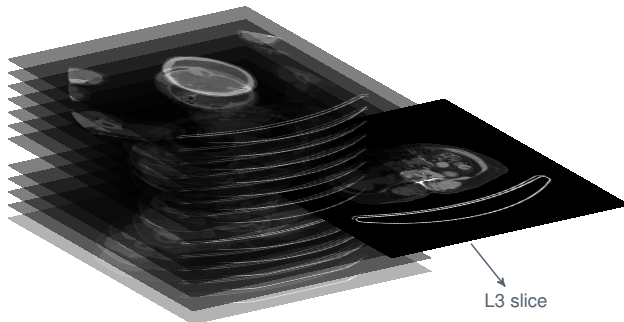
⇒ Need to locate the slice representing the third lumbar vertebra.



Find the L3 slice within a whole CT scan.

1. Sarcopenia: loss of skeletal muscle mass.

Problem setup: L3 slice localization in CT scans



Finding the L3 slice within a whole CT scan.

L3CT1:

a dataset composed of **642 CT scans** provided by Henri-Becquerel center.

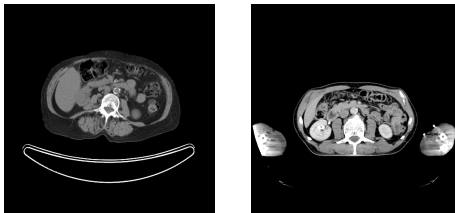
Available annotation:

the **position** of the **3rd lumbar vertebra**. (i.e., the **number** of the **correct slice** in the CT scan)

Problem setup: L3 slice localization in CT scans

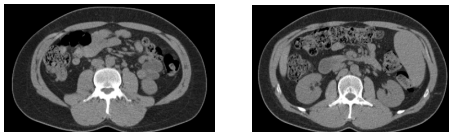
Problems:

- ⚠ Inter-patients **variability**.



L3 slices from two different patients: [Left] Patient A. [Right] Patient B.

- ⚠ Visual **similarity** of the **vertebrae** slices of the same patient.



Two slices from the same patient: [Left] an L3 slice. [Right] a non L3 slice.

- 👉 The need to use the **context** to localize the L3 slice.

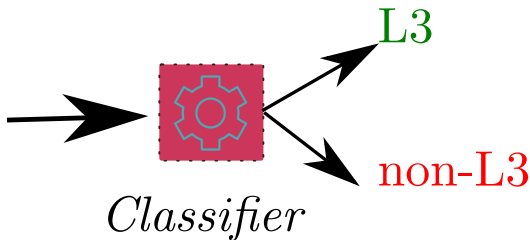
👉 **Machine Learning!**

Classification (discrete value) [X]

Classify each slice for: "L3" or "Not L3":

☞ Simple. 😊

⚠ No context. 😞

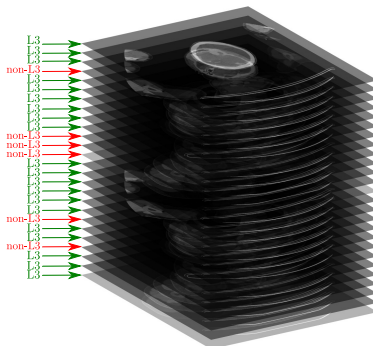
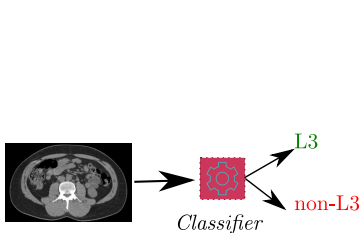


Classification (discrete value) [X]

Classify each slice for: "L3" or "Not L3":

👉 Simple. 😊

⚠️ No context. 😞



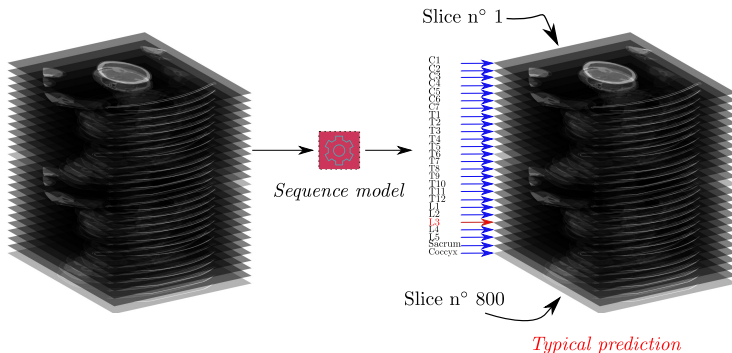
Typical prediction (no context)

L3 problem: Possible solutions > Sequence: [X]

Sequence labeling [X]

Label all the slices (vertebrae): L1, L2, L3, ...:

- ☞ Global analysis: context. 😊
- ☞ Existing work with promising results. 😊
- ⚠ Requires labeling more than one slice. ☹

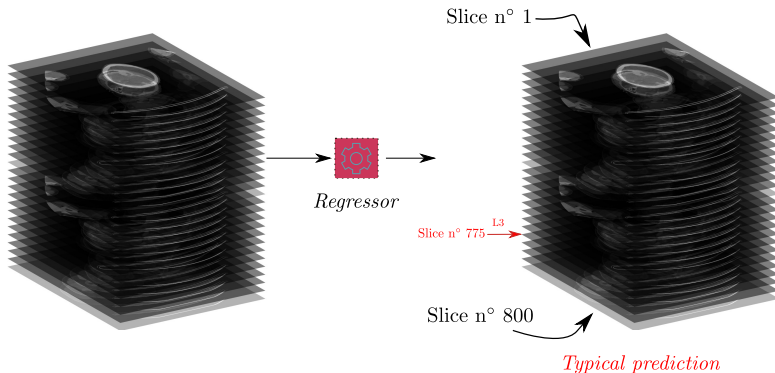


Regression (real value) [✓]

Predict the height (position) of the L3 slice inside the CT scan:

✎ Global analysis: context. 😊

✎ Requires labeling only the L3 slice position. 😊



Which model for regression?

- State of the art in computer vision: Deep learning, **convolutional neural network (CNN)**.
- Requires fixed input size (when using dense layers).
- Needs a large number of training samples.

Issues

- High dimension input: $1 \text{ scan} = N \times 512 \times 512$, with $400 < N < 1200$.
Problem 1: large input space
- Implies: **Variability** of the height of each scan (depends on N).
Problem 2: Different input size
- Dataset with annotated L3 position: **642 patients**. (L3CT1 dataset)
Problem 3: few training data

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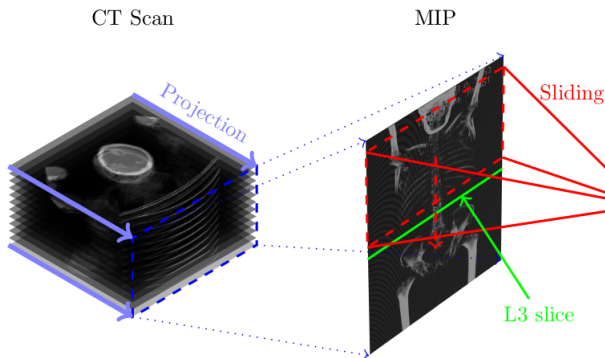
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Proposed approach: Regression for L3 localization

Issue 1: High dimension input > Solution: Frontal MIP

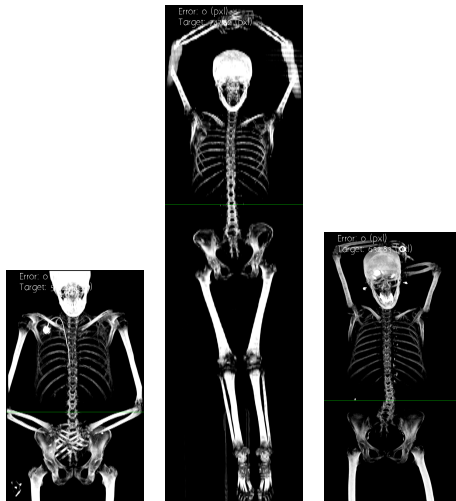
Problem 1: High dimension input

- 131M inputs for one example (large input dimension):
 - Frontal or lateral **Maximum Intensity Projection (MIP)**.
- $512 \times 512 \times N \Rightarrow 512 \times N$.
- Preserves pertinent information (skeletal structure).



Proposed approach: Regression for L3 localization

Issue 2: Different input size > Solution: Sliding window



Examples of normalized frontal MIP images with the L3 slice position.

Problem 2: Different input size

Classical problem in computer vision

👉 Sliding window technique

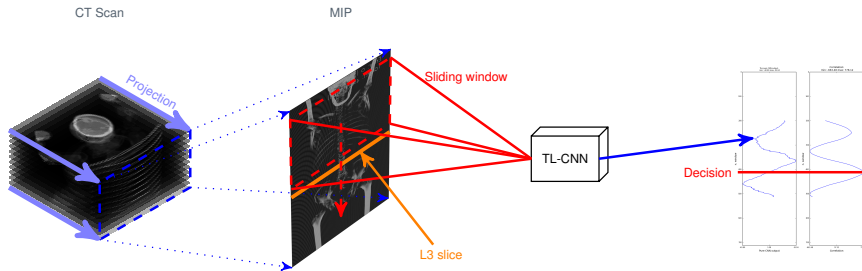
👉 Post-processing



Examples of normalized frontal MIP images with the L3 slice position.

Proposed approach: Regression for L3 localization

Issue 2: Different input size > Solution: Sliding window



1 MIP transformation

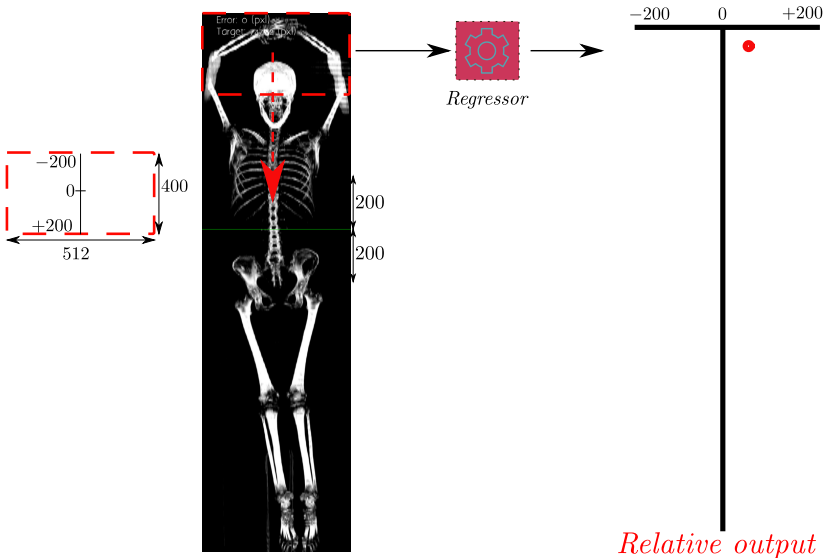
2 CNN prediction

3 Post processing
(Correlation)

Sliding window

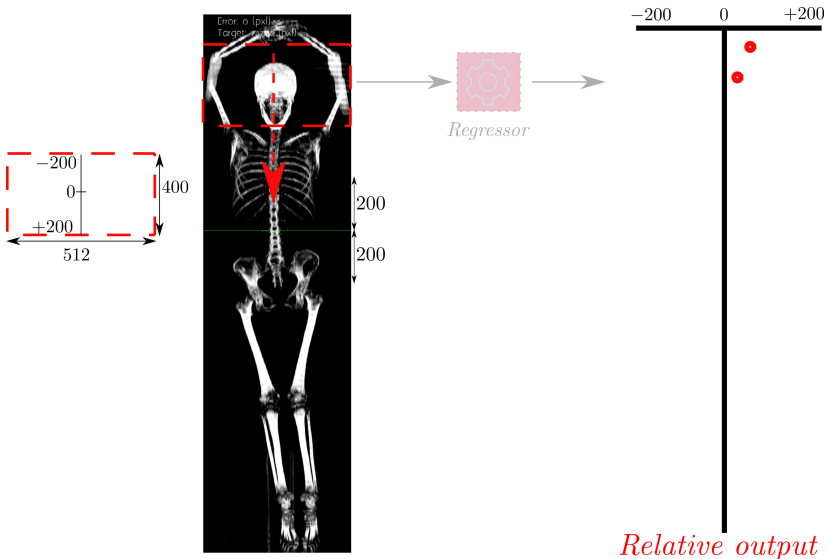
Proposed approach: Regression for L3 localization

Issue 2: Different input size > Solution: Sliding window



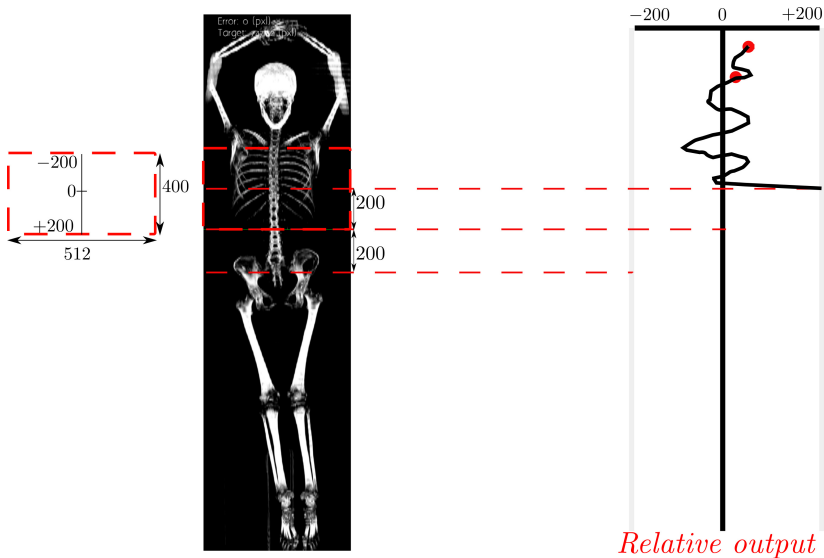
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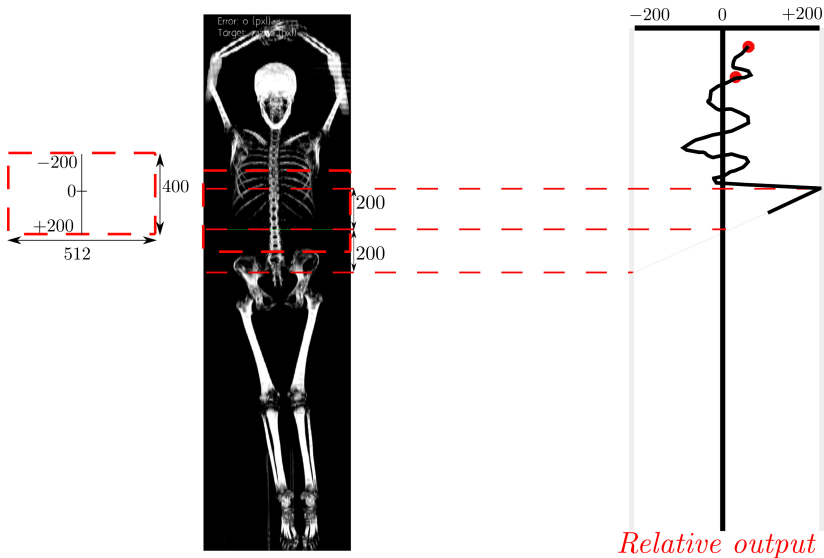
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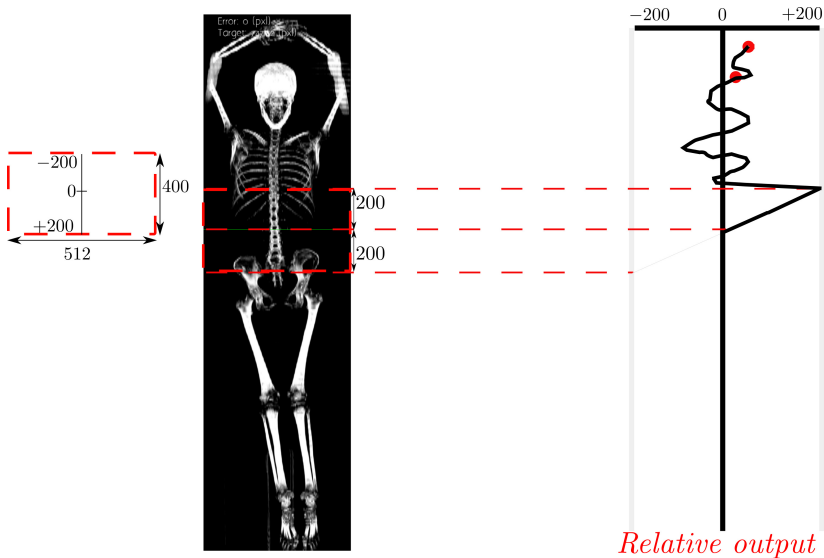
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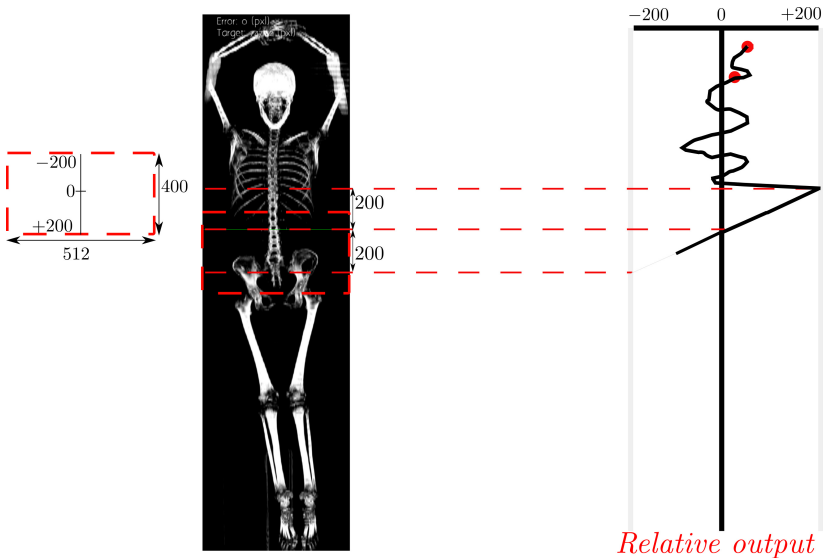
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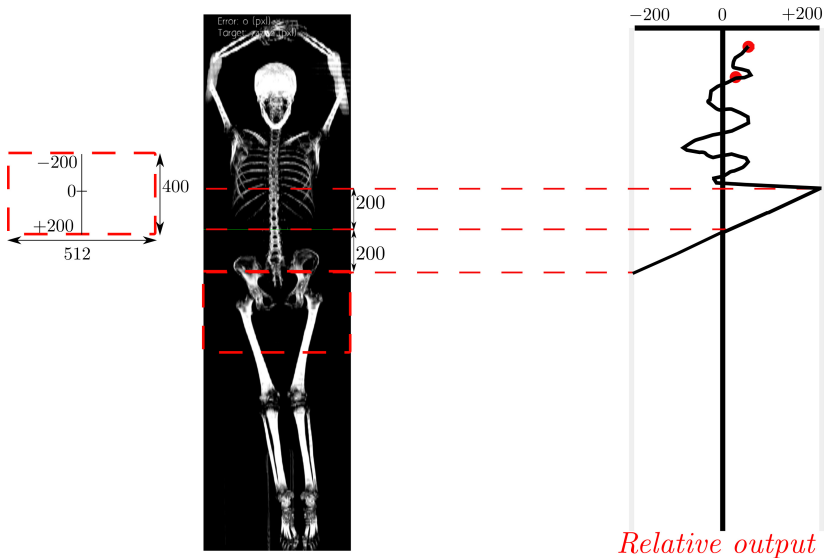
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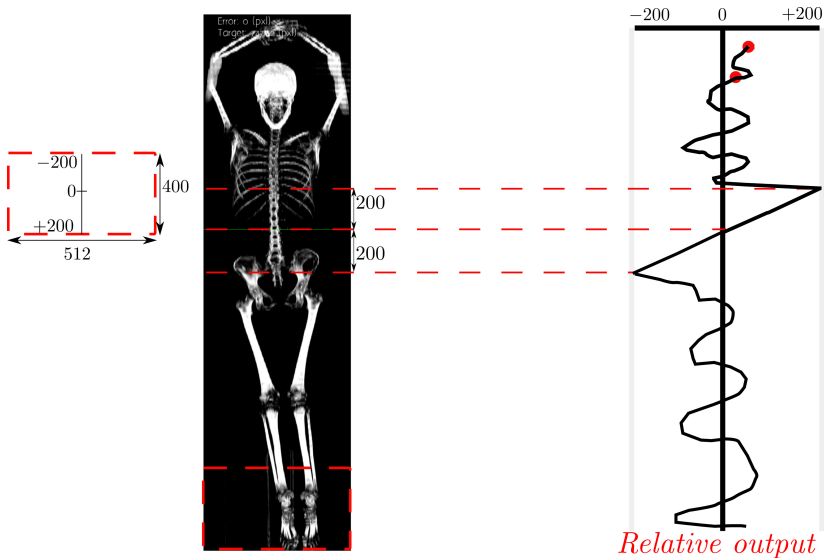
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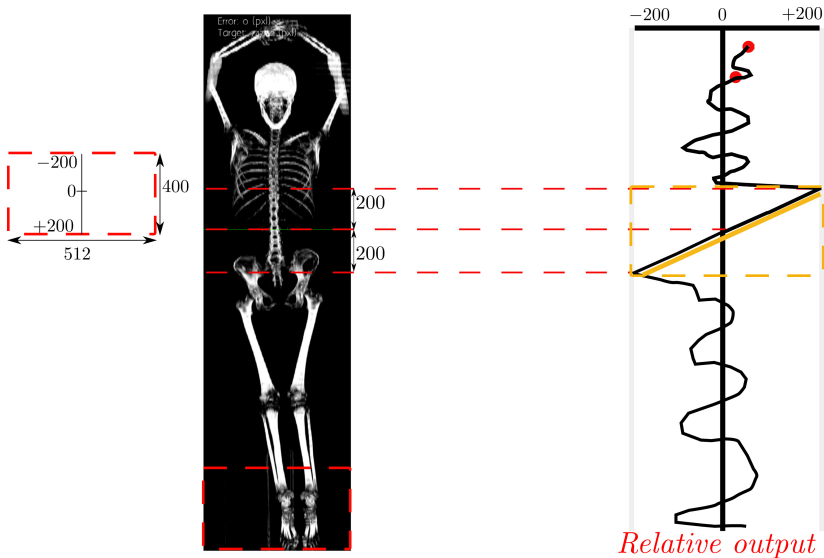
Proposed approach: Regression for L3 localization

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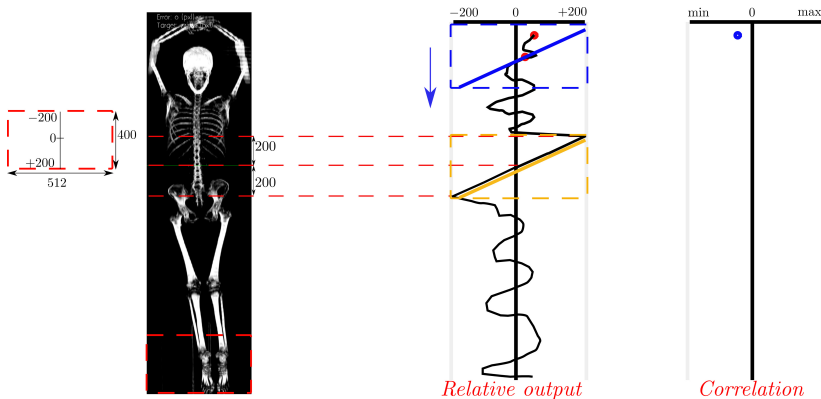
Proposed approach: Regression for L3 localization

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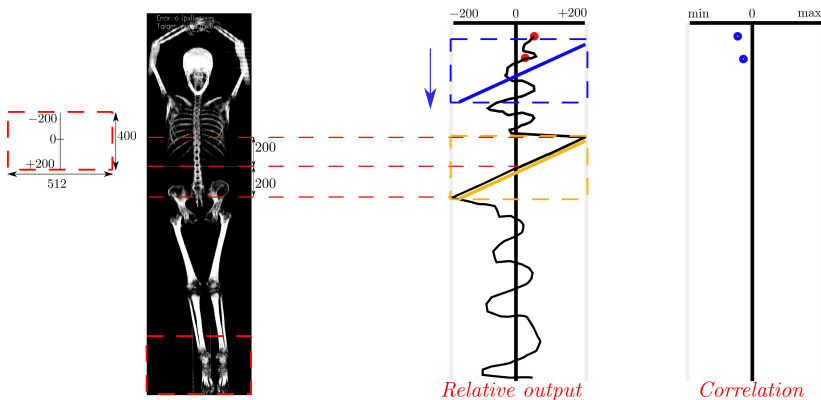
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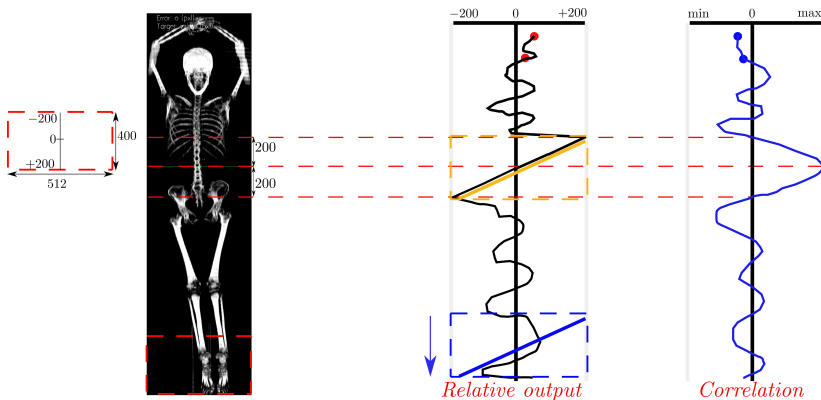
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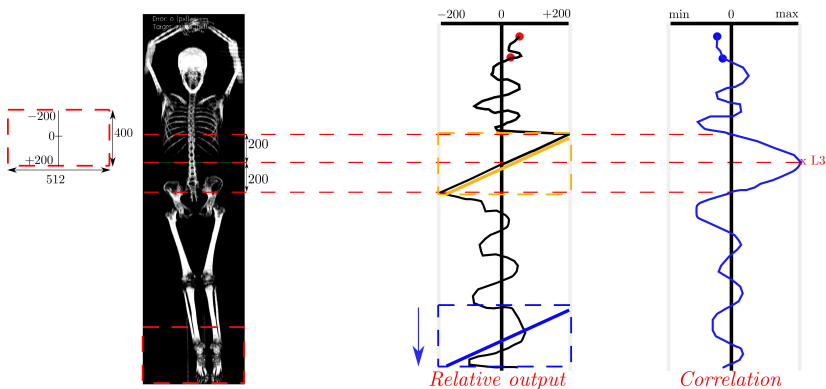
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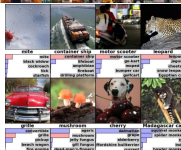
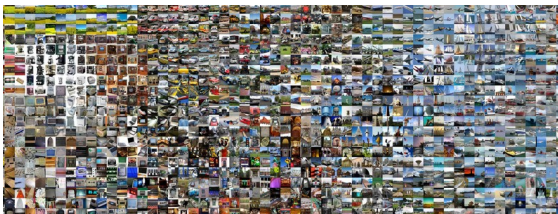


Proposed approach: Regression for L3 localization

Issue 3: Lack of data → Solution: Transfer learning

Problem 2: Few data (642 patients)

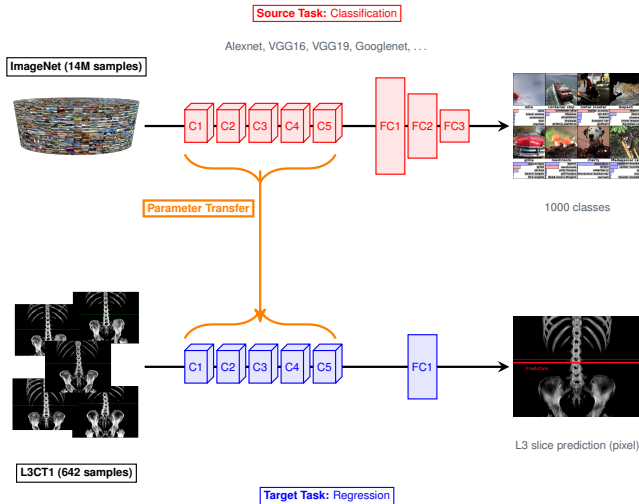
- ✎ Use pre-trained CNNs over **large datasets**
 - ✎ Alexnet, GoogleNet, VGG16, VGG19, ... for **classification**
 - ✎ Pre-trained models over ImageNet: 14 millions of natural images [Fei-Fei and Russakovsky 2013].



Source task with abundant data.

Proposed approach: Regression for L3 localization

Issue 3: Lack of data > Solution: Transfer learning



System training using transfer learning.

Proposed approach: Regression for L3 localization

Experiments: Quantitative results

Cross-validation:

	RF500	CNN4	Pre-trained			
			Alexnet	VGG16	VGG19	Googlenet
Average cross-validation error (5 folds) (slice)	10.50 ± 10.80	2.78 ± 2.48	2.45 ± 2.42	1.82 ± 2.32	1.83 ± 1.83	2.54 ± 4.22
Number of parameters	—	55 K	2 M	14 M	20 M	6 ¹ M
Average processing time (second/CT scan) (K40)	—	04.46	06.37	13.28	16.02	17.75 ¹

RF500 (random forest with 500 decision trees), CNN4 (Homemade model), and Alexnet/VGG16/VGG19/GoogLeNet (Pre-trained models).

Possible speedup: reduce the number of sampled windows \Rightarrow Increase stride.

Example VGG16:

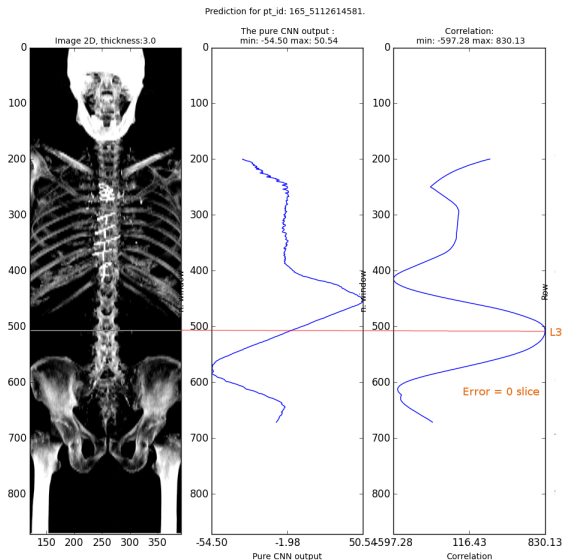
👉 **stride=1:** ~ 13 seconds/CT scan with a an error of **1.82 ± 2.32** .

👉 **stride=4:** ~ 02 seconds/CT scan with a an error of **1.91 ± 2.69** .

1. Due to implementation.

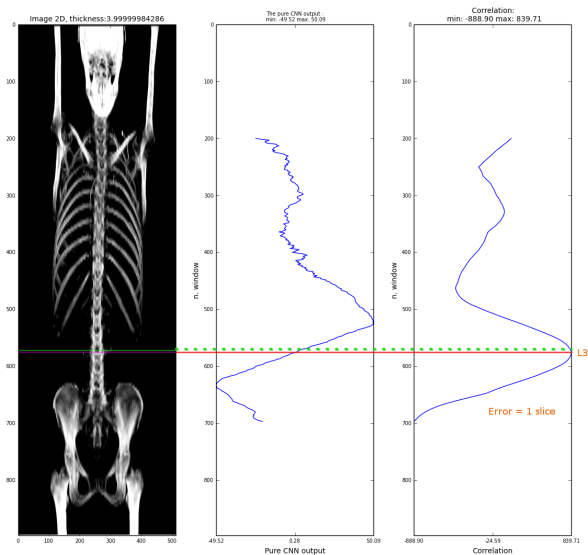
Proposed approach: Regression for L3 localization

Experiments: Qualitative results



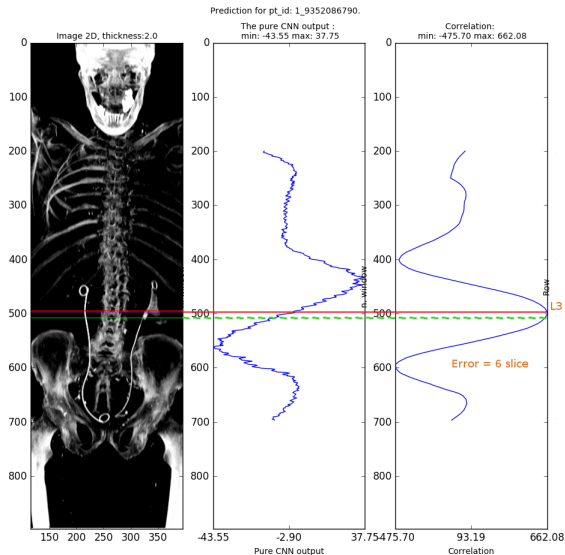
Proposed approach: Regression for L3 localization

Experiments: Qualitative results



Proposed approach: Regression for L3 localization

Experiments: Qualitative results



Setup: Intra-annotator variability

- ➡ New evaluation set: 43 CT scans annotated by the same reference radiologist (who annotated the L3CT1 dataset).
- ➡ Ask 3 other radiologists to localize the L3 slice.
- ➡ Perform this experiment twice: t_1, t_2 .

Errors (slices) / operator	Radiologist #1	Radiologist #2	Radiologist #3
t_1	0.81 ± 0.97	0.72 ± 1.51	0.51 ± 0.62
t_2	0.77 ± 0.68	0.95 ± 1.61	0.86 ± 1.30

Intra-annotator variability.

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Errors (slices) / operator	Radiologist #1	Radiologist #2	Radiologist #3	CNN4	VGG16
t_1	0.81 ± 0.97	0.72 ± 1.51	0.51 ± 0.62	2.37 ± 2.30	1.70 ± 1.65
t_2	0.77 ± 0.68	0.95 ± 1.61	0.86 ± 1.30	2.53 ± 2.27	1.58 ± 1.83

Performance radiologists vs. automatic systems.

Proposed approach: Regression for L3 localization

Conclusion

- Adapted pipeline for L3 localization: pre-processing, CNN, post-processing.
- Obtained average error: 1.82 slice ($< 5mm$) (maximum error: 9 slices).
 - Average thickness of a vertebra $\approx 2.5cm \Rightarrow$ Still within the L3 vertebra.
- Learn context: sliding window (double checked using correlation: context over multiple windows.)
- Generic framework: can be easily adapted for detecting other subjects given the required annotation.
- Use of transfer learning alleviates the lack of training data.

Perspectives: ⚠ Running time of VGG16 over CPUs is time consuming.

- Possible solution: Prune unnecessary convolution filters.

Valorization:

- Integrate this work with the software of the projet “**BodyComp.AI**” (diffused to European centers for cancer treatment).
- “**BodyComp.AI**” has won one of the 2017 French Innovative Unicancer Prize.

Publications:

- S. Belharbia, C. Chatelain, R. Hérault, S. Adam, S. Thureau, M. Chastan, and R. Modzelewski. *Spotting L3 slice in CT scans using deep convolutional network and transfer learning*, Computers in Biology and Medicine, vol. 87, pp. 95-103, 2017.



General conclusion & perspectives

- ➡ Possible **improvements** in the **generalization** of neural networks through the use of **regularization** based on **representation learning** paradigm in different applications (few training data):
 - ➡ Structured output problems: Unsupervised learning.
 - ➡ Classification: Invariant representations prior.
 - ➡ Object localization: Transfer learning.

☞ Improve neural networks generalization through:

☞ Integrating priors/common sense.

☞ Reduce the dependency to statistics.

☞ Require less training data.

☞ Use well studied data representations methods as hidden layers.

☞ Mimic dictionary learning.

Dictionary learning:

$$\arg \min_{D \in \mathbb{C}, r_i \in \mathbb{R}^d} \sum_{i=1}^N \|x_i - Dr_i\|_2^2, \text{ where } \mathbb{C} \equiv \{D \in \mathbb{R}^{d \times K} : \|d_i\|_2 \leq 1 \ \forall i = 1, \dots, K\}.$$



Thank you for your attention!

Questions?

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Clément CHATELAIN



Romain HERAULT



Sébastien ADAM



*In memory of
Frank ROSENBLATT
1928-1971*

Computation resource



CRIANN: Myria



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