

EN.601.482/682 Deep Learning

Unsupervised and Self-supervised Learning

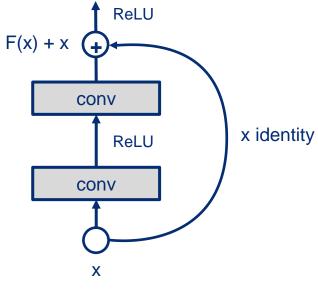
Mathias Unberath, PhD

Assistant Professor

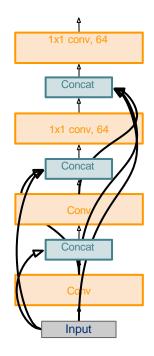
Dept of Computer Science

Johns Hopkins University

Gradient flow

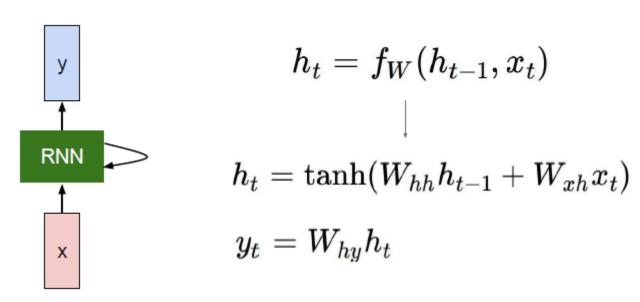


Residual block

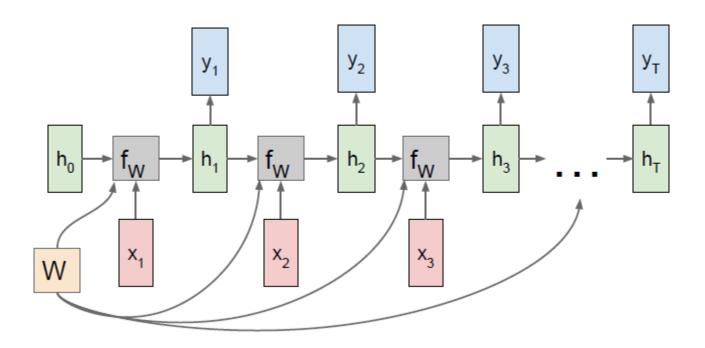


Dense block

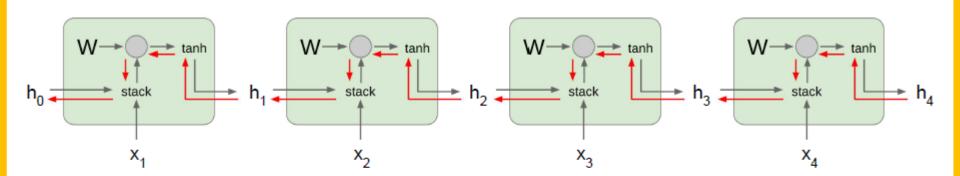
Recurrent Neural Networks: Standard Architecture



Recurrent Neural Networks: Unrolling → Same weights at every timestep!



Recurrent Neural Networks: Gradient flow



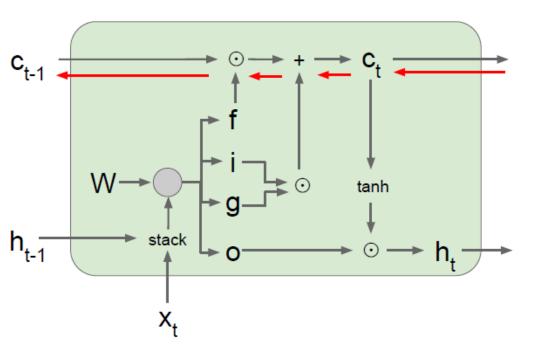
Computing gradient of h₀ involves many factors of W (and repeated tanh)

Largest singular value > 1:

Exploding gradients

Largest singular value < 1: Vanishing gradients

Long Short Term Memory: Mitigating the gradient problem



$$\begin{pmatrix} i \\ f \\ o \\ g \end{pmatrix} = \begin{pmatrix} \sigma \\ \sigma \\ \sigma \\ \tanh \end{pmatrix} W \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix}$$
$$c_t = f \odot c_{t-1} + i \odot g$$
$$h_t = o \odot \tanh(c_t)$$

- 1. Download or collect large database
- 2. Design or download state-of-the-art ConvNet architecture
- 3. Define the desired output targets via loss function (e.g. DICE loss, ...)
- 4. Optimize parameters with respect to loss
- 5. ??

Running example: Image classification

6. Profit



Running example: Image classification in computer vision

- 1. Download or collect large database: ImageNet
- 2. Design or download state-of-the-art ConvNet architecture: ResNet
- 3. Define the desired output targets via loss function (e.g. DICE loss, ...): CE
- 4. Optimize parameters with respect to loss: ADAM

Running example: Image classification in computer vision, but new categories!

- 1. Download or **collect** large database: Proprietary images
- 2. Design or download state-of-the-art ConvNet architecture: ResNet
- 3. Define the desired output targets via loss function (e.g. DICE loss, ...): CE
- 4. Optimize parameters with respect to loss: ADAM

Q: Which assumption are we making?



Running example: Image classification in computer vision, but new categories!

- 1. Download or collect large database: Proprietary images
- 2. Design or download state-of-the-art ConvNet architecture: ResNet
- 3. Define the desired output targets via loss function (e.g. DICE loss, ...): CE
- 4. Optimize parameters with respect to loss: ADAM

We need ground truth labels for every single image to be able to compute such loss.

→ Someone will need to annotate every single image

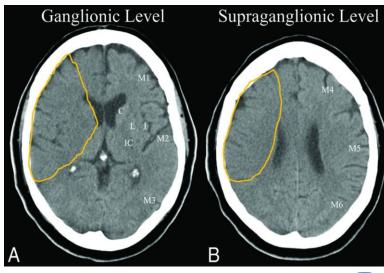
A Bigger Picture

Learning from annotated instances: Supervised learning

Obtaining annotations is among the most critical steps! Why?

Example: Ischemic stroke lesion identification in no-contrast CT (ASPECT scoring)

- Expert-level domain knowledge
- High variation (much data!)
- High dimensional (volumetric labels!)





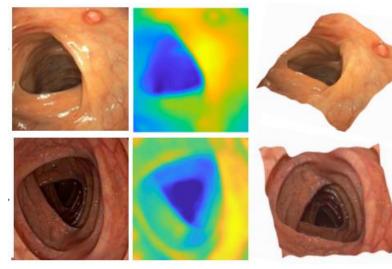
A Bigger Picture

Learning from annotated instances: Supervised learning

Obtaining annotations is among the most critical steps! Why?

Example: Monocular depth prediction from endoscopic video

- "True ground truth": Virtually impossible!
 Would require stereo or RGBD endoscopes
- High variation (much data!)





Today's Lecture

If acquiring data is relatively easy ...

... but annotating data is comparably difficult, ...

... wouldn't it be appealing if we could just learn from data?

Today's Lecture

If acquiring data is relatively easy ...

... but annotating data is comparably difficult, ...

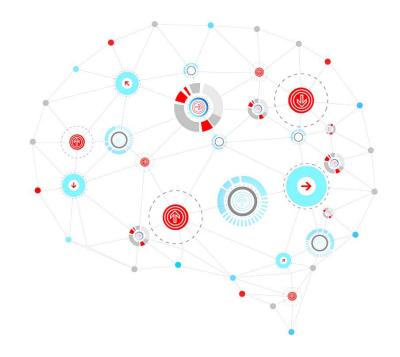
... wouldn't it be appealing if we could just learn from data?

This is known as unsupervised and self-supervised learning! Research in this area is rapidly growing!

- → Training is based on back-propagation of gradients
- → How can we define (un)happiness with the current parameters?

Today's Lecture

Unsupervised and self-supervised learning

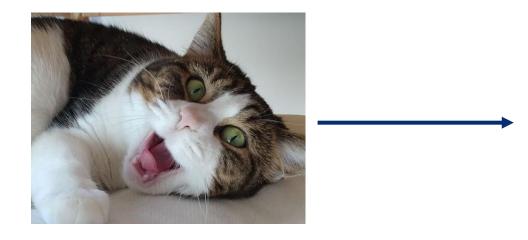


Unsupervised and Self-supervised Learning

ImageNet Classification Without Labels

Image Classification

Assume set of discrete labels is known, e.g. {dog, cat, car, plane, ...} Classification describes a mapping of image onto label



EN.601.482/682 Deep Learning Mathias Unberath

$$\min_{\theta,W} \frac{1}{N} \sum_{i} L\left(g_W(f_{\theta}(x_i)), y_i\right)$$

Input x_i with label y_i



$$\min_{\theta,W} \frac{1}{N} \sum_{i} L\left(g_{W}\left(f_{\theta}(x_{i})\right), y_{i}\right)$$

- Input x_i with label y_i
- f_{Θ} computes high-level representations of x_i



$$\min_{\theta,W} \frac{1}{N} \sum_{i} L\left(g_{W}\left[f_{\theta}(x_{i})\right], y_{i}\right)$$

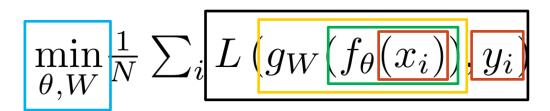
- Input x_i with label y_i
- f_⊙ computes high-level representations of x_i G
- g_W is a classifier that maps representations to labels



$$\min_{\theta,W} \frac{1}{N} \sum_{i} L\left(g_{W}\left(f_{\theta}(x_{i})\right), y_{i}\right)$$

- Input x_i with label y_i
- f_⊙ computes high-level representations of x_i G
- g_W is a classifier that maps representations to labels
- Loss function, e.g. logistic loss (negative log softmax)





Q: We said this was unsupervised. What is y_i?

- Input x_i with label y_i
- f_⊙ computes high-level representations of x_i G
- g_W is a classifier that maps representations to labels
- Loss function, e.g. logistic loss (negative log softmax)
- → Task: Find parameters Θ,W such that loss is optimal



From Embeddings to Pseudo-labels

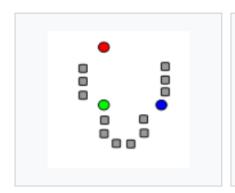
- Let's assume Θ is known → Representations are informative!
- Then, we only need to find W for correct class assignments
- Idea
 - Representations are informative
 - The embedding of images with similar appearance/content will be similar
 - The embedding of images with dissimilar appearance/content will be dissimilar
 - Cluster these embeddings to assign pseudo-labels!

• What clustering to use?

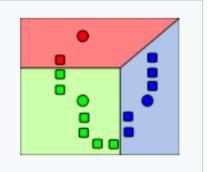


Clustering

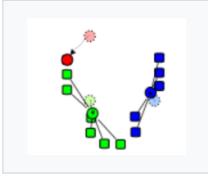
Every image is embedded based on its content/appearance



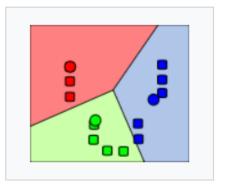
1. *k* initial "means" (in this case *k*=3) are randomly generated within the data domain (shown in color).



2. *k* clusters are created by associating every observation with the nearest mean. The partitions here represent the Voronoi diagram generated by the means.



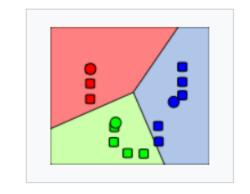
3. The centroid of each of the *k* clusters becomes the new mean.



4. Steps 2 and 3 are repeated until convergence has been reached

Clustering

- Every image is embedded based on its content/appearance
- OK, we have pseudo-labels.
 But assumption was: Θ is already known!
- In reality, Θ is not known. Specifically, at the very first iteration/epoch Θ is not only not known but random!

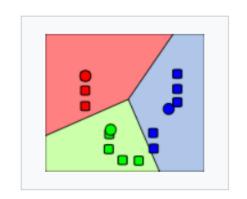


Q: Problem?



Clustering

- Every image is embedded based on its content/appearance
- OK, we have pseudo-labels.
 But assumption was: Θ is already known!
- In reality, Θ is not known. Specifically, at the very first iteration/epoch Θ is not only not known but random!



- Q: Problem?
- Turns out: No problem.
 An MLP classifier on top of random AlexNet achieves 12.5% accuracy!
 Random chance is at 0.1%!



Deep Clustering

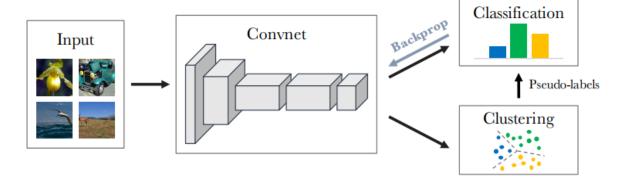


Fig. 1: Illustration of the proposed method: we iteratively cluster deep features and use the cluster assignments as pseudo-labels to learn the parameters of the convnet

- Alternates between
 - 1) clustering features to obtain pseudo-labels and
 - 2) updating the parameters of the ConvNet to predict these pseudo-labels.
- Problem?



Deep Clustering

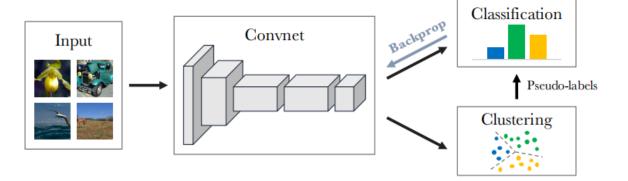


Fig. 1: Illustration of the proposed method: we iteratively cluster deep features and use the cluster assignments as pseudo-labels to learn the parameters of the convnet

- Alternates between
 - 1) clustering features to obtain pseudo-labels and
 - 2) updating the parameters of the ConvNet to predict these pseudo-labels.
- Problem? Assigning all points to a single cluster is an optimal solution.

Deep Clustering

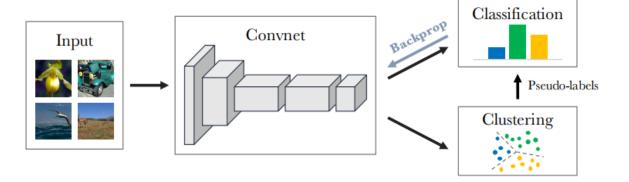


Fig. 1: Illustration of the proposed method: we iteratively cluster deep features and use the cluster assignments as pseudo-labels to learn the parameters of the convnet

- Avoiding trivial solutions
 - Avoiding empty clusters by re-assigning empty clusters
 - If most images are assigned to very few clusters, parameterization can become trivial
 - → This is similar to highly unbalanced data
 - → Sample images based on uniform distribution over the pseudo-labels
- Forward pass on full dataset, k-means clustering, backprop
- AlexNet with labels: 50.5% Top-1 DeepCluster: 38.2% Top-1

Caron, M., Bojanowski, P., Joulin, A., & Douze, M. (2018). Deep clustering for unsupervised learning of visual features. ECCV (pp. 132-149).

Learning Good Representations from Data

- Often times, people make analogies to "how babies learn"
- No semantic information, but once provided, baby can identify the items
- An example:



Learning Good Representations from Data

- Often times, people make analogies to "how babies learn"
- No semantic information, but once provided, baby can identify the items
- And another one: Conceptual model is violated

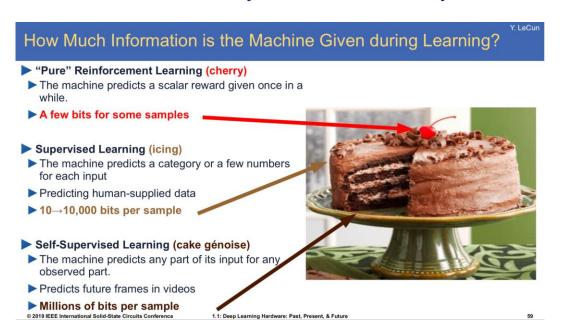




Learning Good Representations from Data

Derive auxiliary tasks from the data itself

Data is high-dimensional, these auxiliary tasks can be very informative!





Unsupervised and Self-supervised Learning

From Images



Jigsaw Puzzle Reassembly



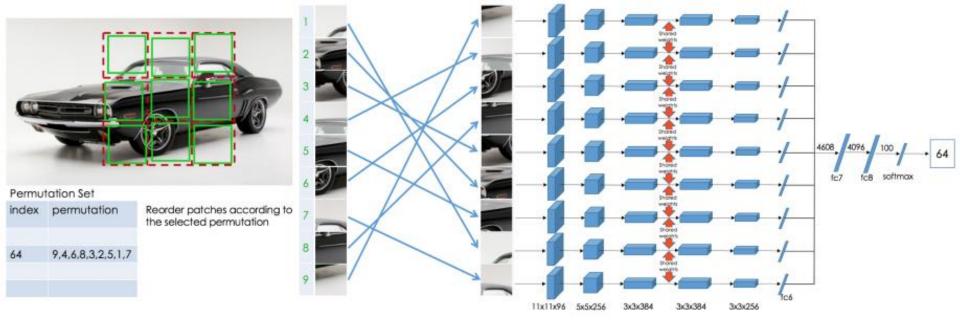
- Introduced 1760 by John Spilsbury for children to learn geography
- Used to assess individual's ability to organize visual stimuli
- → Use puzzles to develop a visuospatial representation of objects in context

Noroozi, M., & Favaro, P. (2016, October). Unsupervised learning of visual representations by solving jigsaw puzzles. ECCV (pp. 69-84).



Jigsaw Puzzle Reassembly

- How to model jigsaw puzzle solving?
- Immediate approach: Stack puzzle tiles along channels (depth)
 - CNN may concentrate on low level statistics
 - → Similar texture patterns at boundaries
 - This does not promote understanding of global object properties
- Idea: Delay computation of statistics across tiles
 - First, compute features/representations of every tile separately
 - Then, determine arrangement only based on this representation!



- Randomly crop 225x225 px window from image (red box)
- Divide into 3x3 cell grid and pick random 64x64 pixel tile from each cell
- 9 tiles are re-ordered randomly according to one of the 9! permutations
- Network predicts premutation index (one-hot)

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Jigsaw Puzzle Reassembly

Q: Any challenges that would prevent generalizable learning?

Jigsaw Puzzle Reassembly

- Q: Any challenges that would prevent generalizable learning? Shortcuts!
 Representations that are suitable for the pre-text but not the target task.
 Features would carry no semantic information
- Shortcut 1: CNN may memorize absolute positions of tiles
 - → Feed in multiple puzzles at once to make absolute positions equally likely
- Shortcut 2: Edge continuity
 - → Random gap between tiles
- Shortcut 3: Pixel intensity / color distributions
 - → Jitter on color channels



Jigsaw Puzzle Reassembly

Table 1: Results on PASCAL VOC 2007 Detection and Classification. The results of the other methods are taken from Pathak et al. [30].

Method	Pretraining time	Supervision	Classification	Detection	Segmentation
Krizhevsky et al. [25]	3 days	1000 class labels	78.2%	$\boldsymbol{56.8\%}$	48.0%
Wang and Gupta[39]	1 week	motion	58.4%	44.0%	-
Doersch et al. [10]	4 weeks	context	55.3%	46.6%	-
Pathak et al. [30]	14 hours	context	56.5%	44.5%	29.7%
Ours	2.5 days	context	$\boldsymbol{67.6\%}$	53.2 %	37.6%

Performs well and is comparably fast to train

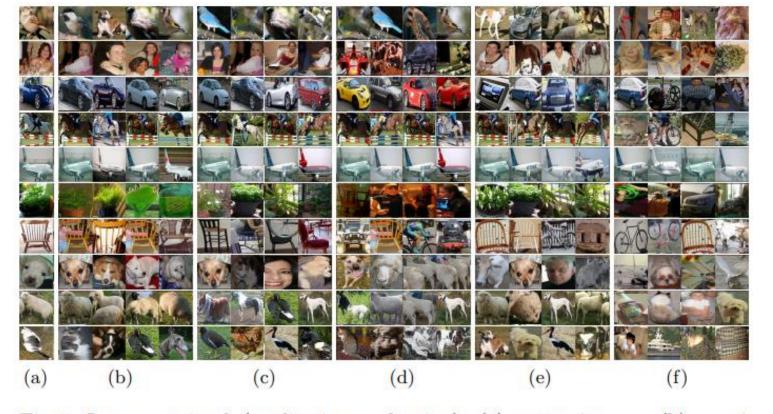


Fig. 5: Image retrieval (qualitative evaluation). (a) query images; (b) top-4 matches with AlexNet; (c) top-4 matches with the CFN trained without blocking chromatic aberration; (d) top-4 matches with Doersch et al. [10]; (e) top-4 matches with Wang and Gupta [39]; (f) top-4 matches with AlexNet with random weights

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Q: When we perform data augmentation, what is our core assumption?

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Dosovitskiy, A., Springenberg, J. T., Riedmiller, M., & Brox, T. (2014). Discriminative unsupervised feature learning with convolutional neural networks. NeurIPS (pp. 766-774).

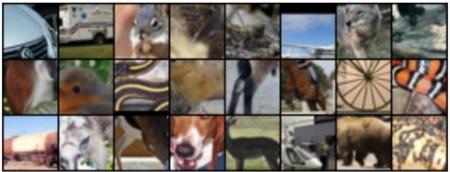




Figure 1: Exemplary patches sampled from the STL unlabeled dataset which are later augmented by various transformations to obtain surrogate data for the CNN training.

Figure 2: Several random transformations applied to one of the patches extracted from the STL unlabeled dataset. The original ('seed') patch is in the top left corner.

- Data augmentation to the max!
- Altering an image will produce an image of the same class! → Pseudo-labels!

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- Family of "exemplar" transformations
 - Translation: vertical or horizontal translation by a distance within 0.2 of the patch size;
 - Scaling: multiplication of the patch scale by a factor between 0.7 and 1.4;
 - Rotation: rotation of the image by an angle up to 20 degrees;
 - Contrast 1: multiply the projection of each patch pixel onto the principal components of the set of all pixels by a factor between 0.5 and 2 (factors are independent for each principal component and the same for all pixels within a patch);
 - Contrast 2: raise saturation and value (S and V components of the HSV color representation) of all pixels to a power between 0.25 and 4 (same for all pixels within a patch), multiply these values by a factor between 0.7 and 1.4, add to them a value between -0.1 and 0.1;
 - Color: add a value between −0.1 and 0.1 to the hue (H component of the HSV color representation) of all pixels in the patch (the same value is used for all pixels within a patch).
- For each patch, sample 300 augmentation parameters



Table 1: Classification accuracies on several datasets (in percent). † Average per-class accuracy $78.0\% \pm 0.4\%$. ‡ Average per-class accuracy $84.4\% \pm 0.6\%$.

Algorithm	STL-10	CIFAR-10(400)	CIFAR-10	Caltech-101	#features
Convolutional K-means Network [26]	60.1 ± 1	70.7 ± 0.7	82.0	_	8000
Multi-way local pooling [28]			_	77.3 ± 0.6	1024×64
Slowness on videos [10]	61.0	61.0		74.6	556
Hierarchical Matching Pursuit (HMP) [27]	64.5 ± 1	_	_	_	1000
Multipath HMP [29]	_ _		_	82.5 ± 0.5	5000
View-Invariant K-means [12]	63.7	72.6 ± 0.7	81.9	_	6400
Exemplar-CNN (64c5-64c5-128f)	67.1 ± 0.3	69.7 ± 0.3	75.7	$79.8 \pm 0.5 \dagger$	256
Exemplar-CNN (64c5-128c5-256c5-512f)	72.8 ± 0.4	$\textbf{75.3} \pm \textbf{0.2}$	82.0	$85.5 \pm 0.4 \ddagger$	960
Supervised state of the art	70.1[30]	_	91.2 [31]	91.44 [32]	

Q: Challenges with this approach?

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Supervised state of the art	70.1[30]	_	91.2 [31]	91.44 [32]	_

- Q: Challenges with this approach?
- Scalability! Exemplars are created via augmentation. How to deal with more complex variation, such as viewpoint changes?

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In order to attribute color to the object, we must recognize the object first

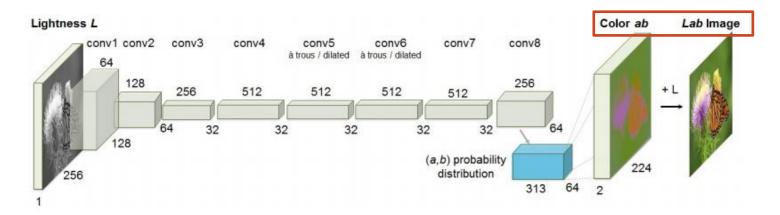


Fig. 2. Our network architecture. Each conv layer refers to a block of 2 or 3 repeated conv and ReLU layers, followed by a BatchNorm [30] layer. The net has no pool layers. All changes in resolution are achieved through spatial downsampling or upsampling between conv blocks.

Zhang, R., Isola, P., & Efros, A. A. (2016, October). Colorful image colorization. ECCV (pp. 649-666).

- Why "CIE Lab" color space? Distances in Lab model perceptual distance
- But using L2 is not a good idea. Q: Why?

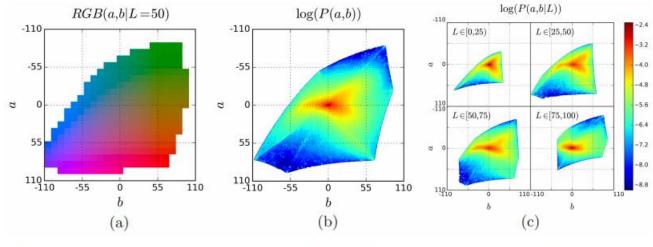


Fig. 3. (a) Quantized *ab* color space with a grid size of 10. A total of 313 *ab* pairs are in gamut. (b) Empirical probability distribution of *ab* values, shown in log scale. (c) Empirical probability distribution of *ab* values, conditioned on *L*, shown in log scale.

- Think about the chameleon. Objects can take multiple different colors!
- Rather than regression → Classification!

Rebalancing needed! See Fig. 3b. Due to background, desaturated pixels are

much more likely!

→ Weighting!

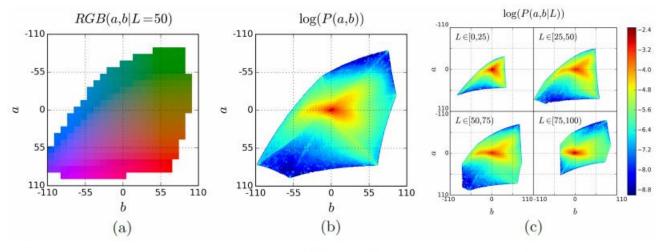


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Author	Training	Immut		[Ref]	Layers					
Author	Training	Input	Params Feats Runtime			[reer]	conv2	conv3	conv4	conv5
Krizhevsky et al. [38]	labels	rgb	1.00	1.00	1.00	_	56.5	56.5	56.5	56.5
Krizhevsky et al. [38]	labels	L	0.99	1.00	0.92	-	50.5	50.5	50.5	50.5
Noroozi & Favaro [43]	imagenet	rgb	1.00	5.60	7.35	[43]	56.0	52.4	48.3	38.1
Gaussian	imagenet	rgb	1.00	1.00	1.00	[43]	41.0	34.8	27.1	12.0
Doersch et al. [14]	imagenet	rgb	1.61	1.00	2.82	[43]	47.6	48.7	45.6	30.4
Wang & Gupta [15]	videos	rgb	1.00	1.00	1.00	[43]	46.9	42.8	38.8	29.8
Donahue et al. [16]	imagenet	rgb	1.00	0.87	0.96	[16]	51.9	47.3	41.9	31.1
Ours	imagenet	L	0.99	0.87	0.84	-	46.6	43.5	40.7	35.2

Table 3. ImageNet classification with nonlinear layers, as proposed in [43]. Note

Jigsaw puzzles



Zhang, R., Isola, P., & Efros, A. A. (2016, October). Colorful image colorization. ECCV (pp. 649-666).









4

Unsupervised and Self-supervised Learning

From Videos



- So far: Image colorization
 - Learn sematic features about objects to assign colors
 - Allows learning of generalizable representations
- Now: Video colorization
 - Naively done, this is just the same as image colorization
 - But, can you think of an interesting twist?



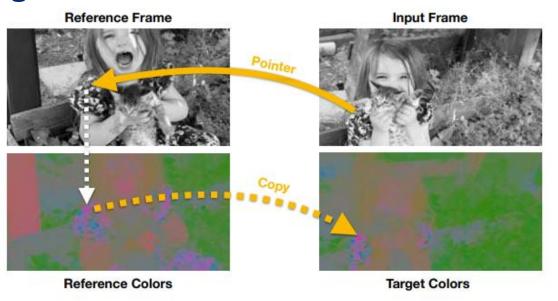


Fig. 1. Self-supervised Tracking: We capitalize on large amounts of unlabeled video to learn a self-supervised model for tracking. The model learns to predict the target colors for a gray-scale input frame by pointing to a colorful reference frame, and copying the color channels. Although we train without ground-truth labels, experiments and visualizations suggest that tracking emerges automatically in this model.

Vondrick, C., Shrivastava, A., Fathi, A., Guadarrama, S., & Murphy, K. (2018). Tracking emerges by colorizing videos. ECCV (pp. 391-408).

- Colorization then is performed using soft assign
- Interestingly, this mechanism discovers object tracking!

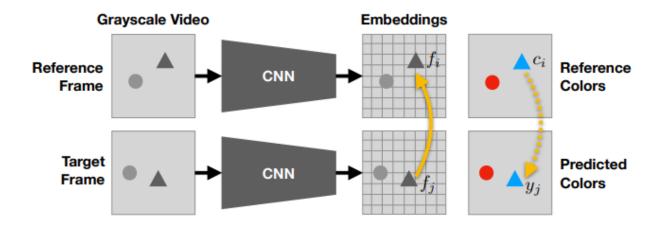


Fig. 2. Model Overview: Given gray-scale frames, the model computes low-dimensional embeddings for each location with a CNN. Using softmax similarity, the model points from the target frame into the reference frame embeddings (solid yellow arrow). The model then copies the color back into the predicted frame (dashed yellow arrow). After learning, we use the pointing mechanism as a visual tracker. Note that the model's pointer is soft, but for illustrations purposes we draw it as a single arrow.











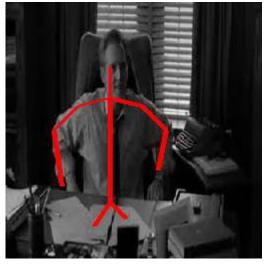


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Unsupervised and Self-supervised Learning

From Multi-modal Data



Can we localize sources of sound in images / a video sequence?



(a) Input image with sound



(b) Where is the sound?

Fig. 1. Where is the sound? Given an input image and sound clip, our method learns, without a single labelled example, to localize the object that makes the sound.

- In order to do so, we first need a network architecture that can process both
 - Video sequences / images
 - Audio
- Then, supervision comes for free from audio-visual synchronization



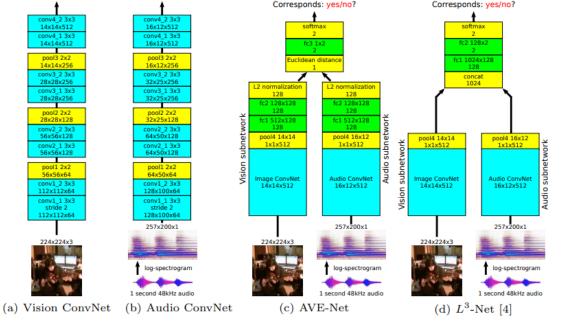
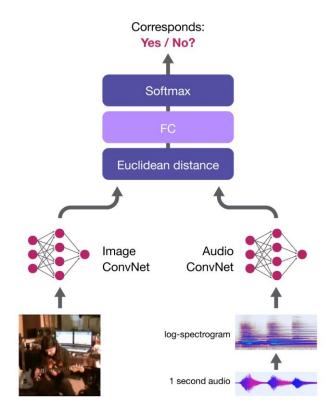


Fig. 2. ConvNet architectures. Each blocks represents a single layer with text providing more information – first row: layer name and optional kernel size, second row: output feature map size. Each convolutional layer is followed by batch normalization [25] and a ReLU nonlinearity, and the first fully connected layer (fc1) is followed by ReLU. All pool layers perform max pooling and their strides are equal to the kernel sizes. (a) and (b) show the vision and audio ConvNets which perform initial feature extraction from the image and audio inputs, respectively. (c) Our AVE-Net is designed to produce aligned vision and audio embeddings as the only information, a single scalar, used to decide whether the two inputs correspond is the Euclidean distance between the embeddings. (d) In contrast, the L^3 -Net [4] architecture combines the two modalities by concatenation and a couple of fully connected layers which produce the corresponds or not classification scores.

- Does the 1s sound clip match my query image?
- Aligns latent spaces
- Can be used for audio clip retrieval
- Shortcuts! Q: Can you think of one?

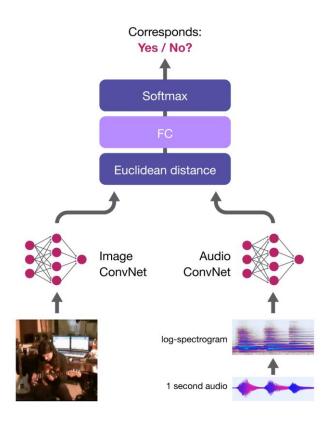


https://deepmind.com/blog/article/objects-that-sound

Arandjelovic, R., & Zisserman, A. (2018). Objects that sound. ECCV (pp. 435-451).



- Does the 1s sound clip match my query image?
- Aligns latent spaces
- Can be used for audio clip retrieval
- Shortcuts!
 - Positives are always sampled at N*0.04s (25fps)
 - Negatives must also be sampled that way!
 Network can identify otherwise, likely due to encoding artifact



https://deepmind.com/blog/article/objects-that-sound

Arandjelovic, R., & Zisserman, A. (2018). Objects that sound. ECCV (pp. 435-451).



 Vision network does not globally pool the features, but operates on 14x14 resolution

FC-layers are converted to fully conv. layers

 Similarities between audio and visual encoding reveal location of objects that sound

Spatial grid of visual representations

Image ConvNet ConvNet log-spectrogram

1 second audio

Corresponds: Yes / No?

Maxpool

Sigmoid

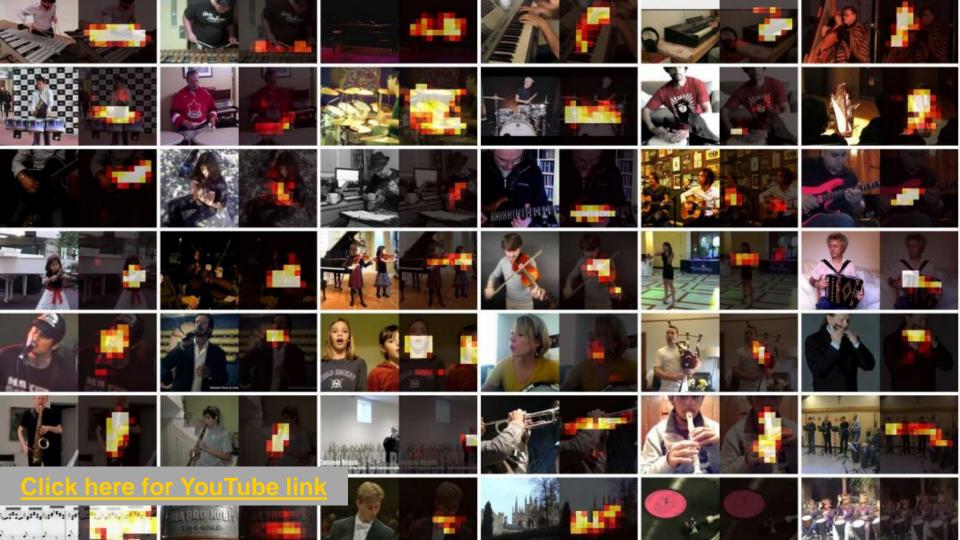
Conv

All pairwise scalar products

Corresponds: Where?

correspondence scares

https://deepmind.com/blog/article/objects-that-sound
Arandielovic, R., & Zisserman, A. (2018). Objects that sound. ECCV (pp. 435-451).



Unsupervised and Self-supervised Learning

Exploiting Domain Knowledge

Extracting Weak Annotations

- In previous applications, we ...
 - ... solved for a surrogate task
 - and then transferred features to our target task
- In some cases, we may be able to target this problem more directly
- Rather than solving for a surrogate task, maybe we can get sparse / weak annotations for our target task?
- Q: Can you find examples for this?

"Error-corrective Boosting"

- Brain segmentation is possible using FreeSurfer
 - Reasonably accurate but takes a very long time (> hours)
 - Manual labels: Even more accurate but even more time consuming

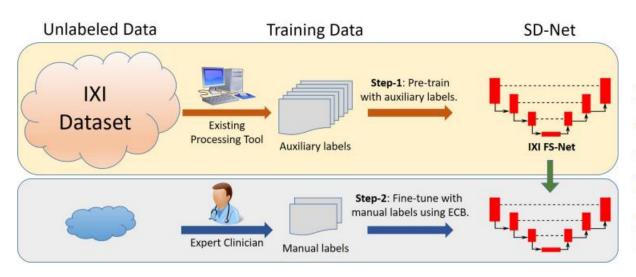


Fig. 1: Illustration of the different steps involved in training of F-CNNs with surplus auxiliary labeled data and limited manually labeled data.

Roy, A. G., Conjeti, S., Sheet, D., Katouzian, A., Navab, N., & Wachinger, C. (2017). Error corrective boosting for learning fully convolutional networks with limited data. MICCAI.

"Error-corrective Boosting"

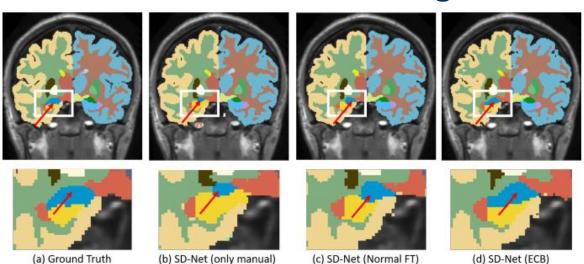


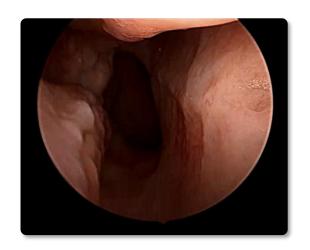
Table 1: Mean and standard deviation of the Dice scores for the different F-CNN models and training procedures on both datasets.

	Mult	ti-Atlas Ch	allenge Dat	aset	MindBoggle Dataset				
Method	IXI FS-Net	Manual	Normal FT	ECB FT	IXI FS-Net	Manual	Normal FT	ECB FT	
		Labels				Labels			
SD-Net	0.74 ± 0.13	0.85 ± 0.08	0.88 ± 0.06	0.91 ± 0.05	0.71 ± 0.17	0.82 ± 0.06	0.86 ± 0.07	0.87 ± 0.06	
SD-Net (No Dice)									
U-Net [4]	0.71 ± 0.15	0.81 ± 0.09	0.82 ± 0.11	0.87 ± 0.06	0.69 ± 0.19	0.76 ± 0.11	0.84 ± 0.07	0.86 ± 0.06	
FCN [1]	0.55 ± 0.23	0.70 ± 0.15	0.78 ± 0.12	0.85 ± 0.07	0.45 ± 0.24	0.64 ± 0.23	0.81 ± 0.08	0.83 ± 0.08	
Spatial Staple [17]		0.89 =	0.05		NA				
PICSL [16]		0.91	± 0.04		NA				

Roy, A. G., Conjeti, S., Sheet, D., Katouzian, A., Navab, N., & Wachinger, C. (2017). Error corrective boosting for learning fully convolutional networks with limited data. MICCAI.

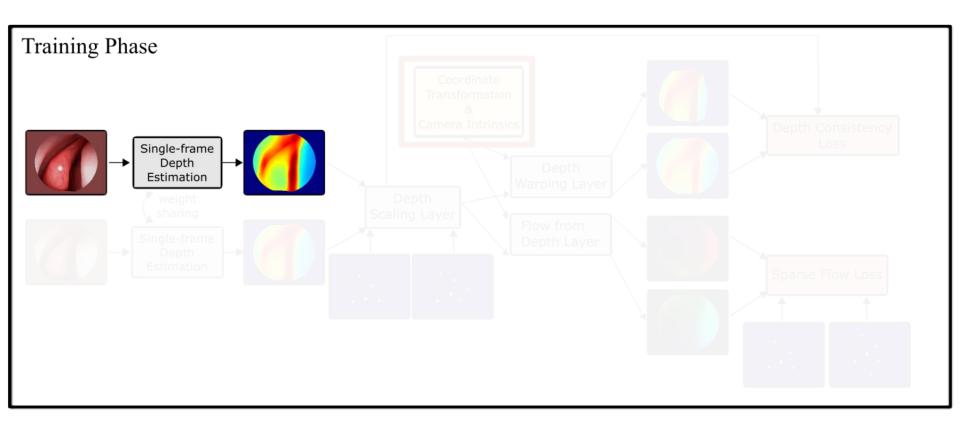
Estimating 3D Geometry from Endoscopic Video

How to obtain 3D representations from endoscopic video?

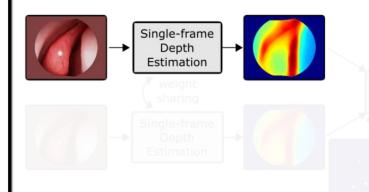








Training Phase



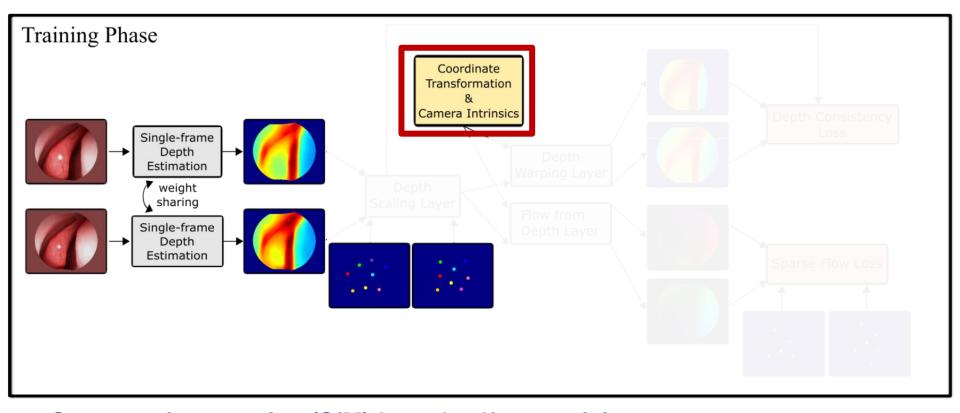
Coordinate Transformation & Camera Intrinsics

Classical – Structure from Motion



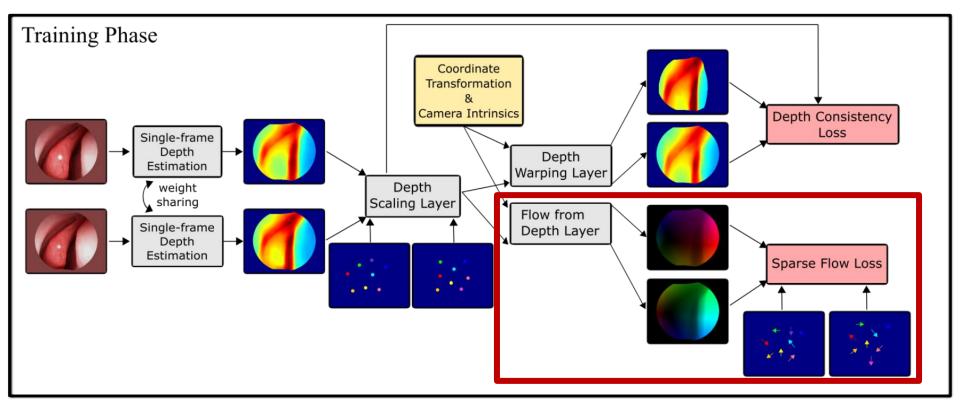
- Feature matching
- Triangulation and bundle adjustment
- → Reconstruction from acquired images

Snavely, N., Seitz, S. M., & Szeliski, R. (2006, July). Photo tourism: exploring photo collections in 3D. In ACM transactions on graphics (TOG) (Vol. 25, No. 3, pp. 835-846). ACM.



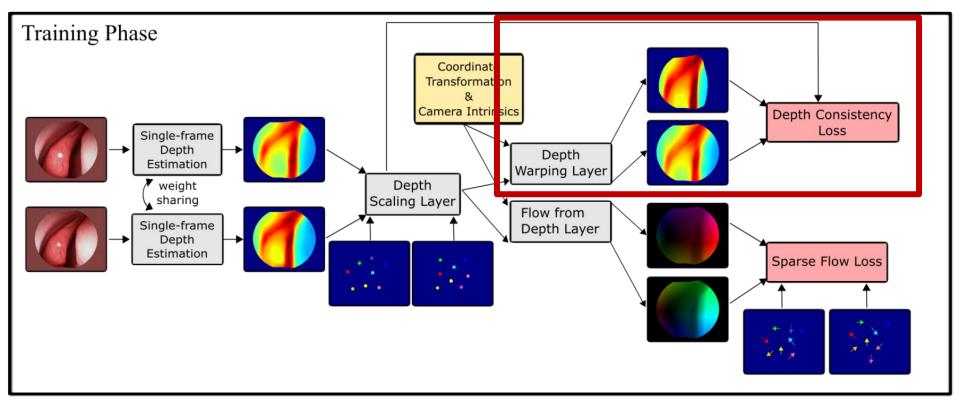
Structure from motion (SfM)-based self-supervision

- Run SfM on short video sequence (15 to 30 frames)
- Siamese network → Process multiple frames



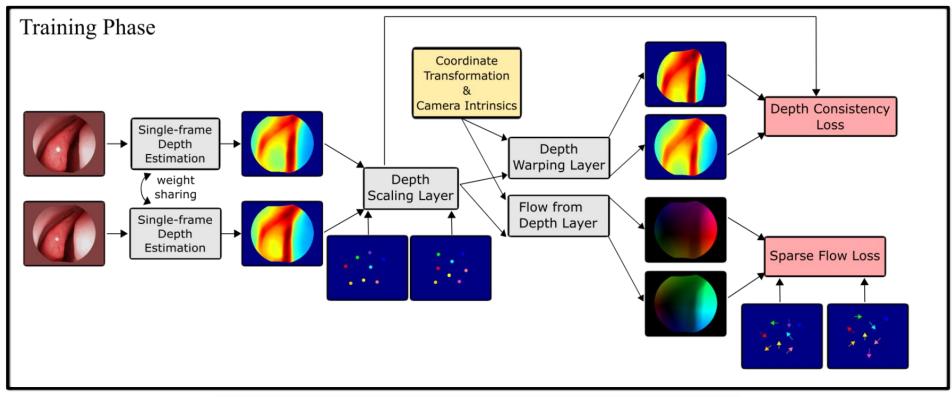
Sparse Flow Loss

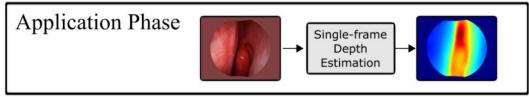
- True 2D optical flow from 3D reconstructed points (SfM)
- Estimated optical flow from depth prediction

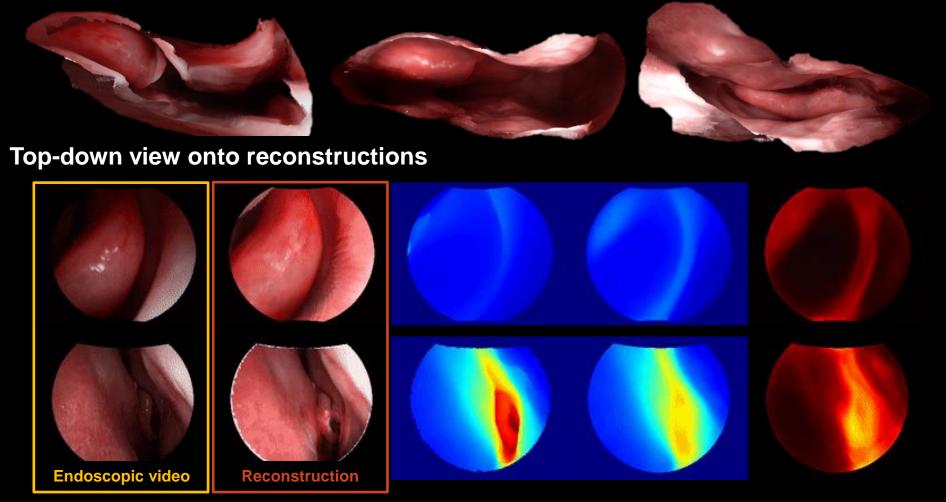


Depth Consistency Loss

- Differentiable warping operation to warp estimated depth into neighbor frame
- Enforces consistency among predictions







Fly-through the reconstructions

Unsupervised and Self-supervised Learning

Questions?

