Identification of Kernels in a Convolutional Neural Network

Jonas Actor
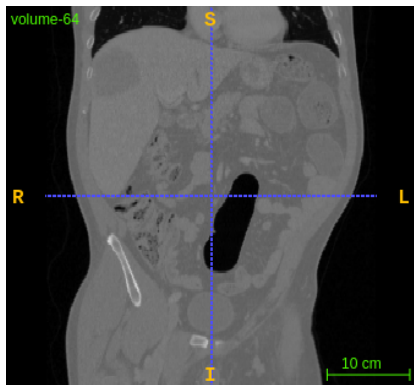
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19 February 2020
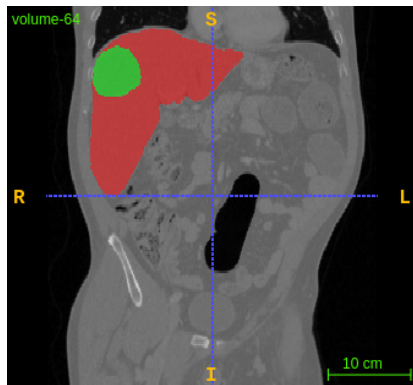
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Target application: medical image segmentation

Abdominal CT scan

Liver and tumor segmentation

Why automate?

- needed for treatment plans
- costly (time+effort) to perform by hand
- less interobserver variability $\rightarrow$ better accuracy

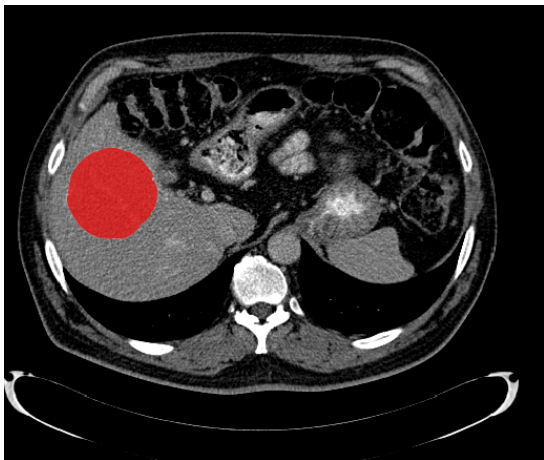errors in segmentation = errors in radiation treatment

Goal: understand why CNNs work so well

1. Compare PDEs to CNNs

2. Build CNNs like PDEs

3. Analyze kernels and explain performance
   - Entrywise comparison
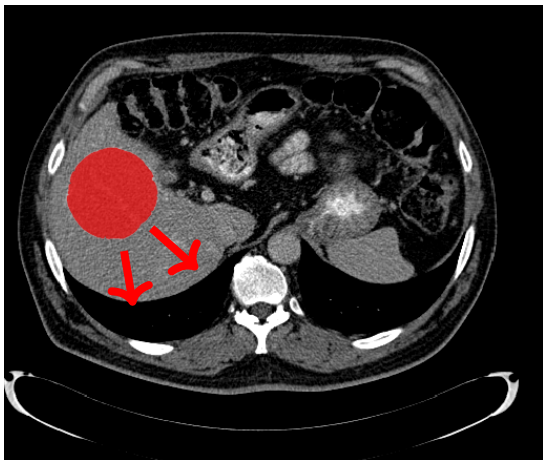   - SVD comparison

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Classical Approach: Solve a PDE

Level Set Equation: time = 200

Classical Approach: Solve a PDE

Level Set Equation: time = 200

Classical Approach: Solve a PDE

Level Set Equation: time = 500

Classical Approach: Solve a PDE
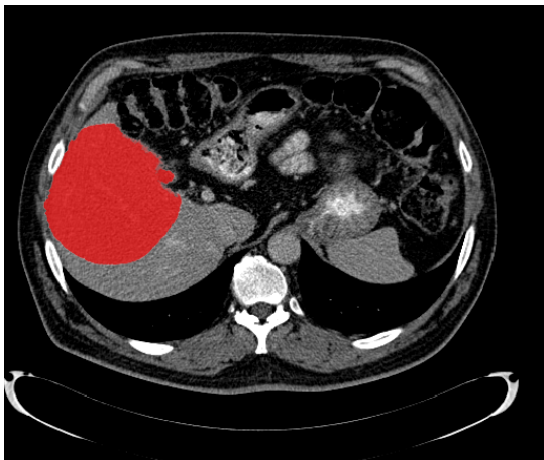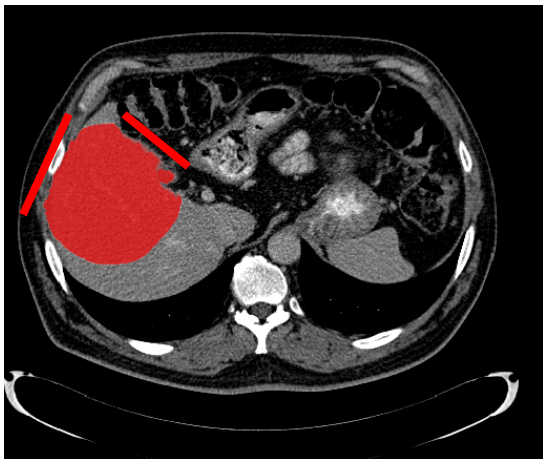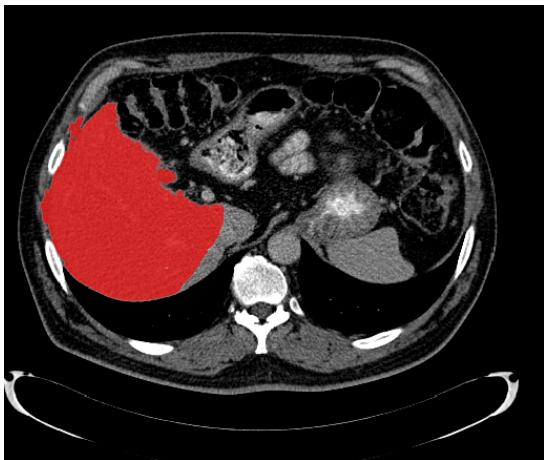

Level Set Equation: time = 500

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Classical Approach: Solve a PDE

Level Set Equation: time = 1100

Classical Approach: Solve a PDE

Level Set Equation: time = 1100

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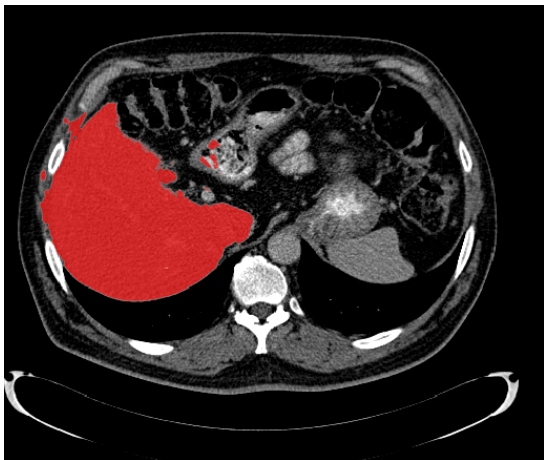
Level Set Equation: time = 1500

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Classical Approach: Level Set Equation

$$\partial_t u - \alpha \underbrace{\|\nabla u\| \, g_I}_{\text{balloon force}} - \beta \underbrace{\|\nabla u\| \, g_I \kappa(u)}_{\text{mean curvature}} - \gamma \underbrace{\nabla g_I \cdot \nabla u}_{\text{convection}} = 0$$

- Well-established theory to analyze approximation, stability
- Upwind finite differences + fast marching method
- Semiautomated : requires initialization by user
- Works for simple problems only : relies on edge information

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Comparison: LSE vs CNN

	Can analyze?	Accurate?
LSE	yes	sometimes
CNN	no	yes

Goal: accurate method we can analyze

Similarities between LSE and CNN

	LSE	CNN
Convolution	finite difference kernel	learned kernel
	$\frac{1}{h^2} \begin{bmatrix} 0 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & 0 \end{bmatrix}$	$\begin{bmatrix} k_{11} & k_{12} & k_{13} \\ k_{21} & k_{22} & k_{23} \\ k_{31} & k_{32} & k_{33} \end{bmatrix}$
ReLU	upwind scheme	activation function
	$\max(0, D^+ * u) + \min(0, D^- * u)$	$\max(0, K * x + b)$

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Build a CNN like a LSE solver

Level Set Equation $\longrightarrow$ Level Set Network

1. Discretize Level Set Equation
   - Explicit forward Euler in time
   - Upwind finite differences in space
2. Forward Euler $\longrightarrow$ residual skip connections
3. Upwind finite differences $\longrightarrow$ convolutions and ReLU

Forward Euler time discretization

$$\frac{u^{(t+1)} - u^{(t)}}{\delta_t} - \alpha \left\| \nabla u^{(t)} \right\| g_I - \beta \left\| \nabla u^{(t)} \right\| g_I \kappa(u^{(t)}) - \gamma \nabla g_I \cdot \nabla u^{(t)} = 0$$

Edge indicator g_I

$$g_I(x) = \frac{1}{1 + \|\nabla I(x)\|^2}$$

becomes

$$g_I(x) = \frac{1}{1 + \sum_{j=1}^{N_{conv}} (\sigma_j * I(x))^2}$$

Convection term: Upwind Finite Differences

$$\nabla g_I \cdot \nabla u^{(k)} = \max\{0, \partial_x g_{\mathcal{I}}\} D_x^+ * u^{(k)} - \max\{0, -\partial_x g_{\mathcal{I}}\} D_x^- * u^{(k)}$$
$$+ \max\{0, \partial_y g_{\mathcal{I}}\} D_y^+ * u^{(k)} - \max\{0, -\partial_y g_{\mathcal{I}}\} D_y^- * u^{(k)}$$

$$= \mathsf{ReLU}(\partial_x g_{\mathcal{I}}) D_x^+ * u^{(k)} - \mathsf{ReLU}(-\partial_x g_{\mathcal{I}}) D_x^- * u^{(k)}$$
$$+ \mathsf{ReLU}(\partial_y g_{\mathcal{I}}) D_y^+ * u^{(k)} - \mathsf{ReLU}(-\partial_y g_{\mathcal{I}}) D_y^- * u^{(k)}$$

Curvature term $\kappa(u)$

$$\kappa(u^{(k)}) = \nabla \cdot \left(\frac{\nabla u^{(k)}}{\|\nabla u^{(k)}\|} \right)$$

becomes

$$\nabla \hat{u}^{(k)} = \sum_{i=1}^{N_{conv}} \rho_i * u^{(k)}$$

$$\kappa(u^{(k)}) = \sum_{j=1}^{N_{conv}} \sigma_j * \frac{\nabla \hat{u}^{(k)}}{\|\nabla \hat{u}^{(k)}\| + \varepsilon}$$

Implementation

- If convolution kernels are finite difference kernels, we recover LSE
- If convolution kenrels are learned, we construct LSN
- Python + Tensorflow / Keras implementation
- Out LSE agrees with ITK-SNAP, a common LSE-segmentation program

LSN: Results

K-Fold	LSE	LSN Test	LSN Validation	UNet
0	0.736	0.837	0.619	0.912
1	0.600	0.847	0.729	0.919
2	0.483	0.116	0.005	0.874
3	0.730	0.827	0.606	0.895
4	0.643	0.831	0.596	0.915
Avg	0.604	0.692	0.511	0.903
Avg$-\{2\}$	0.640	0.837	0.638	0.911

Table: DSC scores for each fold, from training the level set network.

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Identification of Kernels

- Are CNN convolution kernels finite difference stencils?
- Are they *close* to finite difference stencils?
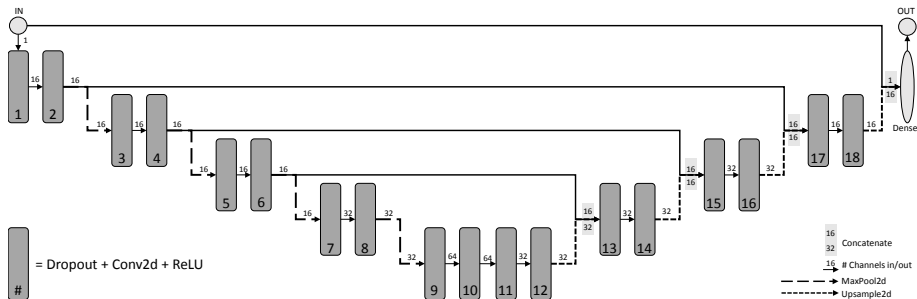- What about other standard image processing kernels?

Numerical analysis kernels

- Laplacian
- Edge detection
- Identity

Image processing kernels

- Gaussian blur
- Local mean
- Sharpen

Setup of CNN

Trained on MICCAI LiTS 2017 dataset for liver segmentation

Kernel Analysis: Comparing entries

- For each layer, separate each channel's 3×3 convolution kernel
- Flatten each 3×3 kernel into a vector $\in \mathbb{R}^9$
- Cluster with k-means
- Project down using PCA
- Project known numerical analysis and image processing kernels
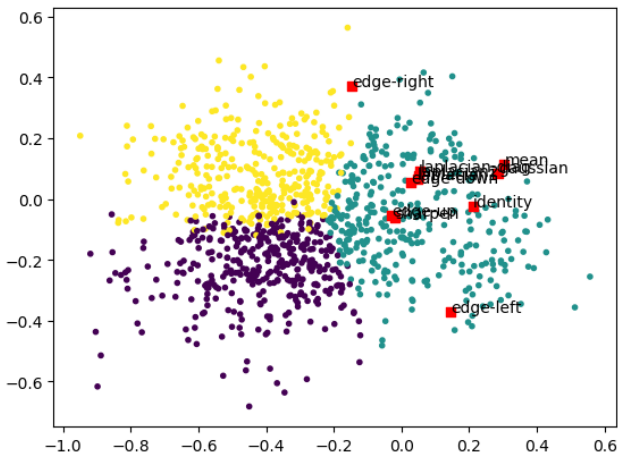
Kernel Clustering Results

Figure: Convolution Layer 11 (encoder)
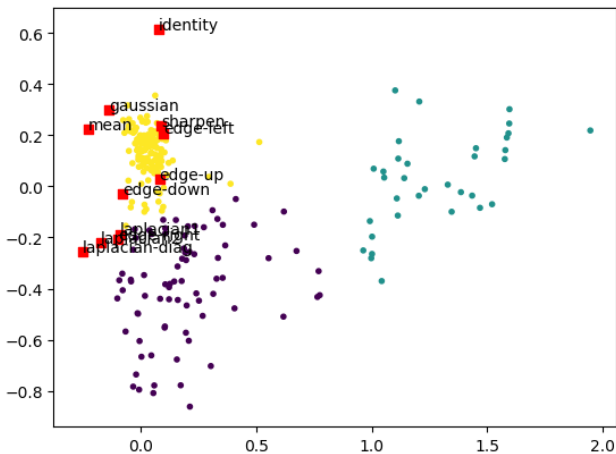
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Kernel Clustering Results

Figure: Convolution Layer 14 (decoder)

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Kernel Analysis: Comparing actions

1. Construct matrix $A_{[K]} \in \mathbb{R}^{n_x n_y \times n_x n_y}$ describing convolution with K
2. Compute singular values of linear operator
3. Compute singular values of clinical image processing kernels
4. Assign closest clinical feature F that has smallest spectral distance to K

Kernel Analysis: Comparing actions

$$\text{Kernel } K = \begin{bmatrix} k_{-1,-1} & k_{-1,0} & k_{-1,1} \\ k_{0,-1} & k_{0,0} & k_{0,1} \\ k_{1,-1} & k_{1,0} & k_{1,1} \end{bmatrix}$$

For $i \in \{-1, 0, 1\}$,

$$T_i = \begin{bmatrix} k_{i,0} & k_{i,1} & & & \\ k_{i,-1} & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & k_{i,1} \\ & & & k_{i,-1} & k_{i,0} \end{bmatrix} \in \mathbb{R}^{n_x \times n_x}$$

$$A_{[K]} = \begin{bmatrix} T_0 & T_1 & & & \\ T_{-1} & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & T_1 \\ & & & T_{-1} & T_0 \end{bmatrix} \in \mathbb{R}^{n_x \, n_y \times n_x \, n_y} \qquad n_y \times n_y \text{ blocks}$$
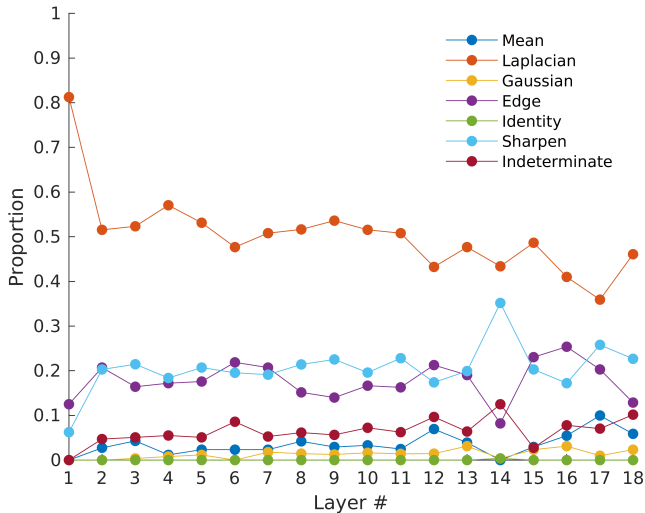
$$A_{[K]} = U_K \Sigma_K V_K^T \qquad \forall K \in \{\text{layers}\}$$
$$A_{[F]} = U_F \Sigma_F V_F^T \qquad \forall F \in \{\text{features}\}$$

$$\text{find} \ \underset{F \in \{\text{features}\}}{\arg\min} \ \|\Sigma_K - \Sigma_F\|_1$$

Label as 'indeterminate' if not within 10% of largest singular value

Kernel Analysis Results

Conclusions

- Level Set Equation $\neq$ Level Set Network $\neq$ UNet
- Framework for using same operations (convolutions + ReLU) for both NNs and PDEs
- Framework for GPU-supported finite differences in Tensorflow
- Examine how learned CNN kernels change across different layers

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