UNCERTAINTY AND THE MEDICAL INTERVIEW

TOWARDS SELF-ASSESSMENT IN MACHINE LEARNING MODELS

Jakob Drachmann Havtorn

DTU Compute
Department of Applied Mathematics and Computer Science

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- Welcome to my PhD defense.
- Thank you to the moderator and the assessment committee for taking part today.
- I will present my work on uncertainty estimation in AI systems for medical domains.
- I will start with an overview of the thesis followed by a brief introduction.
- Then I will present a selection of the research chapters.
- Finally, I will discuss the broader implications of the work.

Thesis

1. The thesis is structured into 10 chapters.
2. The first three chapters are introductory.
3. The next six chapters are research chapters.
4. The final chapter is a discussion and conclusion.

OVERVIEW

Thesis

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Background

Industrial PhD project with Corti AI and DTU Compute.

- **2020-2023**
- **Collaboration** between academia and industry partially funded by InnovationFund Denmark.
- **Corti**: Using machine learning to augment communication in the healthcare sector.
- **Project goal**: Pursue research in machine learning at the interface between academic and company interests.

1. Industrial project, Corti + DTU Compute, InnovationFund Denmark, 2020-2023.
2. Augment communication in healthcare sector.
3. Research in machine learning at the interface of shared interests.

Medical dialogue

Central to an interaction within a healthcare system is the medical dialogue:

- General practitioner
- Nurse
- Midwife
- Emergency medical dispatcher
- Paramedic
- Emergency room
- Health insurance

1. We focus on medical communication.
2. Involves many different parties.
3. Different contexts and purposes.
4. Busy emergency room, calls to emergency medical dispatchers, visits at general practitioners, etc.

Errors in medical dialogue

- Communication is everywhere in healthcare.
- It is complex, involving multiple participants, different contexts, and different purposes.

INTRODUCTION
Errors in medical dialogue
- Communication is everywhere in healthcare.
- It is complex, involving multiple participants, different contexts, and different purposes.

1. So yes communication can be complex and noisy, but what are the consequences?
2. Failure of communication is a leading cause of adverse events.
3. Adverse events are episodes of medical error that result in harm to the patient.
4. Luckily, many of these are preventable, although exact numbers vary.
5. Better communication could help reduce these numbers.

Errors in medical dialogue

- Communication is everywhere in healthcare.
- It is complex, involving multiple participants, different contexts, and different purposes.
- Adverse events: Failure of communication contributes to two out of three adverse events [54].
- Preventability: Many adverse outcomes are preventable [10].

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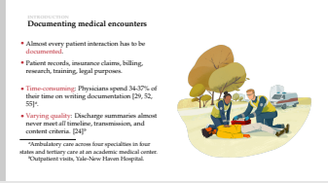
4. (Ambulatory ≡ outpatient care, Tertiary ≡ specialized care)

Documenting medical encounters

- Almost every patient interaction has to be documented.
- Patient records, insurance claims, billing, research, training, legal purposes.
- Time-consuming: Physicians spend 34-37% of their time on writing documentation [29, 52, 55][a].
- Varying quality: Discharge summaries almost never meet *all* timeline, transmission, and content criteria. [24][b]

[a] Ambulatory care across four specialties in four states and tertiary care at an academic medical center.
[b] Outpatient visits, Yale-New Haven Hospital.



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How might machine learning help?

- Assist with documentation.
- Augment communication.
- Improve decision-making.

1. Machine learning can help in many ways.
2. The main goal of augmenting communication is:
   - Reduce the impact.
   - Free up time.

How might machine learning help?

- Assist with documentation.
- Augment communication.
- Improve decision-making.

- Reduce the impact of medical errors and adverse events.
- Free up time spent on documentation for patient care.

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   - Reduce the impact.
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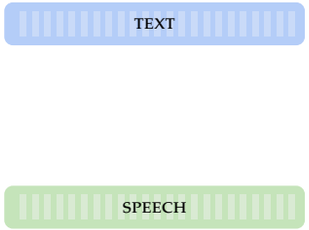
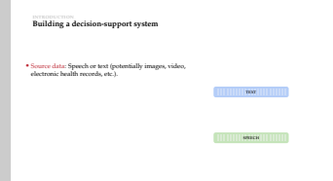
Building a decision-support system

1. We will take a modular approach to building a decision-support system.
2. First we need source data
3. Then we need to convert it into representations useful for downstream tasks.
4. Then we can perform the downstream tasks.
5. Finally, we need to estimate the reliability of our data, representations, and predictions.

Building a decision-support system

- Source data: Speech or text (potentially images, video, electronic health records, etc.).





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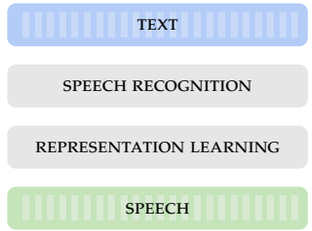

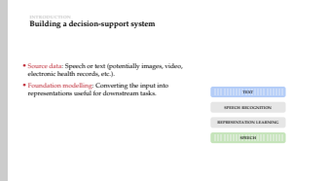

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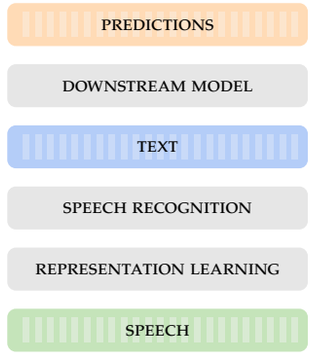

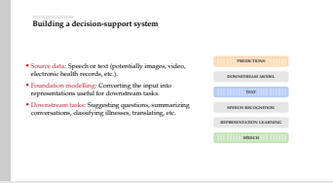

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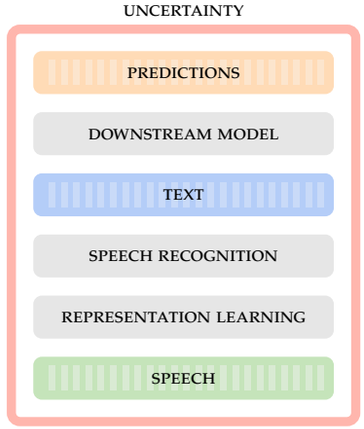
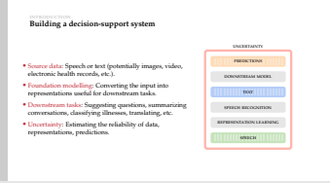
- Downstream tasks: Suggesting questions, summarizing conversations, classifying illnesses, translating, etc.
- Uncertainty: Estimating the reliability of data, representations, predictions.





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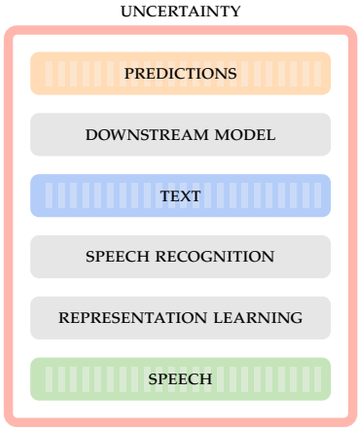

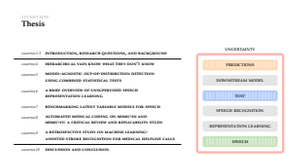

Chp. 4 Examine how a certain class of generative models can be used to detect data that is different from training data.

Chp. 5 Generalize this to be model-agnostic and phrased as a statistical test.

Chp. 6 Step back and provide an overview of modern methods for unsupervised speech representation learning.

Chp. 7 Benchmark some of these methods, generative latent variable models, on likelihood and automatic speech recognition.

Chp. 8 Move to a different domain, medical coding, and provide a critical review of recent works.

Chp. 9 Provide a retrospective study on a machine learning-assisted stroke recognition system for medical helpline calls.

1. So how does the thesis tackle this problem of building such a system?

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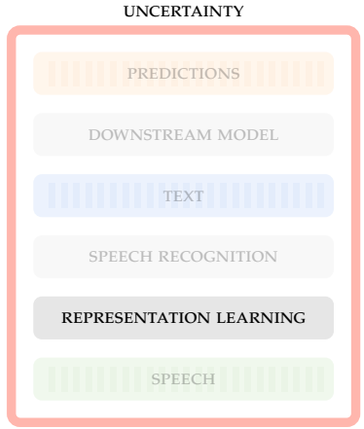

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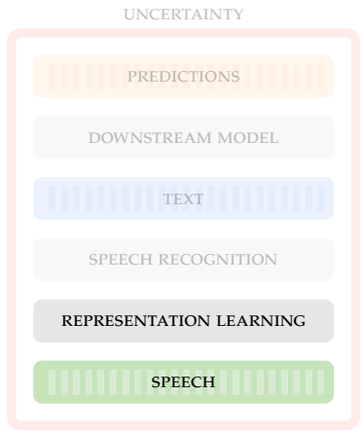

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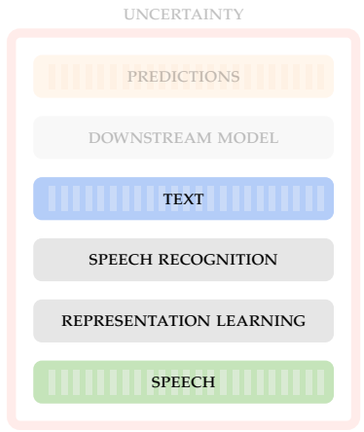

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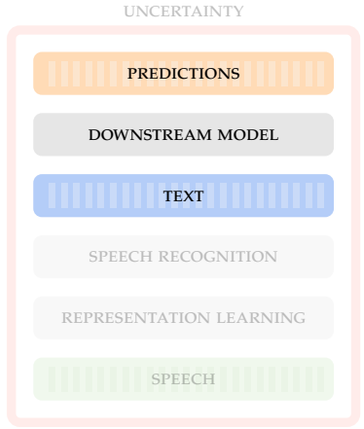

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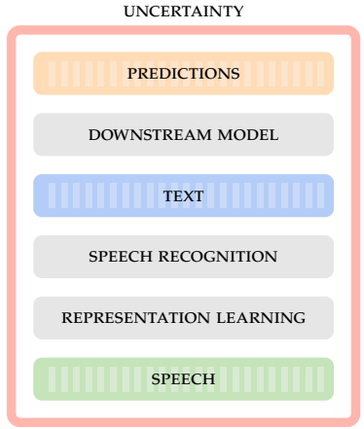

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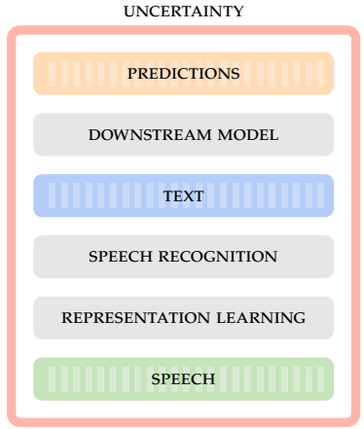

1. We want to keep papers that represent each of the three main themes of the thesis: (Uncertainty estimation, representation learning, and clinical applications)

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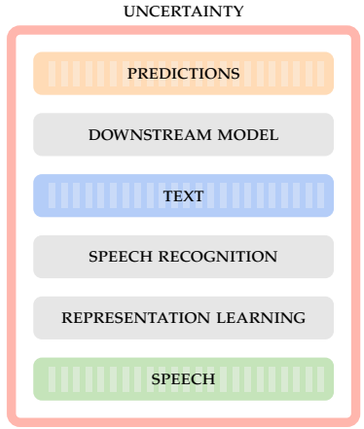

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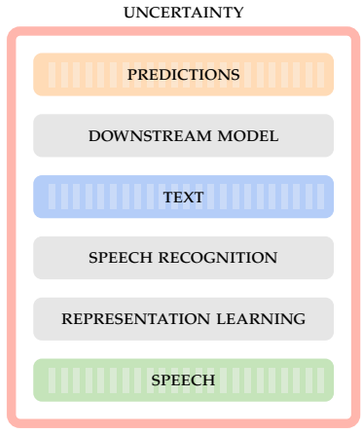

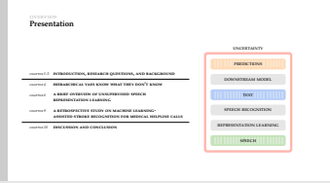

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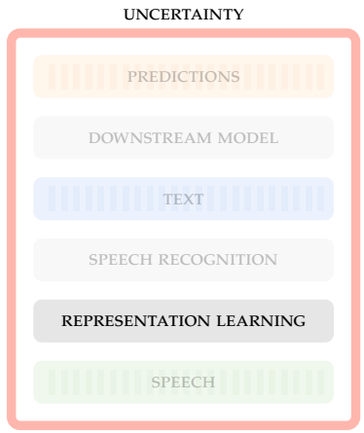
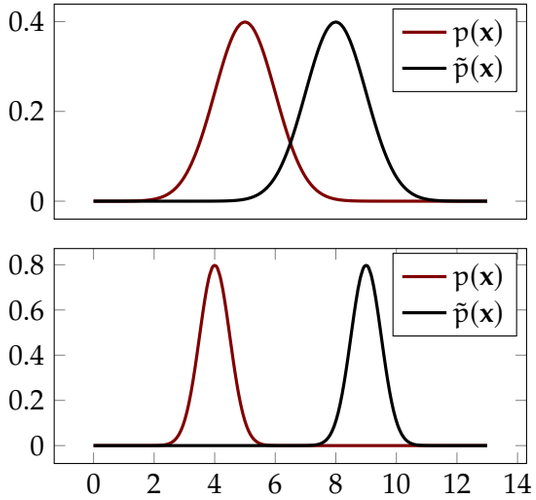


Defining OOD detection

Enable models to distinguish the training data distribution $p(\mathbf{x})$ from any other distribution $\tilde{p}(\mathbf{x})$.

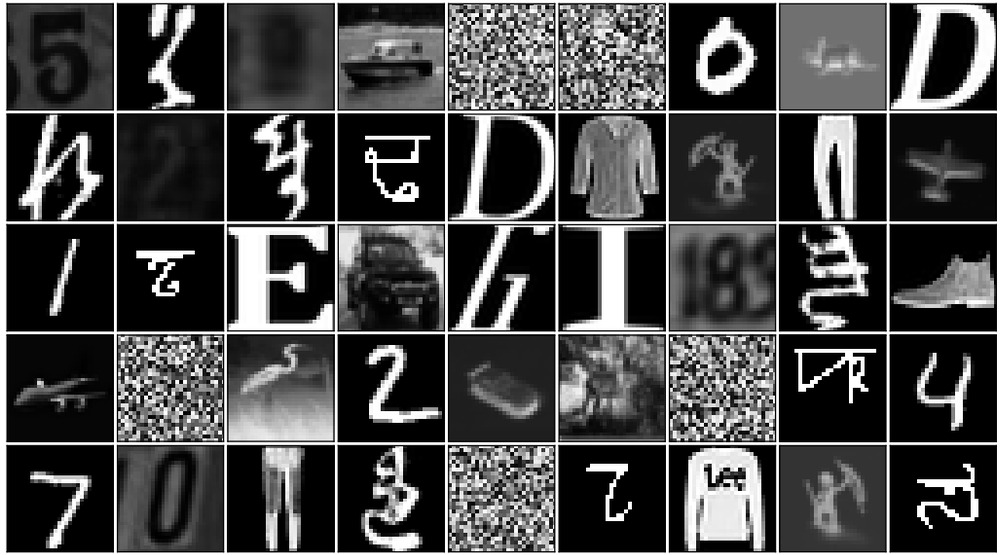
Do this for any given single observation, i.e. answer the question:

"Was $\mathbf{x}$ sampled from $p(\mathbf{x})$ or not?"



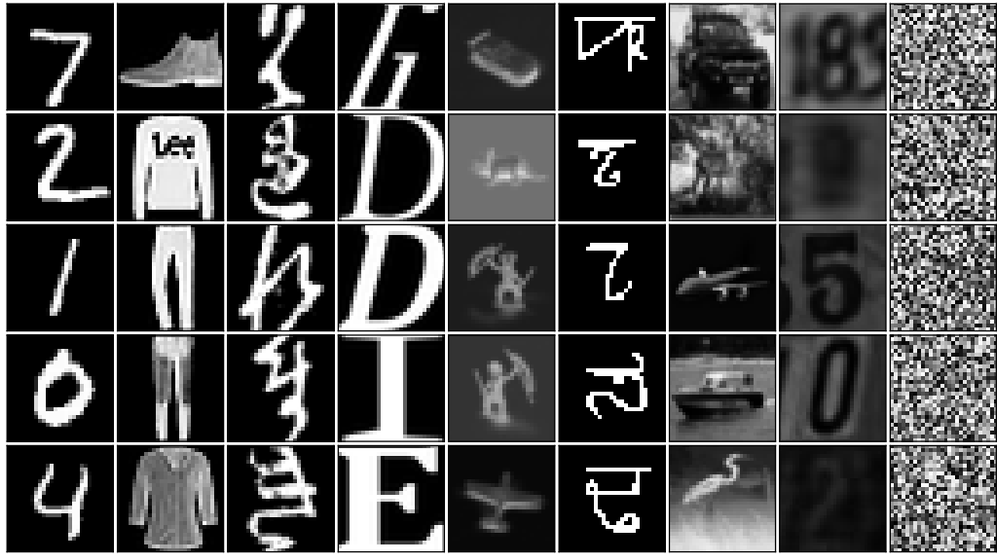
1. Define OOD
2. In 1D it is easy to see when this is possible and when it is not.
3. In higher dimensions it is not as easy to see.

In distribution?



1. Datasets can overlap quite a bit in their raw data space.
2. What we usually care about is a more semantic notion of similarity.

Out of distribution?



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Out-of-distribution detection with generative models

- Generative models learn to approximate the **data distribution** $p(\mathbf{x})$.
- The likelihood of the model given a sample $\mathbf{x}$ is a measure of how well the model **explains the data**.
- **Model likelihood** has long been thought of as useful for OOD detection [5].

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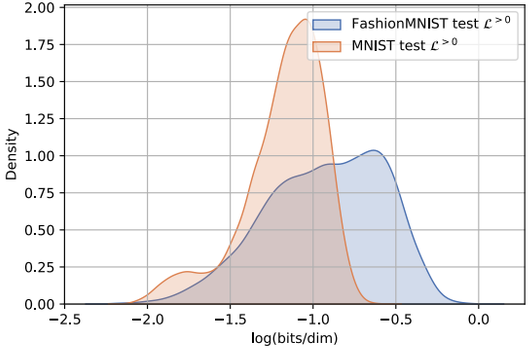
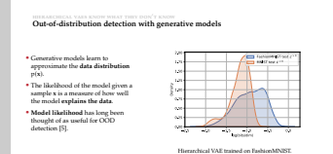


Hierarchical VAE trained on FashionMNIST.



Hierarchical VAE

We choose the hierarchical VAE as our model [33, 48].

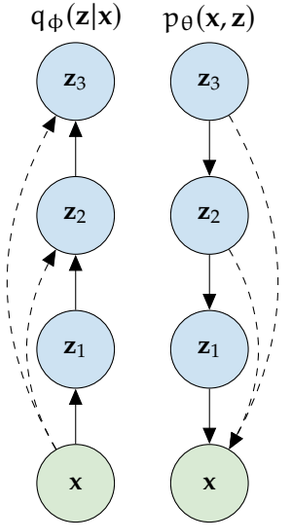
$$p_\theta(\mathbf{x}) = \int p_\theta(\mathbf{x}, \mathbf{z}) d\mathbf{z} = \int p_\theta(\mathbf{x}|\mathbf{z}) p_\theta(\mathbf{z}) d\mathbf{z}$$

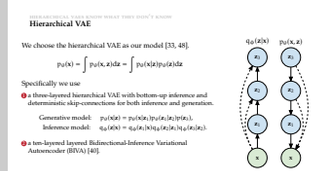
Specifically we use

1. a three-layered hierarchical VAE with bottom-up inference and deterministic skip-connections for both inference and generation.

$$\text{Generative model:} \quad p_\theta(\mathbf{x}|\mathbf{z}) = p_\theta(\mathbf{x}|\mathbf{z}_1) p_\theta(\mathbf{z}_1|\mathbf{z}_2) p(\mathbf{z}_3),$$
$$\text{Inference model:} \quad q_\phi(\mathbf{z}|\mathbf{x}) = q_\phi(\mathbf{z}_1|\mathbf{x}) q_\phi(\mathbf{z}_2|\mathbf{z}_1) q_\phi(\mathbf{z}_3|\mathbf{z}_2).$$

2. a ten-layered layered Bidirectional-Inference Variational Autoencoder (BIVA) [40].





1. We want to explain why HVAEs fail at OOD detection when using their likelihood.
2. And how to fix them.

What is wrong with the ELBO for OOD detection?

We can split the ELBO into two terms

$$\mathcal{L}(\mathbf{x};\theta,\phi) = \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}\left[\log \frac{p_\theta(\mathbf{x},\mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})}\right] = \underbrace{\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log p_\theta(\mathbf{x}|\mathbf{z})]}_{\text{reconstruction likelihood}} - \underbrace{D_{KL}(q_\phi(\mathbf{z}|\mathbf{x}) \parallel p(\mathbf{z}))}_{\text{regularization penalty}} . \quad (1)$$

The first term is high if the data is well-explained by $\mathbf{z}$. The second term we can rewrite as,

$$D_{KL}(q_\phi(\mathbf{z}|\mathbf{x}) \parallel p(\mathbf{z})) = \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}\left[\sum_{i=1}^{L-1} \log \frac{p_\theta(\mathbf{z}_i|\mathbf{z}_{i+1})}{q_\phi(\mathbf{z}_i|\mathbf{z}_{i-1})} + \log \frac{p_\theta(\mathbf{z}_L)}{q_\phi(\mathbf{z}_L|\mathbf{z}_{L-1})}\right] . \quad (2)$$

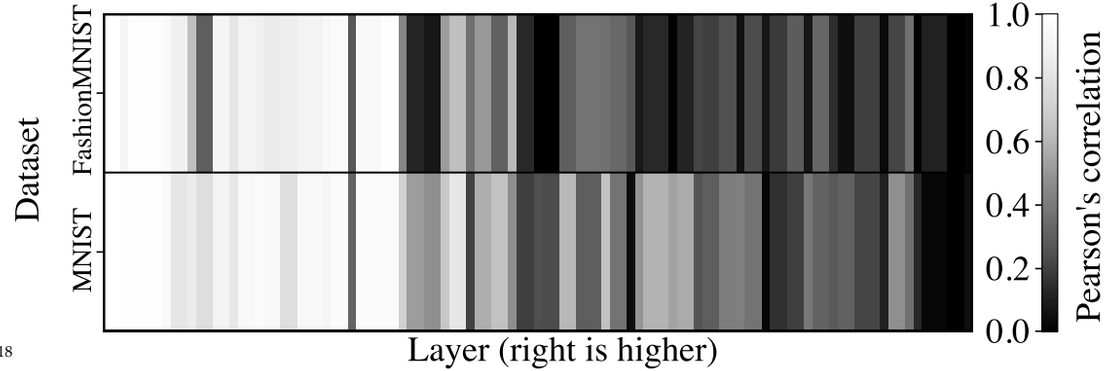
Since the individual terms are computed by summing over the dimensionality of $\mathbf{z}_i$, the absolute log-ratios grow with $\dim(\mathbf{z}_i)$.
Since the lower-most latent variables are usually higher dimensional than top ones, these are weighted higher in the ELBO.

1. There is a tendency for the lower-most latent variables to be weighted higher than the higher ones.

What do the lowest latent variables represent?

Absolute Pearson correlations between data representations in all layers of the inference network of a hierarchical VAE trained on FashionMNIST and of another trained on MNIST.

Correlation computed between the representations of the two different models given the same data, FashionMNIST (top) and MNIST (bottom).



1. Strong evidence that the lowest latent variables are generalizing across datasets.

Likelihood ratios

We suggest to define a likelihood ratio score [9] using the ELBO $\mathcal{L}(\mathbf{x})$ and a relaxed bound $\mathcal{L}^{>k}(\mathbf{x})$.

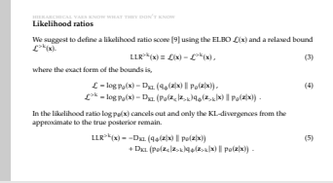
$$\mathrm{LLR}^{>k}(\mathbf{x}) \equiv \mathcal{L}(\mathbf{x}) - \mathcal{L}^{>k}(\mathbf{x}) \,, \tag{3}$$

where the exact form of the bounds is,

$$\begin{aligned} \mathcal{L} &= \log p_\theta(\mathbf{x}) - D_{\mathrm{KL}}\left(q_\phi(\mathbf{z}|\mathbf{x}) \parallel p_\theta(\mathbf{z}|\mathbf{x})\right) , \\ \mathcal{L}^{>k} &= \log p_\theta(\mathbf{x}) - D_{\mathrm{KL}}\left(p_\theta(\mathbf{z}_{\leqslant}|\mathbf{z}_{>k}) q_\phi(\mathbf{z}_{>k}|\mathbf{x}) \parallel p_\theta(\mathbf{z}|\mathbf{x})\right) \,. \end{aligned} \tag{4}$$

In the likelihood ratio $\log p_\theta(\mathbf{x})$ cancels out and only the KL-divergences from the approximate to the true posterior remain.

$$\begin{aligned} \mathrm{LLR}^{>k}(\mathbf{x}) = &-D_{\mathrm{KL}}\left(q_\phi(\mathbf{z}|\mathbf{x}) \parallel p_\theta(\mathbf{z}|\mathbf{x})\right) \\ &+ D_{\mathrm{KL}}\left(p_\theta(\mathbf{z}_{\leqslant}|\mathbf{z}_{>k}) q_\phi(\mathbf{z}_{>k}|\mathbf{x}) \parallel p_\theta(\mathbf{z}|\mathbf{x})\right) \,. \end{aligned} \tag{5}$$



1. Write likelihood-ratio using the exact form of the bounds including intractable KL-divergence.

Importance sampling the ELBO

The importance weighted autoencoder (IWAE) bound is tight with the true likelihood in the limit of infinite samples, $S \to \infty$ [8],

$$\mathcal{L}_S = \mathbb{E}_{q(\mathbf{z}|\mathbf{x})}\left[\log \frac{1}{N}\sum_{s=1}^{S}\frac{p(\mathbf{x},\mathbf{z}^{(s)})}{q(\mathbf{z}^{(s)}|\mathbf{x})}\right] \leqslant \log p_\theta(\mathbf{x})\,, \tag{6}$$

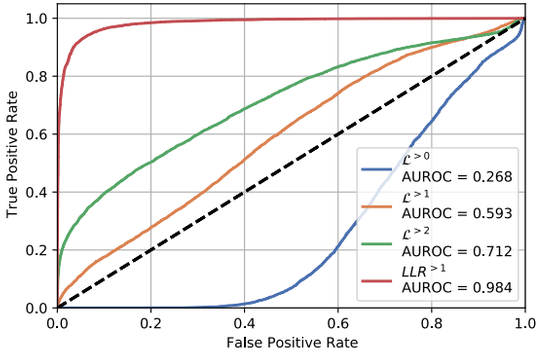
Consequently, by importance sampling the ELBO, $D_{KL}\left(q_\phi(\mathbf{z}|\mathbf{x}) \parallel p_\theta(\mathbf{z}|\mathbf{x})\right) \to 0$ and our likelihood ratio reduces to the KL-divergence of $\mathcal{L}^{>k}$.

$$\mathrm{LLR}_S^{>k}(\mathbf{x}) \to D_{KL}(p(\mathbf{z}_{\leqslant}|\mathbf{z}_{>k})q(\mathbf{z}_{>k}|\mathbf{x}) \parallel p(\mathbf{z}|\mathbf{x}))\,. \tag{7}$$

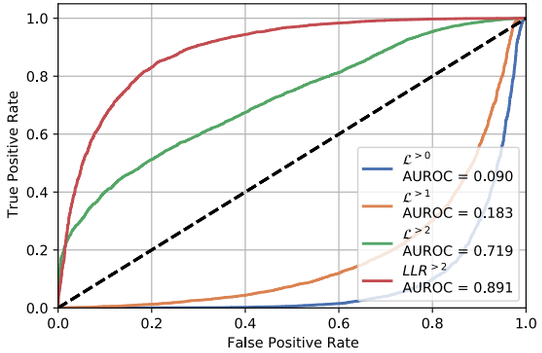
$\mathrm{LLR}_S^{>k}(\mathbf{x})$ performs KL-divergence-based OOD detection using top-most latent variables.

1. We can use the IWAE bound force the KL-divergence of the original ELBO towards zero.
2. Then, the likelihood ratio reduces to the KL-divergence of $\mathcal{L}^{>k}$.
3. We can hope that using the conditional prior for the lowest latent variables will make the KL-divergence more sensitive to OOD data in the top-most latent variables.

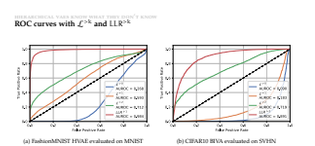
ROC curves with $\mathcal{L}^{>k}$ and $\text{LLR}^{>k}$



(a) FashionMNIST HVAE evaluated on MNIST

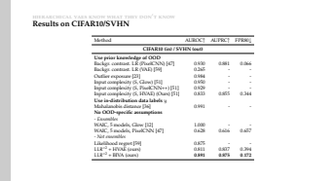


(b) CIFAR10 BIVA evaluated on SVHN



Results on CIFAR10/SVHN

Method	AUROC↑	AUPRC↑	FPR80↓
CIFAR10 (in) / SVHN (out)			
Use prior knowledge of OOD			
Backgr. contrast. LR (PixelCNN) [47]	0.930	0.881	0.066
Backgr. contrast. LR (VAE) [59]	0.265	-	-
Outlier exposure [23]	0.984	-	-
Input complexity (S, Glow) [51]	0.950	-	-
Input complexity (S, PixelCNN++) [51]	0.929	-	-
Input complexity (S, HVAE) (Ours) [51]	0.833	0.855	0.344
Use in-distribution data labels y			
Mahalanobis distance [36]	0.991	-	-
No OOD-specific assumptions			
- Ensembles			
WAIC, 5 models, Glow [12]	1.000	-	-
WAIC, 5 models, PixelCNN [47]	0.628	0.616	0.657
- Not ensembles			
Likelihood regret [59]	0.875	-	-
$\text{LLR}^{>2}$ + HVAE (ours)	0.811	0.837	0.394
$\text{LLR}^{>2}$ + BIVA (ours)	**0.891**	**0.875**	**0.172**



Conclusions

- Key observations:
  - The likelihood of a generative model is not a good score for OOD detection [41].
  - Strong correlations between some latent variables for different datasets.

→ Provide explanation for why the likelihood fails for OODD for HVAEs.

→ Proposed a likelihood-ratio score, $\text{LLR}^{>k}$, that uses the conditional prior for the bottom-most latent variables in the hierarchy and showed its effectiveness.

HIERARCHICAL VAES KNOW WHAT THEY DON'T KNOW
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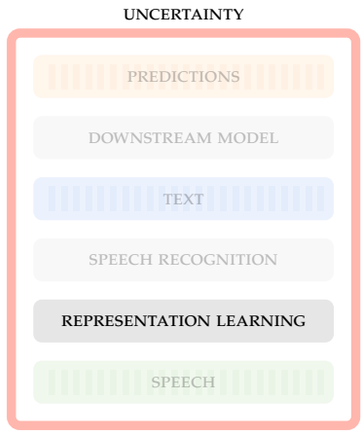
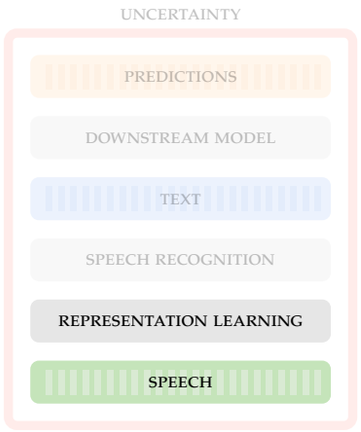
Presentation



1. We now move on to our review paper of speech representation learning.

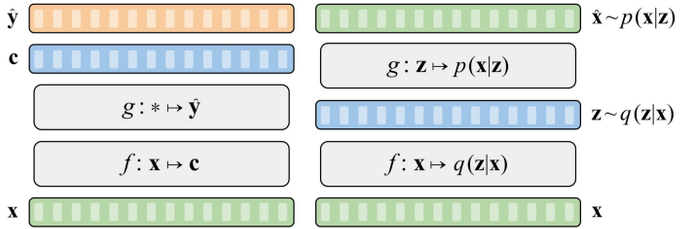
Presentation



1. We now move on to our review paper of speech representation learning.

Overview: Representation Learning for Speech

- Reviews two learning paradigms:
  - Self-supervised learning (SSL)
  - Probabilistic latent variable models (LVMs)
- Recent developments have been driven by self-supervised learning.
- A model-by-model overview for selected self-supervised models.



1. Focus on the self-supervised learning models.

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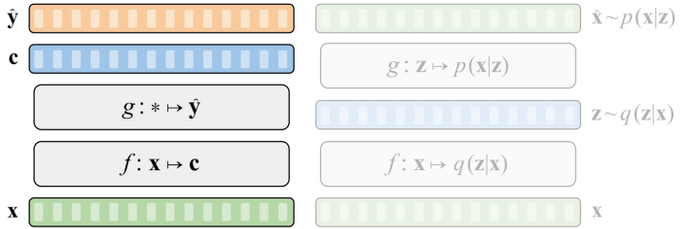
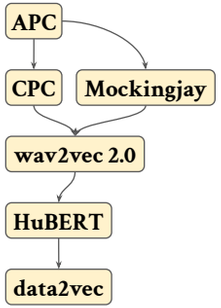


1. Focus on the self-supervised learning models.

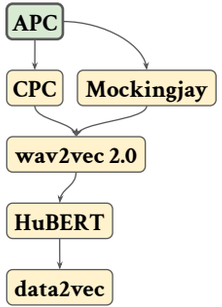
Development of SSL for speech



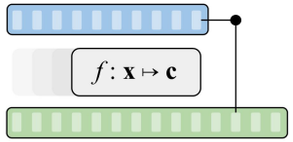
- Common setup: Learn representations from raw audio without supervision.
- Main evaluation: Speech recognition performance.

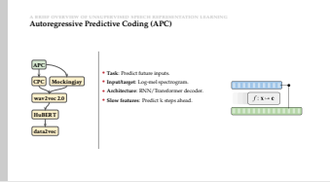
A BRIEF OVERVIEW OF UNSUPERVISED SPEECH REPRESENTATION LEARNING
Development of SSL for speech
APC
CPC
Mockingjay
wav2vec 2.0
HuBERT
data2vec
• Common setup: Learn representations from raw audio without supervision.
• Main evaluation: Speech recognition performance.

Autoregressive Predictive Coding (APC)

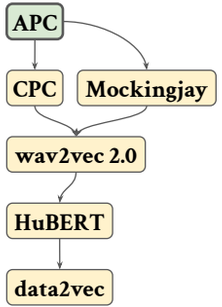


- **Task**: Predict future inputs.
- **Input/target**: Log-mel spectrogram.
- **Architecture**: RNN/Transformer decoder.
- **Slow features**: Predict k steps ahead.

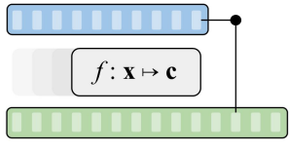


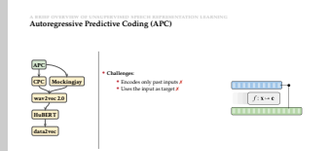


Autoregressive Predictive Coding (APC)



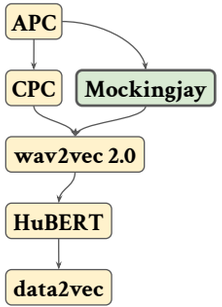
- **Challenges**:
  - Encodes only past inputs ✗
  - Uses the input as target ✗



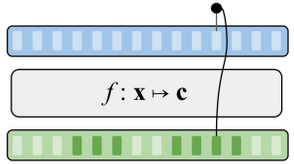


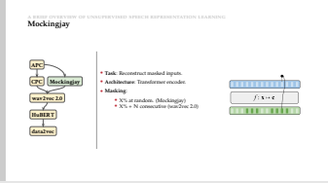
1. Encoding only past inputs limits the model's ability to learn from future context.
2. Input as target limits the model's ability to learn abstract representations.

Mockingjay



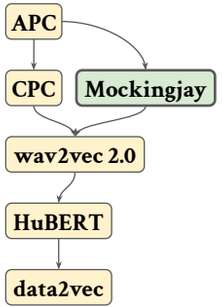
- **Task**: Reconstruct masked inputs.
- **Architecture**: Transformer encoder.
- **Masking**:
  - X% at random. (Mockingjay)
  - X% + N consecutive (wav2vec 2.0)



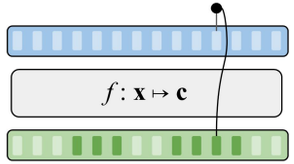


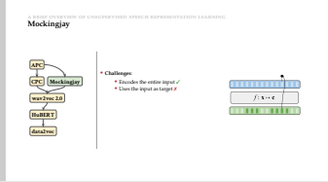
1. Replaces autoregressiveness with a masked reconstruction task.
2. Masking strategy to force learning long-term context.

Mockingjay

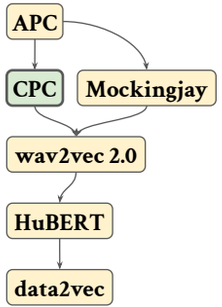


- **Challenges**:
  - Encodes the entire input ✓
  - Uses the input as target ✗

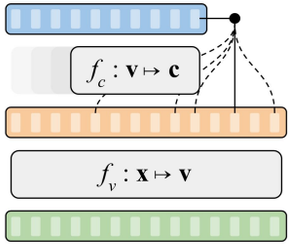


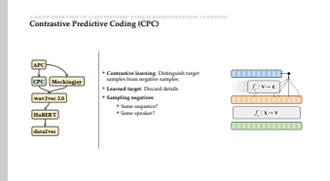


Contrastive Predictive Coding (CPC)



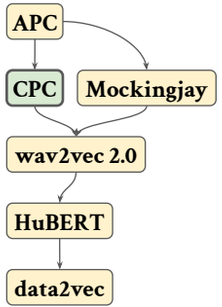
- **Contrastive learning**: Distinguish target samples from negative samples.
- **Learned target**: Discard details.
- **Sampling negatives**:
  - Same sequence?
  - Same speaker?



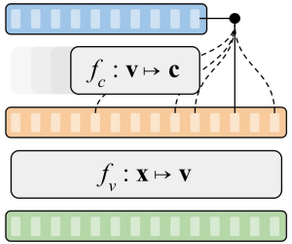


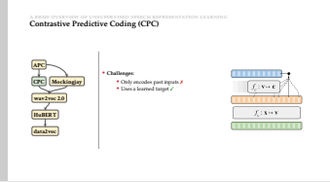
1. Contrastive models allow using a learned target. Discard unimportant details of input.
2. Negative sampling is a challenge and requires careful design.
3. Sampling different speakers as negatives learns strong speaker-identities.

Contrastive Predictive Coding (CPC)



- **Challenges**:
  - Only encodes past inputs ✗
  - Uses a learned target ✓





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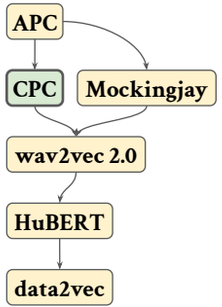
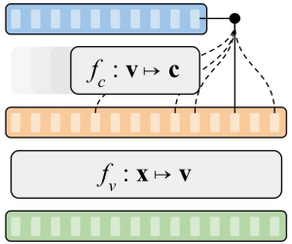
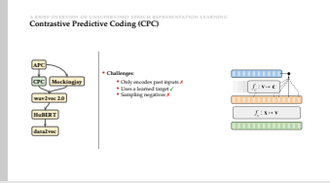
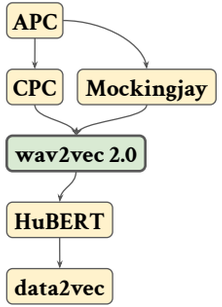


- **Challenges**:
  - Only encodes past inputs ✗
  - Uses a learned target ✓
  - Sampling negatives ✗

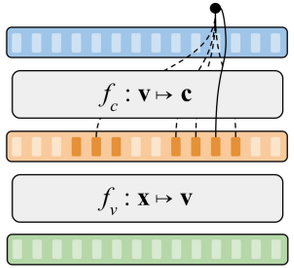


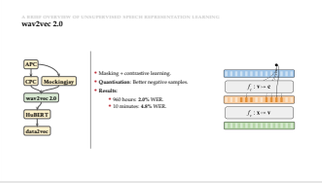


wav2vec 2.0



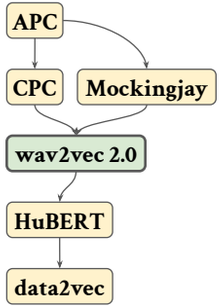
- Masking + contrastive learning.
- **Quantisation**: Better negative samples.
- **Results**:
  - 960 hours: **2.0%** WER.
  - 10 minutes: **4.8%** WER.



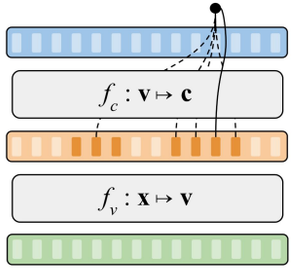


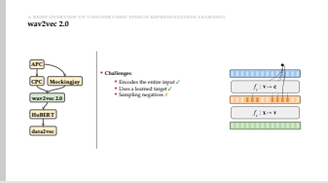
1. Training objective requires identifying the correct quantized latent audio representation in a set of distractors for each masked time step.
2. Quantisation improves negative sampling (requires approximation via Gumbel softmax).

wav2vec 2.0

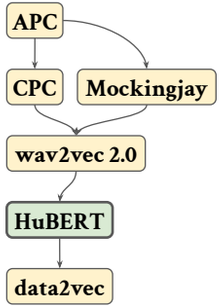


- **Challenges**:
  - Encodes the entire input ✓
  - Uses a learned target ✓
  - Sampling negatives ✗

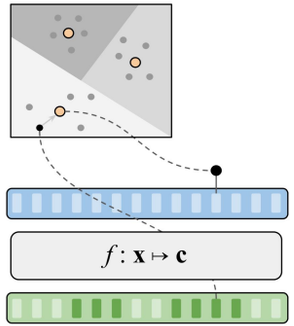


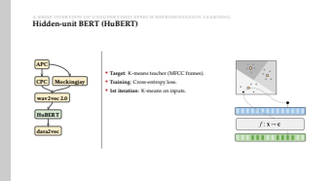


Hidden-unit BERT (HuBERT)



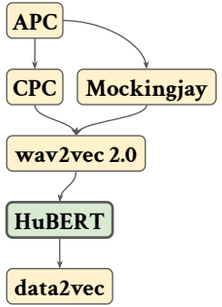
- **Target**: K-means teacher (MFCC frames).
- **Training**: Cross-entropy loss.
- **1st iteration**: K-means on inputs.



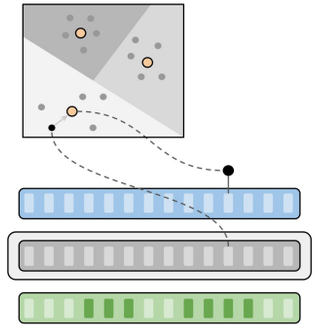


1. HuBERT approach predicts hidden cluster assignments of masked frames

Hidden-unit BERT (HuBERT)

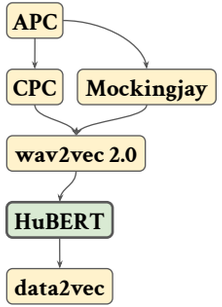


- **Target**: K-means teacher (MFCC frames).
- **Training**: Cross-entropy loss.
- **1st iteration**: K-means on inputs.
- **2nd iteration**: K-means on hidden layers.

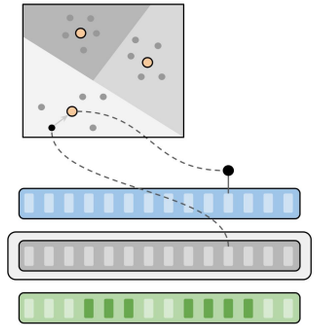


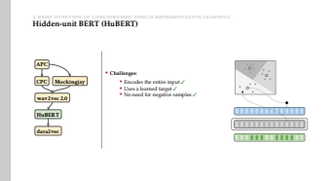
1. HuBERT approach predicts hidden cluster assignments of masked frames

Hidden-unit BERT (HuBERT)



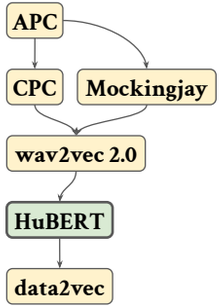
- **Challenges**:
  - Encodes the entire input ✓
  - Uses a learned target ✓
  - No need for negative samples ✓



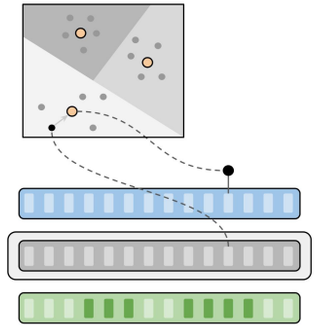


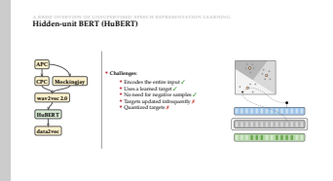
1. HuBERT approach predicts hidden cluster assignments of masked frames
2. Targets are still quantised although we no longer solve a contrastive sampling problem. Might reduce quality.

Hidden-unit BERT (HuBERT)



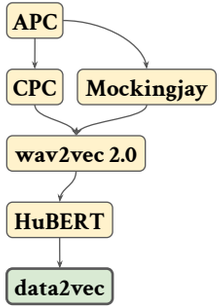
- **Challenges**:
  - Encodes the entire input ✓
  - Uses a learned target ✓
  - No need for negative samples ✓
  - Targets updated infrequently ✗
  - Quantized targets ✗



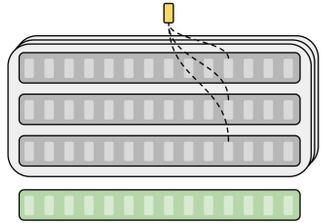


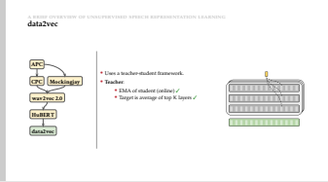
1. HuBERT approach predicts hidden cluster assignments of masked frames
2. Targets are still quantised although we no longer solve a contrastive sampling problem. Might reduce quality.

data2vec

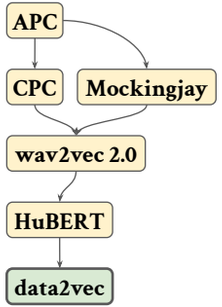


- Uses a teacher-student framework.
- **Teacher**:
  - EMA of student (online) ✓
  - Target is average of top K layers ✓

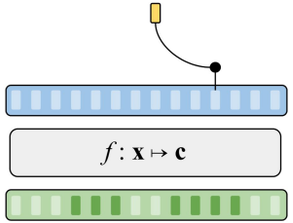


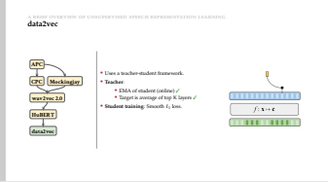


data2vec

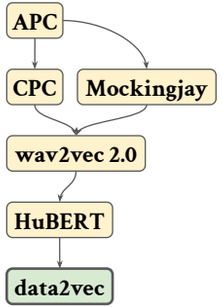


- Uses a teacher-student framework.
- **Teacher**:
  - EMA of student (online) ✓
  - Target is average of top K layers ✓
- **Student training**: Smooth ℓ_1 loss.

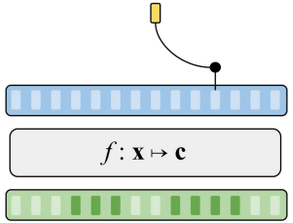


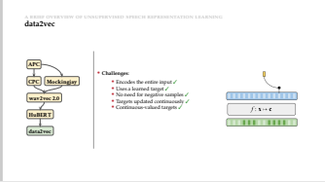


data2vec



- **Challenges**:
  - Encodes the entire input ✓
  - Uses a learned target ✓
  - No need for negative samples ✓
  - Targets updated continuously ✓
  - Continuous-valued targets ✓



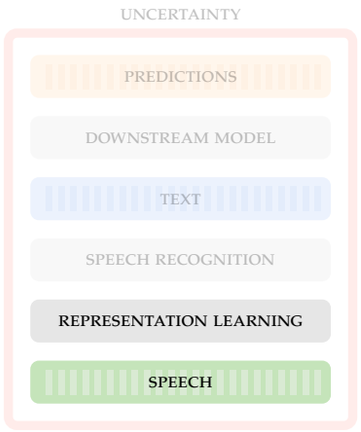


Conclusions

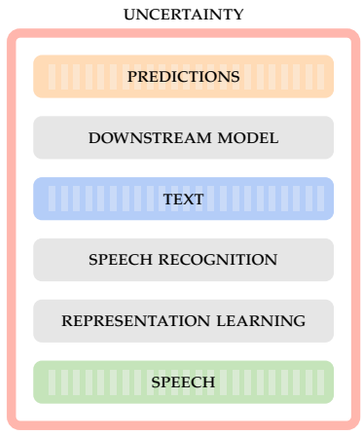
- **Main conclusions**:
  - The most popular self-supervised speech models can be compactly described by a few core design choices.
  - Many of these design choices are mirrored in earlier work on speech embedding models.
- **Open questions and limitations**:
  - Which design choices benefit which downstream tasks?
  - It is difficult to compare methods as model size and evaluation procedures differ widely between papers.

1. Predictive, Contrastive, Masking, Learned targets, Quantization, Teacher-student
2. Audio Word2vec, Speech2Vec, Unspeech which also used masking, and predictive and contrastive setups.

Presentation



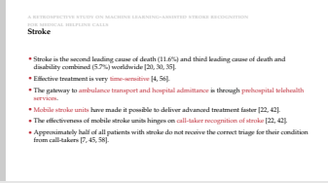
Presentation



Stroke

- Stroke is the second leading cause of death (11.6%) and third leading cause of death and disability combined (5.7%) worldwide [20, 30, 35].
- Effective treatment is very time-sensitive [4, 56].
- The gateway to ambulance transport and hospital admittance is through prehospital telehealth services.
- Mobile stroke units have made it possible to deliver advanced treatment faster [22, 42].
- The effectiveness of mobile stroke units hinges on call-taker recognition of stroke [22, 42].
- Approximately half of all patients with stroke do not receive the correct triage for their condition from call-takers [7, 45, 58].

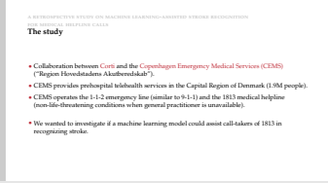
1. [45]: Systematic review, recall = 41-83%, precision = 42-68%.
2. [58]: 1-1-2 calls at CEMS, recall = 66.2%, precision = 30.2%.
3. [7]: Systematic review, recall = 66.2%, precision = 30.2%.
4. Recognition rates also vary widely by call-center.



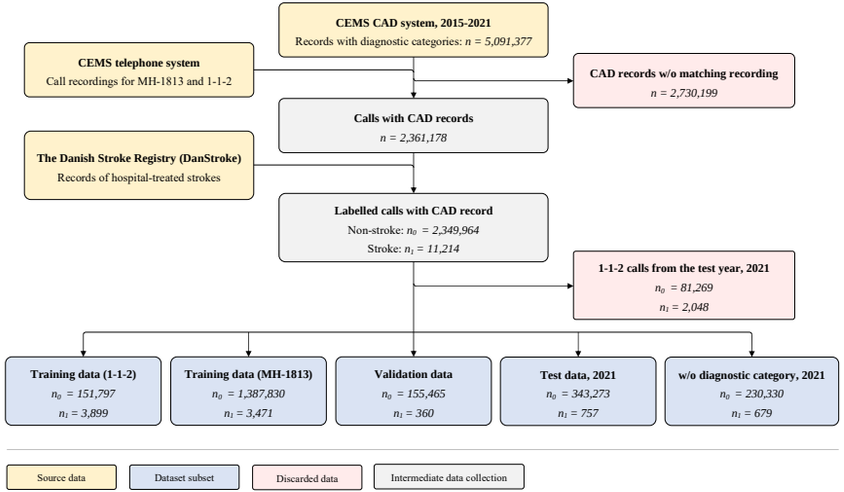
The study

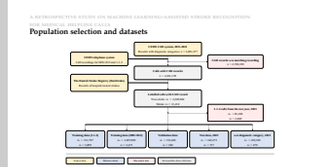
- Collaboration between Corti and the Copenhagen Emergency Medical Services (CEMS) ("Region Hovedstadens Akutberedskab").
- CEMS provides prehospital telehealth services in the Capital Region of Denmark (1.9M people).
- CEMS operates the 1-1-2 emergency line (similar to 9-1-1) and the 1813 medical helpline (non-life-threatening conditions when general practitioner is unavailable).

- We wanted to investigate if a machine learning model could assist call-takers of 1813 in recognizing stroke.



Population selection and datasets





1. Test data is MH-1813 2021.
2. All 1-1-2 data is used for training except 2021.
3. Validation data is sampled with stratified sampling from MH-1813 from 2015-2020.

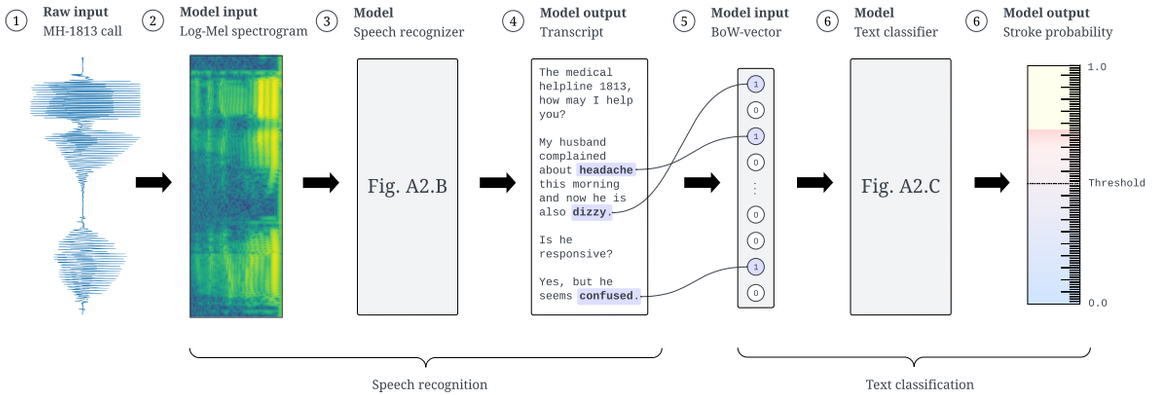
Population characteristics of test set

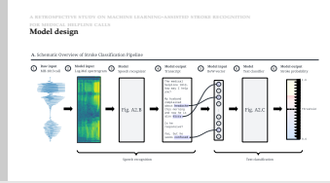
Subset	*All calls*	*Stroke calls*	*Non-stroke*
Num. calls	344,030	757	343,273
Female	190,974 (55.51%)	349 (46.10%)	190,625 (55.53%)
Male	153,050 (44.49%)	408 (53.90%)	152,642 (44.47%)
65+ years	65,652 (19.08%)	555 (73.32%)	65,097 (18.96%)
Age (mean ± std.)	44.31 ± 20.10	71.51 ± 13.41	44.25 ± 20.08

1. Prevalence of stroke is less than a quarter percent, one in every 400 calls.
2. The mean age of stroke calls is 71.5 years, older than general callers.
3. Males are a bit more likely to call with a stroke compared to females.
4. Other datasets (training, validation) have similar characteristics.

Model design

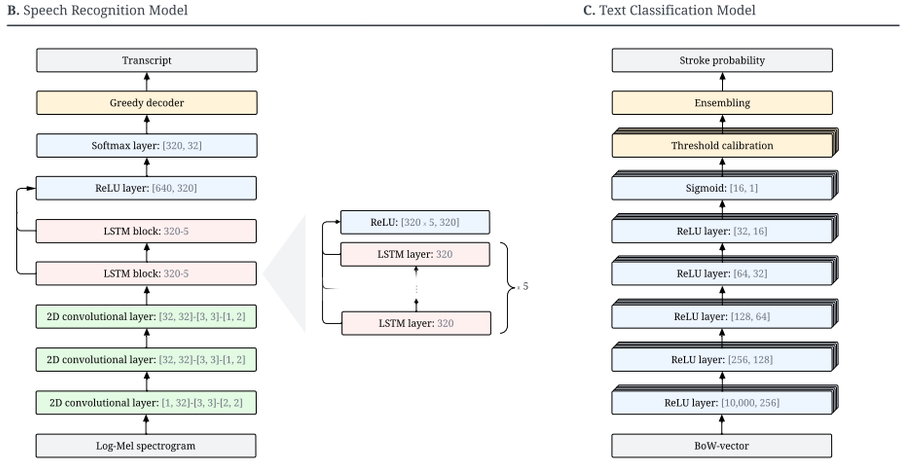
A. Schematic Overview of Stroke Classification Pipeline





1. Same structure as the decision-support system sketched in the overview slides.

Model design



1. ASR model somewhat old-school, but performant for this task with noisy calls.
2. Classification model is ensemble of five models.

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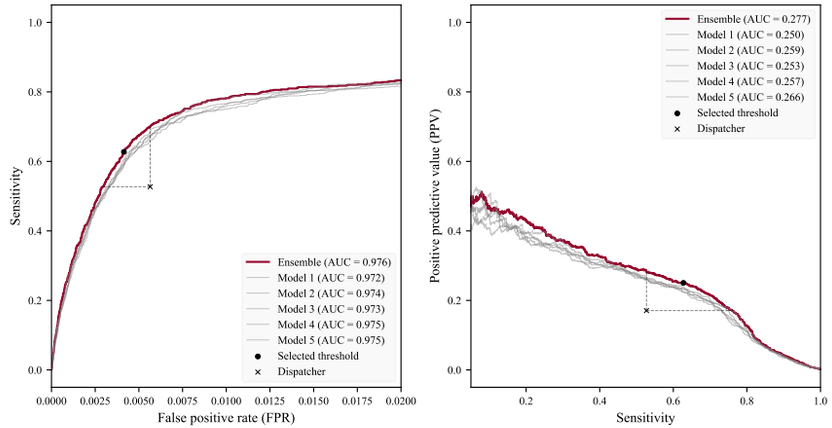
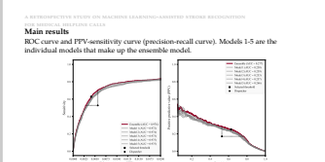
Main results

ROC curve and PPV-sensitivity curve (precision-recall curve). Models 1-5 are the individual models that make up the ensemble model.



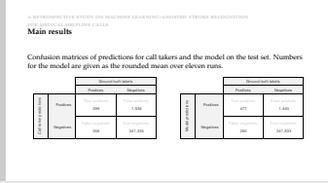


Main results

Confusion matrices of predictions for call takers and the model on the test set. Numbers for the model are given as the rounded mean over eleven runs.

		Ground truth labels	
		Positives	Negatives
Call taker predictions	Positives	True positives 399	False positves 1,938
	Negatives	False negatives 358	True negatives 341,335

		Ground truth labels	
		Positives	Negatives
Model predictions	Positives	True positives 477	False positves 1,440
	Negatives	False negatives 280	True negatives 341,833



1. In absolute numbers, the model correctly identifies 78 cases of stroke missed by call-takers.
2. The model also reduces the number of false positives by about 500 from 1938 to 1440.

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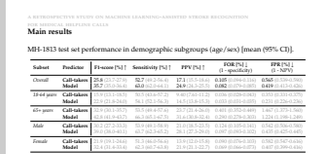
Main results

MH-1813 test set performance in demographic subgroups (age/sex) [mean (95% CI)].

Subset	Predictor	F1-score [%] ↑	Sensitivity [%] ↑	PPV [%] ↑	FOR [%] ↓ (1 - specificity)	FPR [%] ↓ (1 - NPV)
Overall	**Call-takers**	25.8 (23.7-27.9)	52.7 (49.2-56.4)	17.1 (15.5-18.6)	0.105 (0.094-0.116)	0.565 (0.539-0.590)
	Model	35.7 (35.0-36.4)	63.0 (62.0-64.1)	24.9 (24.3-25.5)	0.082 (0.079-0.085)	0.419 (0.413-0.426)
18-64 years	**Call-takers**	15.9 (13.1-18.5)	50.5 (43.6-57.2)	9.40 (7.61-11.2)	0.036 (0.028-0.043)	0.353 (0.331-0.375)
	Model	22.9 (21.8-24.0)	54.1 (52.1-56.3)	14.5 (13.8-15.3)	0.033 (0.031-0.035)	0.231 (0.226-0.236)
65+ years	**Call-takers**	32.9 (30.1-35.7)	53.5 (49.4-57.6)	23.7 (21.4-26.0)	0.401 (0.352-0.449)	1.467 (1.373-1.560)
	Model	42.8 (41.9-43.7)	66.3 (65.1-67.5)	31.6 (30.8-32.4)	0.290 (0.278-0.303)	1.224 (1.198-1.249)
Male	**Call-takers**	30.2 (27.2-33.3)	53.9 (49.1-58.9)	21.0 (18.5-23.5)	0.124 (0.105-0.141)	0.542 (0.506-0.580)
	Model	39.0 (38.0-40.1)	63.7 (62.3-65.2)	28.1 (27.3-29.0)	0.097 (0.093-0.102)	0.435 (0.425-0.445)
Female	**Call-takers**	21.9 (19.1-24.6)	51.3 (46.0-56.6)	13.9 (12.0-15.8)	0.090 (0.076-0.103)	0.582 (0.547-0.616)
	Model	32.4 (31.4-33.4)	62.3 (60.7-63.8)	21.9 (21.1-22.7)	0.069 (0.066-0.073)	0.407 (0.399-0.416)



corti DTU

Occlusion analysis — Which features are evidence?

Features with positive ranking score ($r^{(w)} > 0$) **computed on stroke positive predictions** (D = 1,897)					
Rank	Word, *w (translated)*	Occurrences, $D^{(w)}$	Rank	Word, *w (translated)*	Occurrences, $D^{(w)}$
1.	Ambulance	1,680	16.	Difficulties speaking	44
2.	Blood clot	895	17.	Hemorrhagic stroke	133
3.	Left	1,108	18.	Hand	297
4.	Right	1,050	19.	The ambulance	521
5.	Double vision	84	20.	Slurred speech	58
6.	The words	344	21.	Blood clots	224
7.	Suddenly	783	22.	Fast	663
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12.	Control	134	27.	Reduced	528
13.	Call	39	28.	Hangs	628
14.	Numb	94	29.	Transient	48
15.	Minutes	763	30.	Not making sense	14

[Recognition, Symptom, Urgency/Time]

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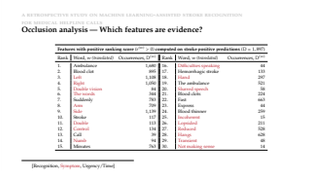

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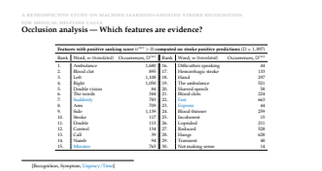

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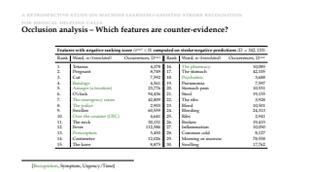
Features with negative ranking score ($r^{(w)} < 0$) **computed on stroke-negative predictions** ($D = 342,133$)

Rank	Word, w *(translated)*	Occurrences, $D^{(w)}$	Rank	Word, w *(translated)*	Occurrences, $D^{(w)}$
1.	Tetanus	4,378	16.	The pharmacy	10,085
2.	Pregnant	8,749	17.	The stomach	42,105
3.	Cut	7,592	18.	Psychiatric	3,688
4.	Bandage	4,561	19.	Pneumonia	7,597
5.	Amager (a location)	23,776	20.	Stomach pain	10,551
6.	O'clock	94,436	21.	Stool	19,155
7.	The emergency room	42,809	22.	The ribs	3,928
8.	The police	2,903	23.	Bleed	10,501
9.	Swollen	60,559	24.	Bleeding	24,313
10.	Over the counter (OTC)	4,641	25.	Ribs	2,941
11.	The neck	30,151	26.	Broken	19,415
12.	Fever	112,586	27.	Inflammation	10,050
13.	Prescription	5,450	28.	Common cold	8,127
14.	Centimeter	12,026	29.	Morning or morrow	78,558
15.	The knee	8,875	30.	Swelling	17,762

[Recognition, Symptom, Urgency/Time]



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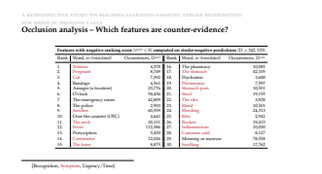

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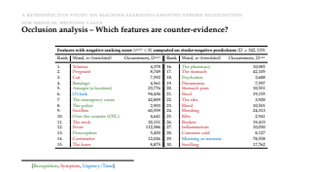
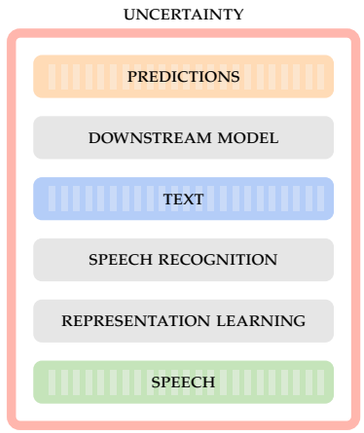


Future work

- Machine learning
  - Learning to predict directly from audio data (SSL).
  - Learning to defer to predict methods [57].
- Clinical applications
  - Mental health: Screening for suicide risk in emergency and medical helpline calls.
  - Maternity ward: Screening for serious pregnancy complications.

1. Learning to defer to predict is related to uncertainty estimation.

Presentation



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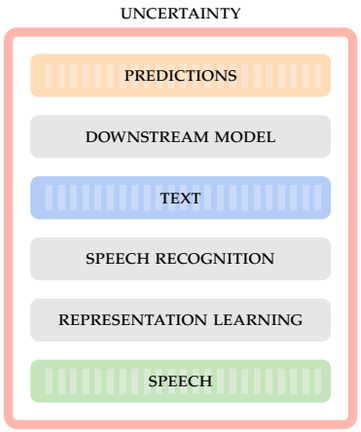

The broad picture: The thesis topic since 2020

2020 **Project start**

- Out-of-distribution detection with generative models: Mysterious new topic.
- Speech representation/recognition: Inflection point between supervised methods and new self-supervised approaches.

DISCUSSION
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2020 Project start
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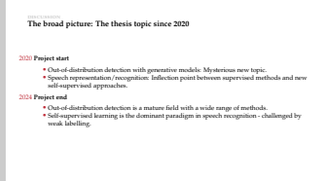
- Out-of-distribution detection is a mature field with a wide range of methods.
- Self-supervised learning is the dominant paradigm in speech recognition - challenged by weak labelling.



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2024 **Project end**

- Out-of-distribution detection is a mature field with a wide range of methods.
- Self-supervised learning is the dominant paradigm in speech recognition - challenged by weak labelling.
- Clinical research is increasingly becoming interested in the use of machine learning.

What lies ahead

- Selective out-of-distribution detection

  Two pairs of distributions may have identical divergence, but in different dimensions. How do we control features in black-box models?

- Self-supervised learning in the wild

  Does the recent progress on academic datasets translate to the real-world setting?

  Speech recognition has been the cornerstone benchmarking task. How do we target spoken language understanding directly?

- Large language models in medical dialogue

  LLMs will likely play a central role in the future of medical documentation and communication. How do we get a grip of their uncertainty?

1. We saw how certain features can dominate an uncertainty score. How do we properly control which features we want to use to detect out-of-distribution data?
2. Self-supervised learning has made great strides in academic benchmarks. How does this translate to real-world settings?
3. LLMs will be important for medical documentation and communication going forward. What does uncertainty look like in this context?

DISCUSSION

The role of uncertainty in an operational decision support system

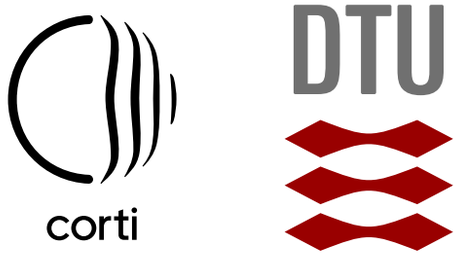
- Are true uncertainty estimates really feasible? Pragmatism versus idealism.
- Role of explainability compared to uncertainty estimates.
- European Parliamentary Research Services [18]:

"Future AI solutions for healthcare should be implemented by integrating uncertainty estimation, a relatively new field of research that aims to provide clinicians with clinically useful indications on the degree of confidence in AI predictions"

DISCUSSION
The role of uncertainty in an operational decision support system
• Are true uncertainty estimates really feasible? Pragmatism versus idealism.
• Role of explainability compared to uncertainty estimates.
• European Parliamentary Research Services [18]:
"Future AI solutions for healthcare should be implemented by integrating uncertainty estimation, a relatively new field of research that aims to provide clinicians with clinically useful indications on the degree of confidence in AI predictions"

1. LVMs were difficult to scale to the problems we care about.
2. LVMs did not convincingly outperform more pragmatic approaches (e.g. deferring).
3. Bayesian methods, deferring to predict, discriminative uncertainty.
4. What will happen if uncertainty estimates become a regulatory requirement?

Thank you for your attention.



Thank you for your attention.

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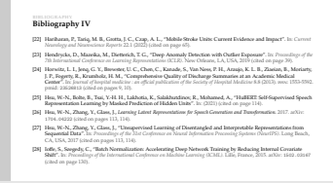

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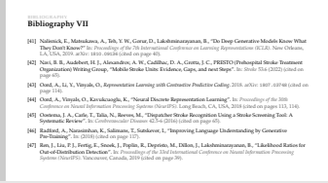

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Extra slides

- Introduction
- Hierarchical VAEs Know What They Don't Know
- A Brief Overview of Unsupervised Speech Representation Learning
- VAE background and the Ladder VAE

Reliability of machine learning systems

- Data: Quality, quantity, diversity, bias, privacy, ethics.
- Task: Context, domain, language, culture, purpose.

1. So what are the challenges holding us back in implementing such systems?
2. – Strong requirements of data.
   – Tasks that span different contexts, domains, languages, and cultures.
   – Regulatory requirements for transparency and accountability.
   – Trust and understanding of predictions.

Reliability of machine learning systems

- Data: Quality, quantity, diversity, bias, privacy, ethics.
- Task: Context, domain, language, culture, purpose.

- Interpretability of how a model works (transparency, accountability, regulation).
- Explainability of model predictions (trust, understanding, feedback).
- Fairness in treatment of different groups of people.
- Robustness to noise, outliers, distribution shift, and adversarial attacks.

1. So what are the challenges holding us back in implementing such systems?
2. – Strong requirements of data.
   – Tasks that span different contexts, domains, languages, and cultures.
   – Regulatory requirements for transparency and accountability.
   – Trust and understanding of predictions.

An alternative likelihood bound, $\mathcal{L}^{>k}$

An alternative version of the ELBO that only partially uses the approximate posterior can be written as [40]

$$\mathcal{L}^{>k}(\mathbf{x};\theta,\phi) = \mathbb{E}_{p_\theta(\mathbf{z}_{\leqslant k}|\mathbf{z}_{>k})q_\phi(\mathbf{z}_{>k}|\mathbf{x})}\left[\log \frac{p_\theta(\mathbf{x}|\mathbf{z})p_\theta(\mathbf{z}_{>k})}{q_\phi(\mathbf{z}_{>k}|\mathbf{x})}\right] \tag{8}$$

Here, we have replaced the approximate posterior $q_\phi(\mathbf{z}|\mathbf{x})$ with a different proposal distribution that combines part of the approximate posterior with the conditional prior, namely

$$p_\theta(\mathbf{z}_{\leqslant k}|\mathbf{z}_{>k})q_\phi(\mathbf{z}_{>k}|\mathbf{x})$$

This bound uses the conditional prior for the lowest latent variables in the hierarchy.

1. So can we come up with a new bound that does not use the lowest latent variables in the same way?
2. So we could use this for OOD detection (as done in BIVA).

Likelihood ratios

We can use our new bound to compute the score used in a standard likelihood ratio test [9].

$$\mathrm{LLR}^{>k}(\mathbf{x}) \equiv \mathcal{L}(\mathbf{x}) - \mathcal{L}^{>k}(\mathbf{x}) \,. \tag{9}$$

We can inspect what this likelihood-ratio measures by considering the exact form of our bounds.

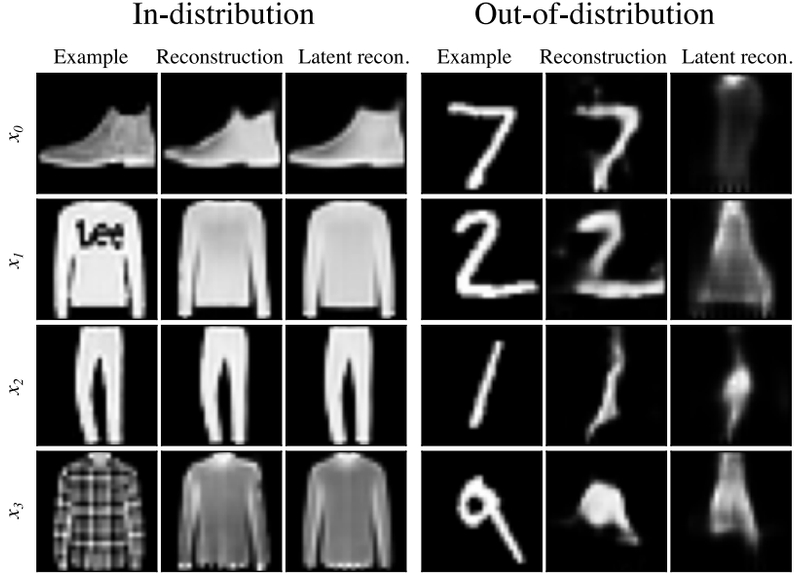
$$\begin{aligned} \mathcal{L} &= \log p_\theta(\mathbf{x}) - D_{KL}\left(q_\phi(\mathbf{z}|\mathbf{x}) \parallel p_\theta(\mathbf{z}|\mathbf{x})\right), \\ \mathcal{L}^{>k} &= \log p_\theta(\mathbf{x}) - D_{KL}\left(p_\theta(\mathbf{z}_{\leqslant}|\mathbf{z}_{>k}) q_\phi(\mathbf{z}_{>k}|\mathbf{x}) \parallel p_\theta(\mathbf{z}|\mathbf{x})\right) . \end{aligned} \tag{10}$$

In the likelihood ratio the reconstruction terms cancel out and only the KL-divergences from the approximate to the true posterior remain.

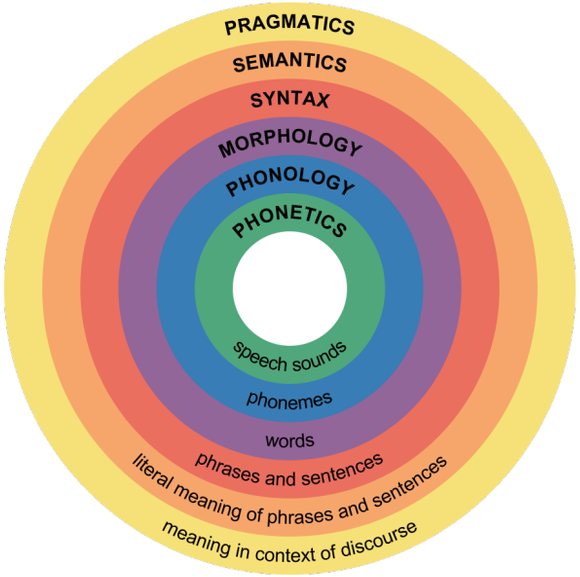
$$\begin{aligned} \mathrm{LLR}^{>k}(\mathbf{x}) = &-D_{KL}\left(q_\phi(\mathbf{z}|\mathbf{x}) \parallel p_\theta(\mathbf{z}|\mathbf{x})\right) \\ &+ D_{KL}\left(p_\theta(\mathbf{z}_{\leqslant}|\mathbf{z}_{>k}) q_\phi(\mathbf{z}_{>k}|\mathbf{x}) \parallel p_\theta(\mathbf{z}|\mathbf{x})\right) . \end{aligned} \tag{11}$$

1. Write likelihood-ratio using the exact form of the bounds including intractable KL-divergence.

Reconstructions of ID and OOD data



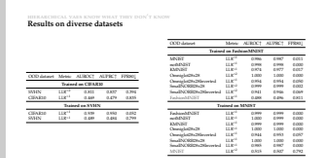
Hierarchy of speech features



Results on diverse datasets

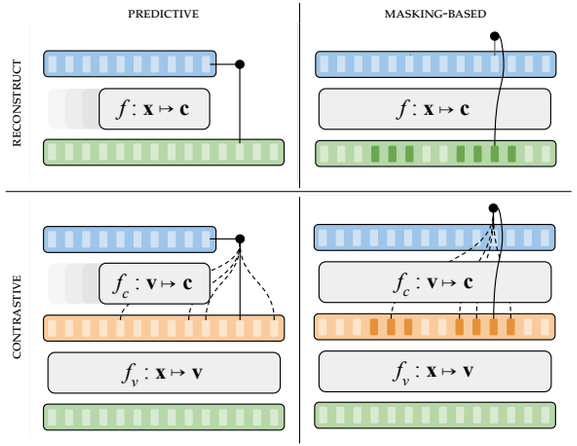
OOD dataset	Metric	AUROC↑	AUPRC↑	FPR80↓
Trained on CIFAR10				
SVHN	$LLR^{>2}$	0.811	0.837	0.394
CIFAR10	$LLR^{>1}$	0.469	0.479	0.835
Trained on SVHN				
CIFAR10	$LLR^{>1}$	0.939	0.950	0.052
SVHN	$LLR^{>1}$	0.489	0.484	0.799

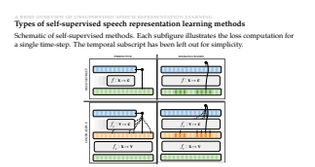
OOD dataset	Metric	AUROC↑	AUPRC↑	FPR80↓
Trained on FashionMNIST				
MNIST	$LLR^{>1}$	0.986	0.987	0.011
notMNIST	$LLR^{>1}$	0.998	0.998	0.000
KMNIST	$LLR^{>1}$	0.974	0.977	0.017
Omniglot28x28	$LLR^{>2}$	1.000	1.000	0.000
Omniglot28x28Inverted	$LLR^{>1}$	0.954	0.954	0.050
SmallNORB28x28	$LLR^{>2}$	0.999	0.999	0.002
SmallNORB28x28Inverted	$LLR^{>2}$	0.941	0.946	0.069
FashionMNIST	$LLR^{>1}$	0.488	0.496	0.811
Trained on MNIST				
FashionMNIST	$LLR^{>1}$	0.999	0.999	0.000
notMNIST	$LLR^{>1}$	1.000	0.999	0.000
KMNIST	$LLR^{>1}$	0.999	0.999	0.000
Omniglot28x28	$LLR^{>1}$	1.000	1.000	0.000
Omniglot28x28Inverted	$LLR^{>1}$	0.944	0.953	0.057
SmallNORB28x28	$LLR^{>1}$	1.000	1.000	0.000
SmallNORB28x28Inverted	$LLR^{>1}$	0.985	0.987	0.000
MNIST	$LLR^{>2}$	0.515	0.507	0.792



Types of self-supervised speech representation learning methods

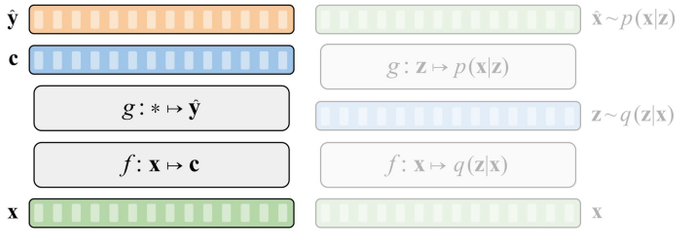
Schematic of self-supervised methods. Each subfigure illustrates the loss computation for a single time-step. The temporal subscript has been left out for simplicity.





Overview: Representation Learning for Speech

- We focus on two primary categories:
  - Self-supervised learning (SSL)
  - Probabilistic latent variable models (LVMs)
- Recent developments have been driven by self-supervised learning.
- A model-by-model overview: Focus on speech recognition.



Overview: Representation Learning for Speech

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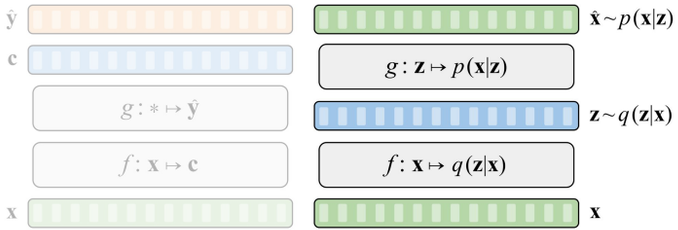
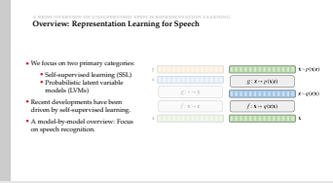
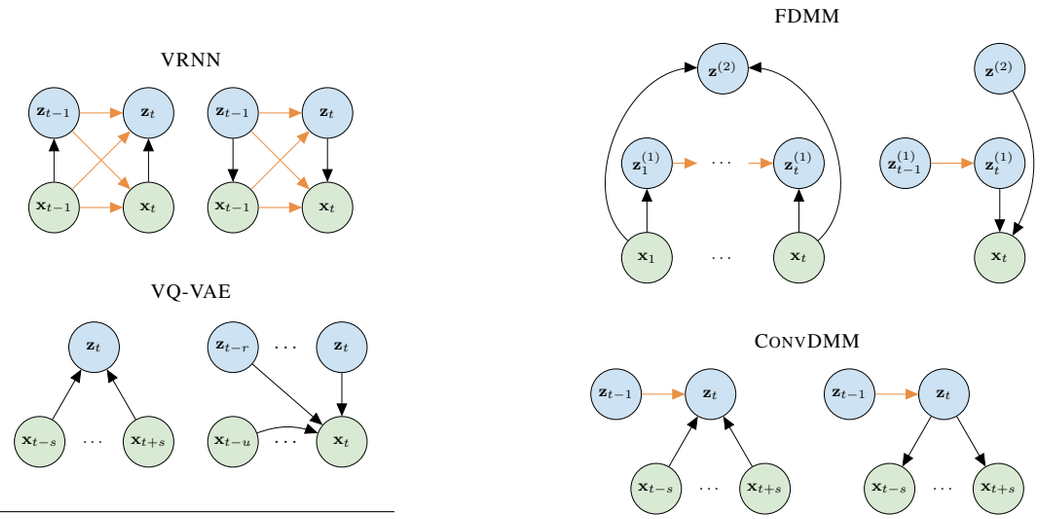
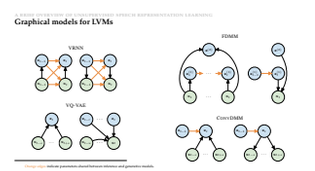




Graphical models for LVMs

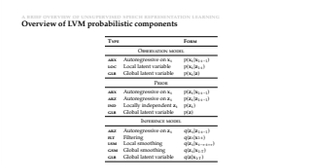


Orange edges indicate parameters shared between inference and generative models.



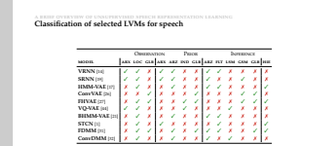
Overview of LVM probabilistic components

Type		Form
	Observation model	
ARX	Autoregressive on $\mathbf{x}_t$	$p(\mathbf{x}_t \vert \mathbf{x}_{1:t-1})$
LOC	Local latent variable	$p(\mathbf{x}_t \vert \mathbf{z}_{1:t})$
GLB	Global latent variable	$p(\mathbf{x}_t \vert \mathbf{z})$
	Prior	
ARX	Autoregressive on $\mathbf{x}_t$	$p(\mathbf{z}_t \vert \mathbf{x}_{1:t-1})$
ARZ	Autoregressive on $\mathbf{z}_t$	$p(\mathbf{z}_t \vert \mathbf{z}_{1:t-1})$
IND	Locally independent $\mathbf{z}_t$	$p(\mathbf{z}_t)$
GLB	Global latent variable	$p(\mathbf{z})$
	Inference model	
ARZ	Autoregressive on $\mathbf{z}_t$	$q(\mathbf{z}_t \vert \mathbf{z}_{1:t-1})$
FLT	Filtering	$q(\mathbf{z}_t \vert \mathbf{x}_{1:t})$
LSM	Local smoothing	$q(\mathbf{z}_t \vert \mathbf{x}_{t-r:t+r})$
GSM	Global smoothing	$q(\mathbf{z}_t \vert \mathbf{x}_{1:T})$
GLB	Global latent variable	$q(\mathbf{z} \vert \mathbf{x}_{1:T})$



Classification of selected LVMs for speech

	Observation			Prior				Inference					
Model	**ARX**	**LOC**	**GLB**	**ARX**	**ARZ**	**IND**	**GLB**	**ARZ**	**FLT**	**LSM**	**GSM**	**GLB**	**HIE**
VRNN [14]	✓	✓	✗	✓	✓	✗	✗	✓	✓	✗	✗	✗	✗
SRNN [19]	✓	✓	✗	✓	✓	✗	✗	✓	✗	✗	✓	✗	✗
HMM-VAE [17]	✗	✓	✗	✗	✓	✗	✗	✓	✓	✗	✗	✗	✓
ConvVAE [26]	✗	✗	✓	✗	✗	✗	✓	✗	✗	✗	✓	✓	✗
FHVAE [27]	✗	✓	✓	✗	✗	✓	✓	✗	✗	✗	✓	✓	✓
VQ-VAE [44]	✓	✓	✗	✗	✗	✓	✗	✗	✗	✓	✗	✗	✗
BHMM-VAE [21]	✗	✓	✗	✗	✓	✗	✗	✓	✓	✗	✗	✗	✗
STCN [1]	✗	✓	✗	✓	✗	✗	✗	✗	✓	✗	✗	✗	✓
FDMM [31]	✗	✓	✓	✗	✓	✗	✓	✓	✓	✗	✗	✓	✓
ConvDMM [32]	✗	✓	✗	✗	✓	✗	✗	✓	✗	✓	✗	✗	✗



Comparison of LVMs and SSL methods

		MODEL AND TASK DESIGN						RESOLUTION			USAGE	
	MODEL	MSK	PRD	CON	REC	QTZ	GEN	LOC	GLB	VAR	FRZ	FTN
SELF-SUPERVISED MODELS	**CPC** [43]	✗	✓	✓	✗	✗	✗	✓	✗	✗	✓	✗
	APC [13]	✗	✓	✗	✓	✗	✗	✓	✗	✗	✓	✗
	wav2vec [50]	✗	✓	✓	✗	✗	✗	✓	✗	✗	✓	✗
	Mockingjay [39]	✓	✗	✗	✓	✗	✗	✓	✗	✗	✓	✓
	wav2vec 2.0 [3]	✓	✗	✓	✗	✓	✗	✓	✗	✗	✗	✓
	NPC [38]	✓	✗	✗	✓	✓	✗	✓	✗	✗	✓	✗
	DeCoAR 2.0 [37]	✓	✗	✗	✓	✓	✗	✓	✗	✗	✓	✗
	HuBERT [25]	✓	✗	✗	✗	✓	✗	✓	✗	✗	✗	✓
	data2vec [2]	✓	✗	✗	✗	✗	✗	✓	✗	✗	✗	✓
LATENT VARIABLE MODELS	**VRNN** [14]	✗	✗	✗	✓	✗	✓	✓	✗	✗	✓	✗
	SRNN [19]	✗	✗	✗	✓	✗	✓	✓	✗	✗	✓	✗
	ConvVAE [26]	✗	✗	✗	✓	✗	✓	✗	✓	✗	✓	✗
	FHVAE [27]	✗	✗	✗	✓	✗	✓	✓	✓	✗	✓	✗
	VQ-VAE [44]	✗	✗	✗	✓	✓	✓	✓	✗	✗	✓	✗
	STCN [1]	✗	✗	✗	✓	✗	✓	✓	✗	✗	✓	✗
	FDMM [31]	✗	✗	✗	✓	✗	✓	✓	✓	✗	✓	✗
	ConvDMM [32]	✗	✗	✗	✓	✗	✓	✓	✗	✗	✓	✗

Simulated prospective study

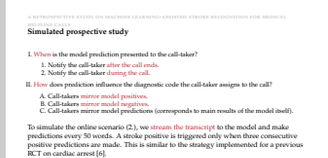
I. When is the model prediction presented to the call-taker?

1. Notify the call-taker after the call ends.
2. Notify the call-taker during the call.

II. How does prediction influence the diagnostic code the call-taker assigns to the call?

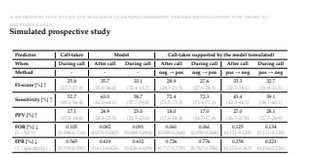
A. Call-takers mirror model positives.
B. Call-takers mirror model negatives.
C. Call-takers mirror model predictions (corresponds to main results of the model itself).

To simulate the online scenario (2.), we stream the transcript to the model and make predictions every 50 words. A stroke positive is triggered only when three consecutive positive predictions are made. This is similar to the strategy implemented for a previous RCT on cardiac arrest [6].



Simulated prospective study

Predictor	Call-taker	Model		Call-taker supported by the model (simulated)			
When	During call	After call	During call	After call	During call	After call	During call
Method	-	-	-	neg → pos	neg → pos	pos → neg	pos → neg
F1-score [%] ↑	25.8 (23.7-27.9)	35.7 (35.0-36.4)	33.1 (32.4-33.7)	28.9 (28.3-29.5)	27.6 (27.0-28.1)	33.3 (32.5-34.1)	32.7 (31.8-33.5)
Sensitivity [%] ↑	52.7 (49.2-56.4)	63.0 (62.0-64.1)	58.7 (57.7-59.8)	72.4 (71.5-73.3)	72.3 (71.4-73.3)	43.4 (42.3-44.5)	39.1 (38.1-40.1)
PPV [%] ↑	17.1 (15.5-18.6)	24.9 (24.3-25.5)	23.0 (22.5-23.6)	18.0 (17.6-18.4)	17.0 (16.7-17.4)	27.0 (26.3-27.8)	28.1 (27.3-28.9)
FOR [%] ↓ (1 - NPV)	0.105 (0.094-0.116)	0.082 (0.079-0.085)	0.091 (0.088-0.094)	0.061 (0.059-0.064)	0.061 (0.059-0.064)	0.125 (0.121-0.129)	0.134 (0.131-0.138)
FPR [%] ↓ (1 - specificity)	0.565 (0.539-0.590)	0.419 (0.413-0.426)	0.432 (0.426-0.439)	0.726 (0.717-0.735)	0.776 (0.767-0.786)	0.258 (0.253-0.263)	0.221 (0.216-0.226)

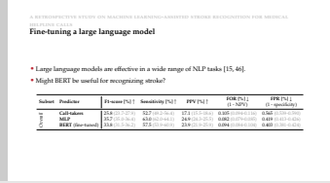


corti DTU

Fine-tuning a large language model

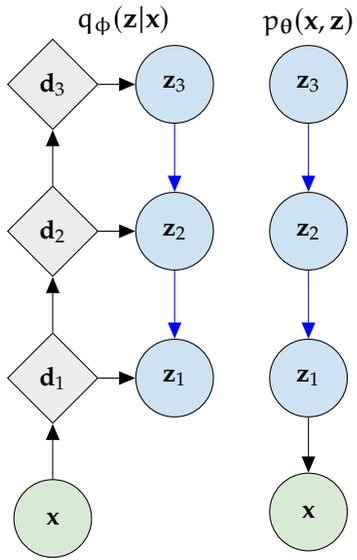
- Large language models are effective in a wide range of NLP tasks [15, 46].
- Might BERT be useful for recognizing stroke?

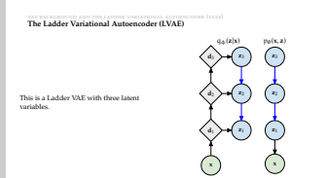
Subset	Predictor	F1-score [%] ↑	Sensitivity [%] ↑	PPV [%] ↑	FOR [%] ↓ (1 - NPV)	FPR [%] ↓ (1 - specificity)
Overall	**Call-takers**	25.8 (23.7-27.9)	52.7 (49.2-56.4)	17.1 (15.5-18.6)	0.105 (0.094-0.116)	0.565 (0.539-0.590)
	MLP	35.7 (35.0-36.4)	63.0 (62.0-64.1)	24.9 (24.3-25.5)	0.082 (0.079-0.085)	0.419 (0.413-0.426)
	BERT (fine-tuned)	33.8 (31.5-36.2)	57.5 (53.9-60.9)	23.9 (21.9-25.9)	0.094 (0.084-0.104)	0.403 (0.381-0.424)



The Ladder Variational Autoencoder (LVAE)

This is a Ladder VAE with three latent variables.





Overview

Understanding the Ladder VAE is not so much about understanding the specific architecture as it is about:

a) understanding the reason for choosing it,

b) which other options were available,

c) and why they don't work as well.

VAE BACKGROUND AND THE LADDER VARIATIONAL AUTOENCODER (LVAE)
Overview
Understanding the Ladder VAE is not so much about understanding the specific architecture as it is about:
a) understanding the reason for choosing it,
b) which other options were available,
c) and why they don't work as well.

A generative model from latent variables

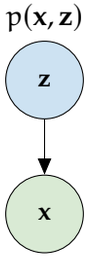
Suppose data $\mathbf{x} \sim p(\mathbf{x})$ is generated via some underlying *latent* variable $\mathbf{z}$. Then

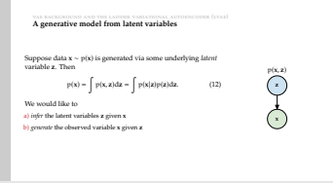
$$p(\mathbf{x}) = \int p(\mathbf{x}, \mathbf{z}) d\mathbf{z} = \int p(\mathbf{x}|\mathbf{z}) p(\mathbf{z}) d\mathbf{z}. \quad (12)$$

We would like to

a) *infer* the latent variables $\mathbf{z}$ given $\mathbf{x}$

b) *generate* the observed variable $\mathbf{x}$ given $\mathbf{z}$





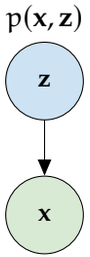
Exact inference

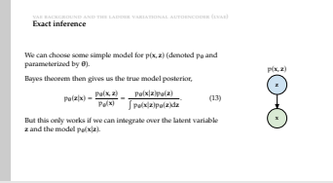
We can choose some simple model for $p(\mathbf{x}, \mathbf{z})$ (denoted p_θ and parameterized by $\boldsymbol{\theta}$).

Bayes theorem then gives us the true model posterior,

$$p_\theta(\mathbf{z}|\mathbf{x}) = \frac{p_\theta(\mathbf{x}, \mathbf{z})}{p_\theta(\mathbf{x})} = \frac{p_\theta(\mathbf{x}|\mathbf{z})p_\theta(\mathbf{z})}{\int p_\theta(\mathbf{x}|\mathbf{z})p_\theta(\mathbf{z})d\mathbf{z}}. \tag{13}$$

But this only works if we can integrate over the latent variable $\mathbf{z}$ and the model $p_\theta(\mathbf{x}|\mathbf{z})$.





Exact inference becomes intractable

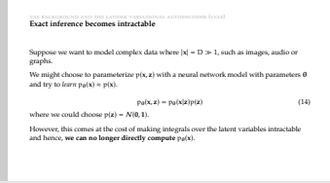
Suppose we want to model complex data where $|\mathbf{x}| = D \gg 1$, such as images, audio or graphs.

We might choose to parameterize $p(\mathbf{x}, \mathbf{z})$ with a neural network model with parameters $\boldsymbol{\theta}$ and try to *learn* $p_{\boldsymbol{\theta}}(\mathbf{x}) \approx p(\mathbf{x})$.

$$p_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{z}) = p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})p(\mathbf{z}) \tag{14}$$

where we could choose $p(\mathbf{z}) = \mathcal{N}(\mathbf{0}, \mathbf{1})$.

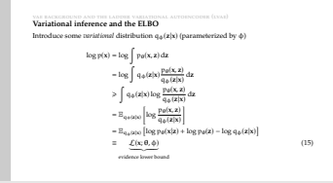
However, this comes at the cost of making integrals over the latent variables intractable and hence, **we can no longer directly compute** $p_{\boldsymbol{\theta}}(\mathbf{x})$.



Variational inference and the ELBO

Introduce some *variational* distribution $q_\phi(\mathbf{z}|\mathbf{x})$ (parameterized by ϕ)

$$
\begin{aligned}
\log p(\mathbf{x}) &= \log \int p_\theta(\mathbf{x}, \mathbf{z})\, d\mathbf{z} \\
&= \log \int q_\phi(\mathbf{z}|\mathbf{x}) \frac{p_\theta(\mathbf{x}, \mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})}\, d\mathbf{z} \\
&\geqslant \int q_\phi(\mathbf{z}|\mathbf{x}) \log \frac{p_\theta(\mathbf{x}, \mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})}\, d\mathbf{z} \\
&= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} \left[\log \frac{p_\theta(\mathbf{x}, \mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})} \right] \\
&= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} \left[\log p_\theta(\mathbf{x}|\mathbf{z}) + \log p_\theta(\mathbf{z}) - \log q_\phi(\mathbf{z}|\mathbf{x}) \right] \\
&\equiv \underbrace{\mathcal{L}(\mathbf{x}; \boldsymbol{\theta}, \phi)}_{\text{evidence lower bound}} \qquad (15)
\end{aligned}
$$



The variational autoencoder (VAE)

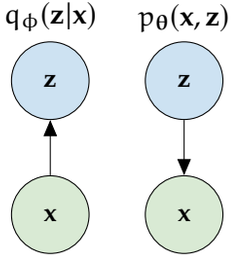
Suppose we parameterize $q_\phi(\mathbf{z}|\mathbf{x})$ by a model with parameters ϕ. Then we can optimize both $\{\boldsymbol{\theta}, \phi\}$ jointly by maximizing the ELBO.

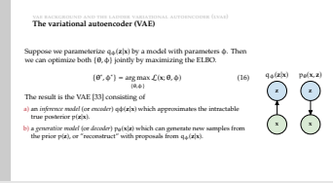
$$\{\boldsymbol{\theta}^*, \phi^*\} = \arg\max_{\{\boldsymbol{\theta}, \phi\}} \mathcal{L}(\mathbf{x}; \boldsymbol{\theta}, \phi) \tag{16}$$

The result is the VAE [33] consisting of

a) an *inference model* (or *encoder*) $q\phi(\mathbf{z}|\mathbf{x})$ which approximates the intractable true posterior $p(\mathbf{z}|\mathbf{x})$.

b) a *generative model* (or *decoder*) $p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})$ which can generate new samples from the prior $p(\mathbf{z})$, or "reconstruct" with proposals from $q_\phi(\mathbf{z}|\mathbf{x})$.

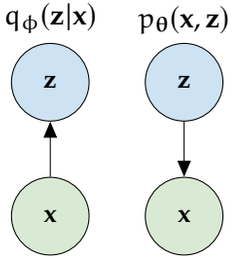




Limitations of VAEs

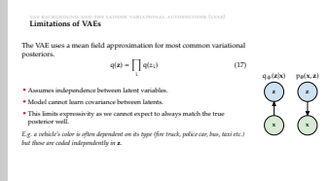
The VAE uses a mean field approximation for most common variational posteriors.

$$q(\mathbf{z}) = \prod_i q(z_i) \tag{17}$$



- Assumes independence between latent variables.
- Model cannot learn covariance between latents.
- This limits expressivity as we cannot expect to always match the true posterior well.

E.g. a vehicle's color is often dependent on its type (fire truck, police car, bus, taxi etc.) but these are coded independently in $\mathbf{z}$.



Hierarchical VAE

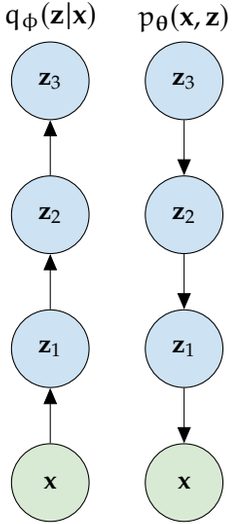
To avoid these limitations, we can introduce a hierarchy of additional latent variables $\mathbf{z} = \mathbf{z}_1, \ldots, \mathbf{z}_L$. For $L = 3$,

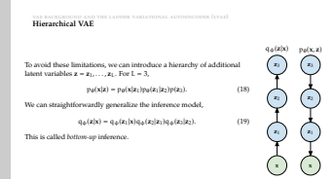
$$p_\theta(\mathbf{x}|\mathbf{z}) = p_\theta(\mathbf{x}|\mathbf{z}_1)p_\theta(\mathbf{z}_1|\mathbf{z}_2)p(\mathbf{z}_3). \tag{18}$$

We can straightforwardly generalize the inference model,

$$q_\phi(\mathbf{z}|\mathbf{x}) = q_\phi(\mathbf{z}_1|\mathbf{x})q_\phi(\mathbf{z}_2|\mathbf{z}_1)q_\phi(\mathbf{z}_3|\mathbf{z}_2). \tag{19}$$

This is called *bottom-up* inference.



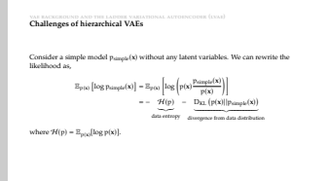


Challenges of hierarchical VAEs

Consider a simple model $p_{\text{simple}}(\mathbf{x})$ without any latent variables. We can rewrite the likelihood as,

$$\begin{aligned}\mathbb{E}_{p(\mathbf{x})}\left[\log p_{\text{simple}}(\mathbf{x})\right] &= \mathbb{E}_{p(\mathbf{x})}\left[\log\left(p(\mathbf{x})\frac{p_{\text{simple}}(\mathbf{x})}{p(\mathbf{x})}\right)\right] \\ &= -\underbrace{\mathcal{H}(p)}_{\text{data entropy}} - \underbrace{D_{KL}\left(p(\mathbf{x})||p_{\text{simple}}(\mathbf{x})\right)}_{\text{divergence from data distribution}}\end{aligned}$$

where $\mathcal{H}(p) = \mathbb{E}_{p(\mathbf{x})}[\log p(\mathbf{x})]$.



Challenges of hierarchical VAEs

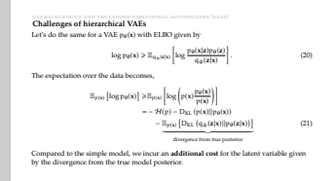
Let's do the same for a VAE $p_\theta(\mathbf{x})$ with ELBO given by

$$\log p_\theta(\mathbf{x}) \geqslant \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}\left[\log \frac{p_\theta(\mathbf{x}|\mathbf{z})p_\theta(\mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})}\right]. \tag{20}$$

The expectation over the data becomes,

$$\begin{aligned}\mathbb{E}_{p(\mathbf{x})}\left[\log p_\theta(\mathbf{x})\right] \geqslant & \mathbb{E}_{p(\mathbf{x})}\left[\log\left(p(\mathbf{x})\frac{p_\theta(\mathbf{x})}{p(\mathbf{x})}\right)\right] \\ = & -\mathcal{H}(p) - D_{KL}\left(p(\mathbf{x})||p_\theta(\mathbf{x})\right) \\ & \underbrace{-\mathbb{E}_{p(\mathbf{x})}\left[D_{KL}\left(q_\phi(\mathbf{z}|\mathbf{x})||p_\theta(\mathbf{z}|\mathbf{x})\right)\right]}_{\text{divergence from true posterior}}\end{aligned} \tag{21}$$

Compared to the simple model, we incur an **additional cost** for the latent variable given by the divergence from the true model posterior.



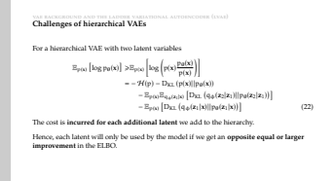
Challenges of hierarchical VAEs

For a hierarchical VAE with two latent variables

$$\begin{aligned}\mathbb{E}_{p(\mathbf{x})}\left[\log p_\theta(\mathbf{x})\right] \geqslant & \mathbb{E}_{p(\mathbf{x})}\left[\log\left(p(\mathbf{x})\frac{p_\theta(\mathbf{x})}{p(\mathbf{x})}\right)\right] \\ = & -\mathcal{H}(p) - D_{KL}\left(p(\mathbf{x})||p_\theta(\mathbf{x})\right) \\ & - \mathbb{E}_{p(\mathbf{x})}\mathbb{E}_{q_\phi(\mathbf{z}_1|\mathbf{x})}\left[D_{KL}\left(q_\phi(\mathbf{z}_2|\mathbf{z}_1)||p_\theta(\mathbf{z}_2|\mathbf{z}_1)\right)\right] \\ & - \mathbb{E}_{p(\mathbf{x})}\left[D_{KL}\left(q_\phi(\mathbf{z}_1|\mathbf{x})||p_\theta(\mathbf{z}_1|\mathbf{x})\right)\right] \end{aligned} \tag{22}$$

The cost is **incurred for each additional latent** we add to the hierarchy.

Hence, each latent will only be used by the model if we get an **opposite equal or larger improvement** in the ELBO.

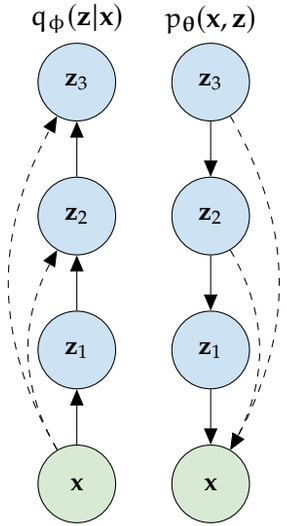


(Failing to) Dodge the challenges

There's a few common ways to try and dodge these issues:

- Skip connections [16, 40]
- Free bits in the KL-terms [34]
- Deterministic warmup [53]
- Batch normalization/weight normalization [28, 49]

None of them work for more than around 5 latent variables.

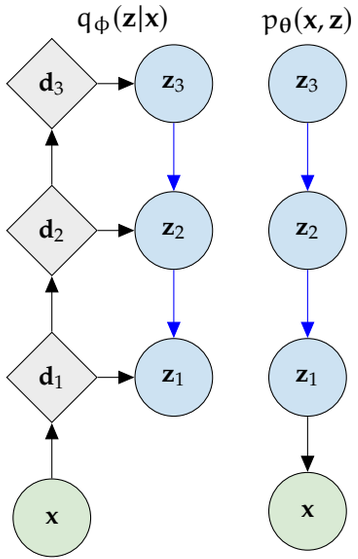


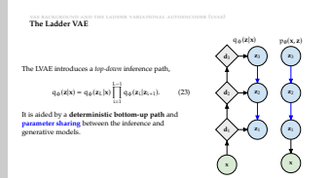
The Ladder VAE

The LVAE introduces a *top-down* inference path,

$$q_\phi(\mathbf{z}|\mathbf{x}) = q_\phi(\mathbf{z}_L|\mathbf{x}) \prod_{i=1}^{L-1} q_\phi(\mathbf{z}_i|\mathbf{z}_{i+1}). \qquad (23)$$

It is aided by a **deterministic bottom-up path** and **parameter sharing** between the inference and generative models.





Benchmarks

Model	$\geqslant \log p(\mathbf{x})$
VAE + NF (L = 1)	-85.10
IWAE (L = 2, K = 1)	-85.33
IWAE (L = 2, K = 50)	-82.90
VAE + VGP (L = 2)	-81.90
LVAE (L = 5)	-82.12
LVAE + finetuning (L = 5)	-81.84
LVAE + finetuning (L = 5, K = 10)	-81.74

Table 1: Results on dynamically binarized MNIST.

Latent space activation

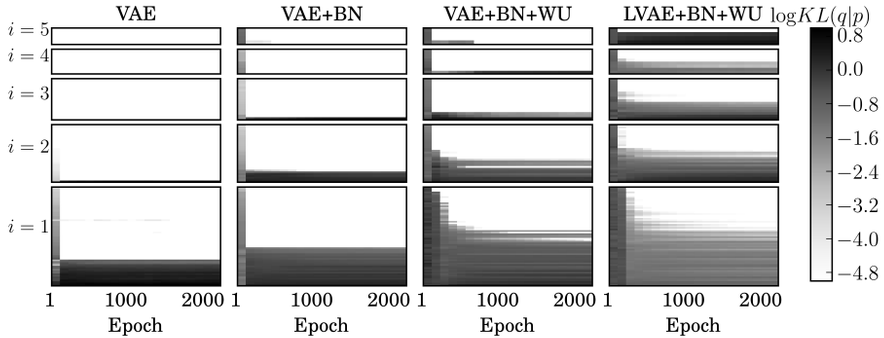
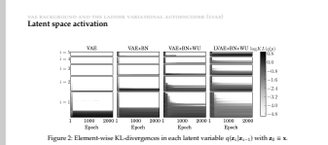


Figure 2: Element-wise KL-divergences in each latent variable $q(\mathbf{z}_i|\mathbf{z}_{i-1})$ with $\mathbf{z}_0 \equiv \mathbf{x}$.



Latent space representation

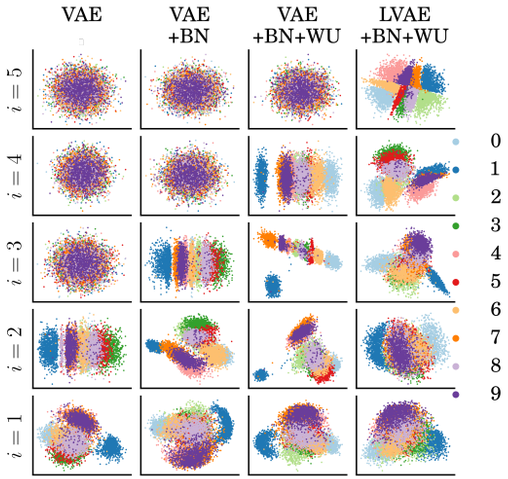
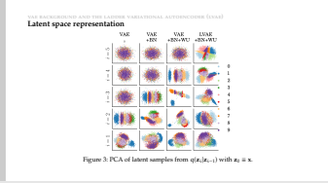


Figure 3: PCA of latent samples from $q(\mathbf{z}_i|\mathbf{z}_{i-1})$ with $\mathbf{z}_0 \equiv \mathbf{x}$.



Recent work

Figure 4: Samples from the generative model of [11] with more than 70 latents.

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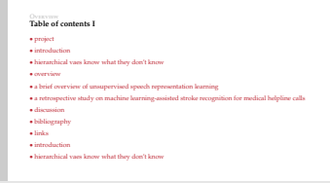

Table of contents II

- a brief overview of unsupervised speech representation learning
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- vae background and the ladder variational autoencoder (lvae)

Overview
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