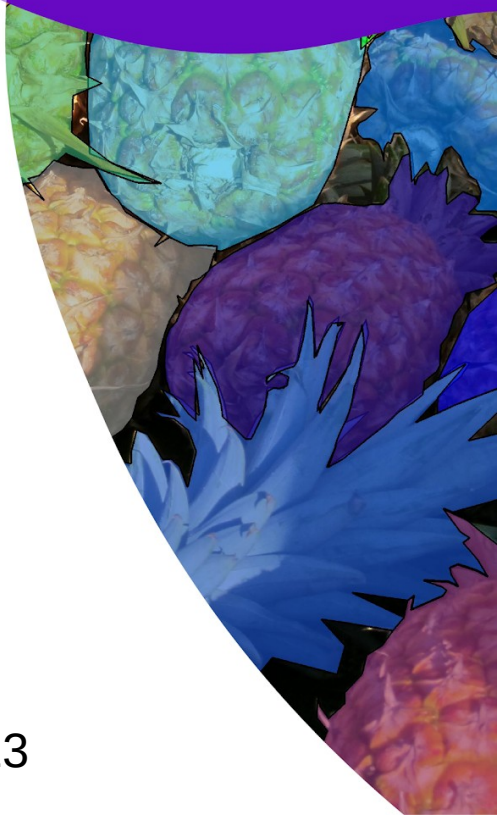
NEW YORK UNIVERSITY

The Energy-Based View of Self-Supervised Learning



Yann LeCun
NYU - Courant Institute & Center for Data Science
Facebook AI Research
http://yann.lecun.com

Nvidia GTC 2021-04-13

Three challenges for AI & Machine Learning

- **1. Learning with fewer labeled samples and/or fewer trials**
  - Supervised and reinforcement learning require too much samples/trails
  - Self-supervised learning / learning dependencies / to fill in the blanks
    - learning to represent the world in a non task-specific way

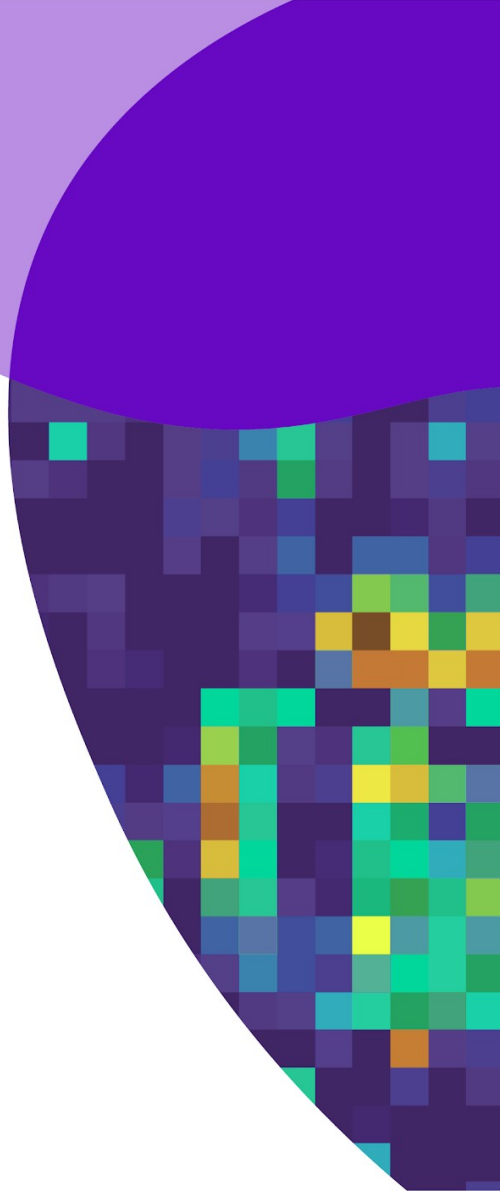
- **2. Learning to reason,** like Daniel Kahneman's "System 2"
  - Beyond feed-forward, System 1 subconscious computation.
  - Making reasoning compatible with learning.

- **3. Learning to plan complex action sequences**
  - Learning hierarchical representations of action plans

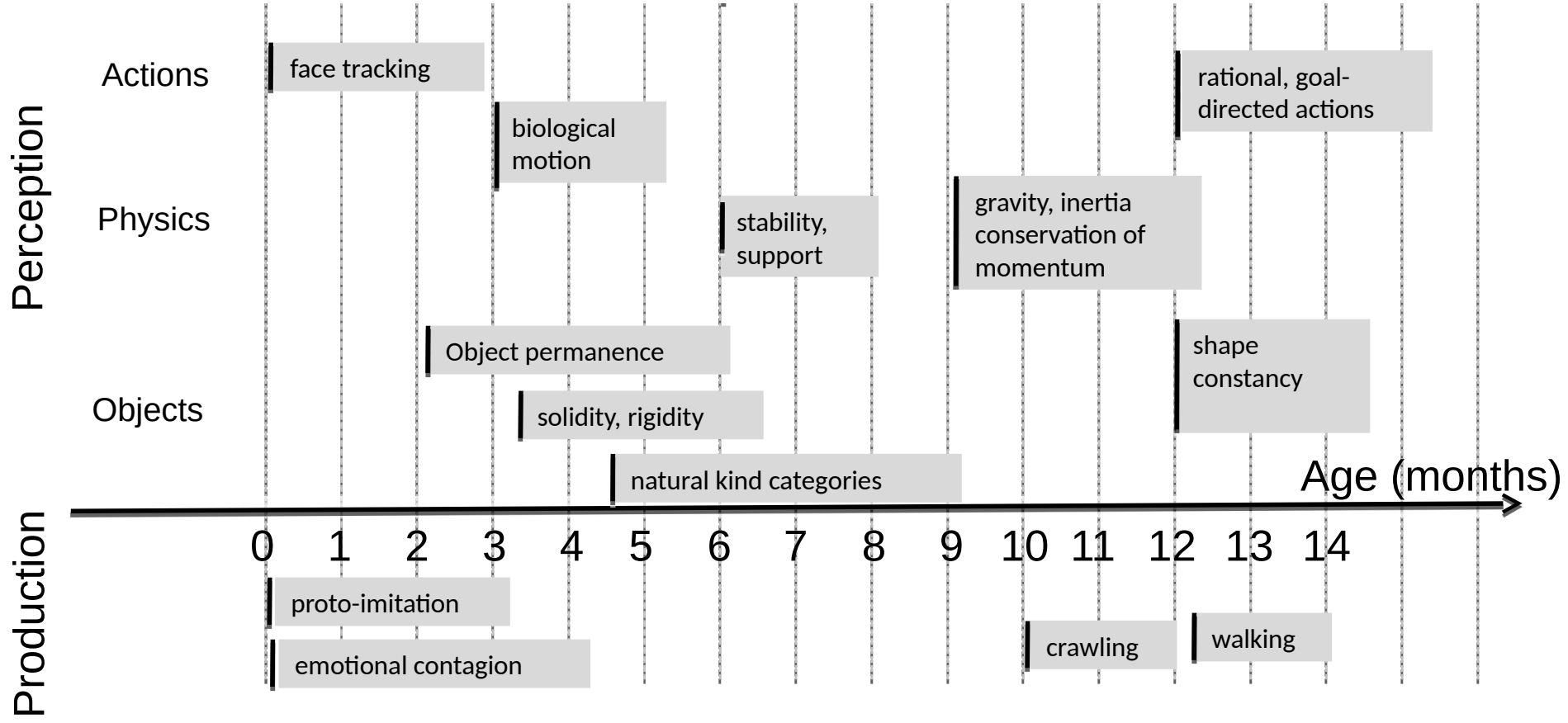
FACEBOOK AI

How do humans and animals learn so quickly?

Not supervised.
Not Reinforced.



When infants learn models of the world [after Emmanuel Dupoux]



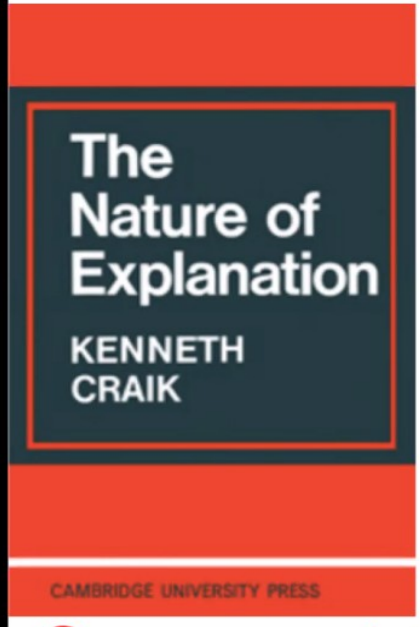
How do Human and Animal Babies Learn?

- **How do they learn how the world works?**
- **Largely by observation, with remarkably little interaction (initially).**
- **They accumulate enormous amounts of background knowledge**
  - About the structure of the world, like intuitive physics.
- **Perhaps common sense emerges from this knowledge?**

Photos courtesy of Emmanuel Dupoux

Common sense is a collection of models of the world

AI systems need to build "mental models"



If the organism carries a `small-scale model' of external reality and of its own possible actions within its head, it is able to try out various alternatives, conclude which is the best of them, react to future situations before they arise, utilize the knowledge of past events in dealing with the present and the future, and in every way to react in a much fuller, safer, and more competent manner to the emergencies which face it (Craik, 1943,Ch. 5, p.61)

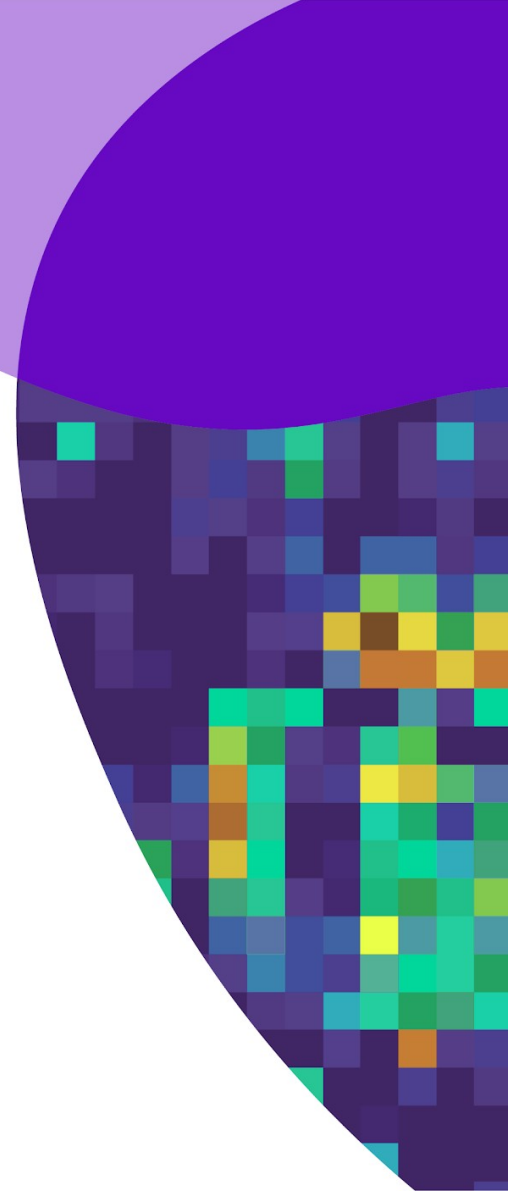
Commonsense is not just facts, it is a collection of models

Jitendra Malik

FACEBOOK AI

Self-Supervised Learning

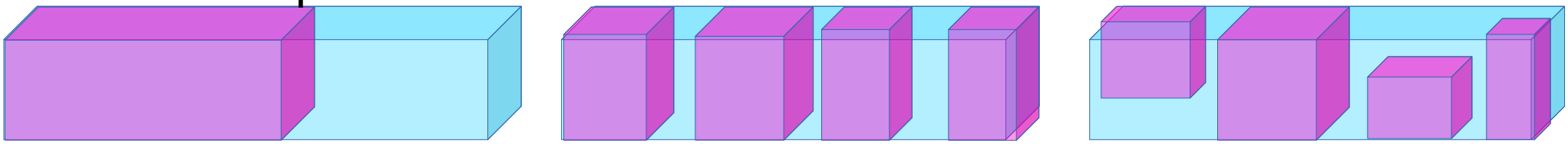
Capture dependencies.
Predict everything from everything else.



Self-Supervised Learning = Learning to Fill in the Blanks

- **Reconstruct the input or Predict missing parts of the input.**

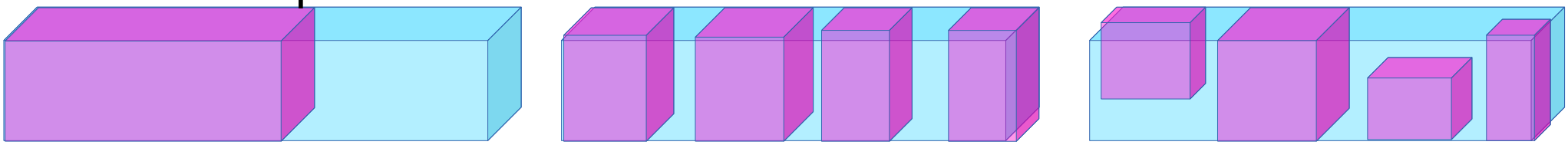
time or space →



Self-Supervised Learning = Learning to Fill in the Blanks

- **Reconstruct the input or Predict missing parts of the input.**

time or space →



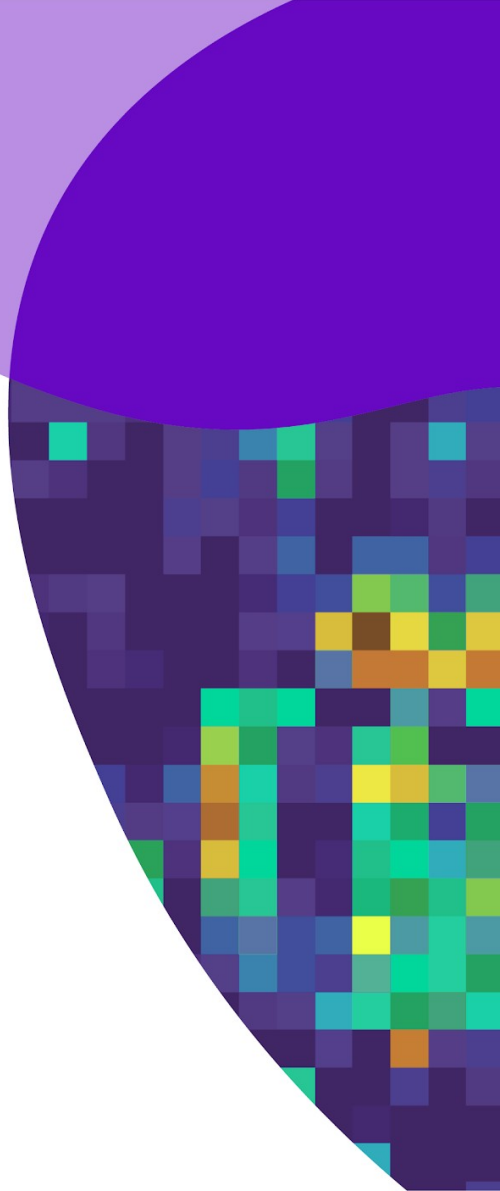
Two Uses for Self-Supervised Learning

- **1. Learning hierarchical representations of the world**
  - SSL pre-training precedes a supervised or RL phase
- **2. Learning predictive (forward) models of the world**
  - Learning models for Model-Predictive Control, policy learning for control, or model-based RL.
- **Question: how to represent uncertainty & multi-modality in the prediction?**

FACEBOOK AI

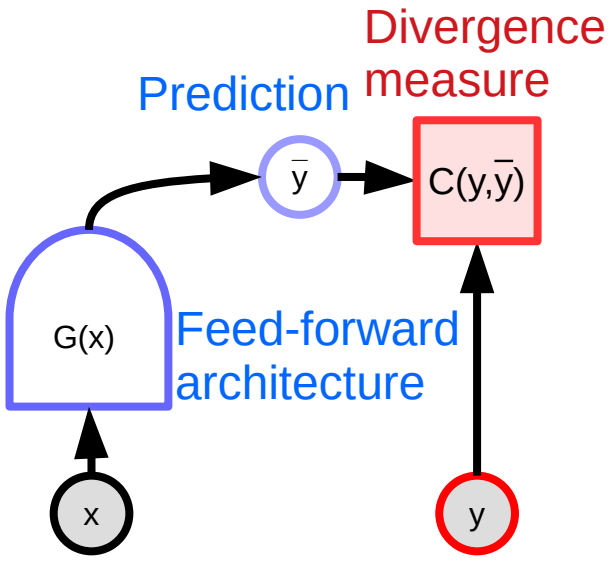
Energy-Based Models

Capture dependencies through an energy function.

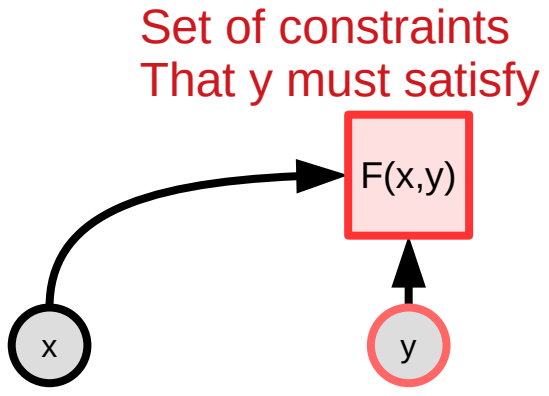


Energy-Based Models

- **Feed-forward nets use a finite number of steps to produce a single output.**
- **What if…**
  - The problem requires a complex computation to produce its output? (complex inference)
  - There are multiple possible outputs for a single input? (e.g. predicting future video frames)

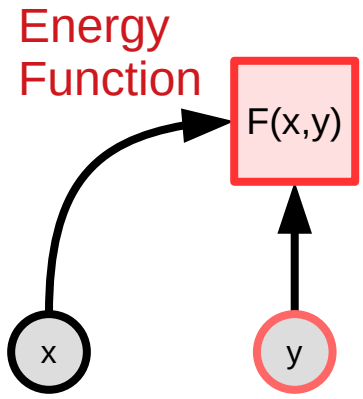


- **Inference through constraint satisfaction**
  - Finding an output that satisfies constraints: e.g a linguistically-correct translation or a transcription of speech into text.
  - Maximum likelihood inference in graphical models



Energy-Based Models (EBM)

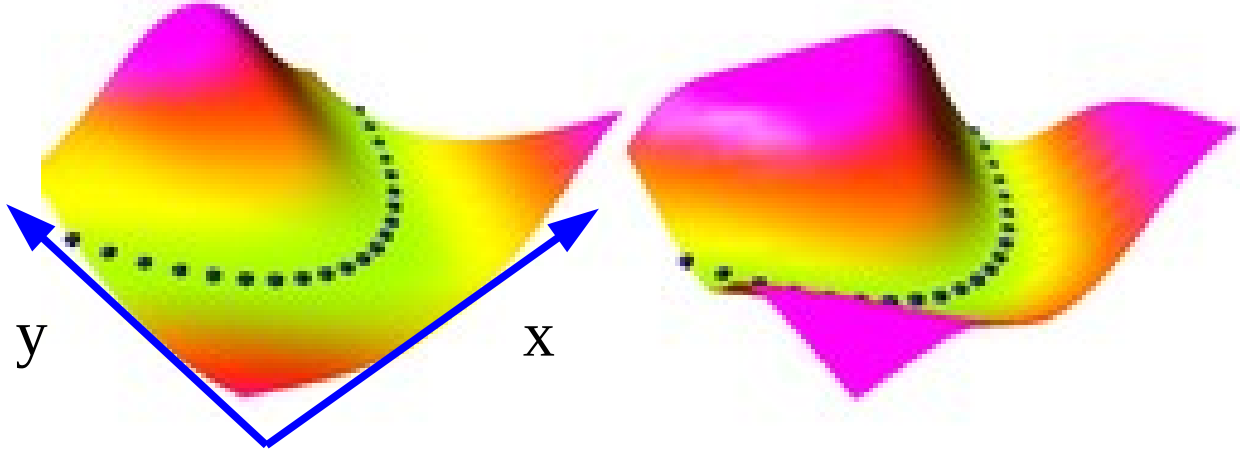
- **Energy function F(x,y) scalar-valued.**
  - Takes low values when y is compatible with x and higher values when y is less compatible with x
- **Inference: find values of y that make F(x,y) small.**
  - There may be multiple solutions



$$\check{y} = \text{argmin}_y F(x, y)$$

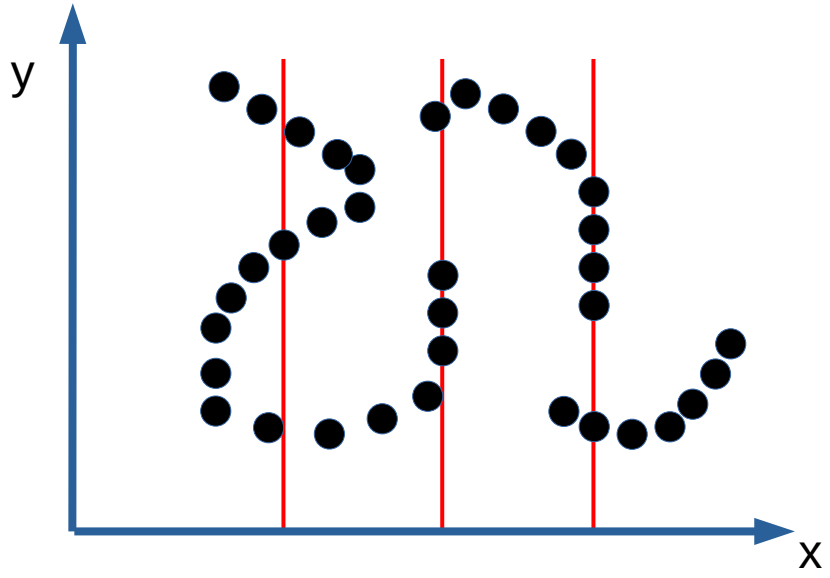
- **Note: the energy is used for inference, not for learning**

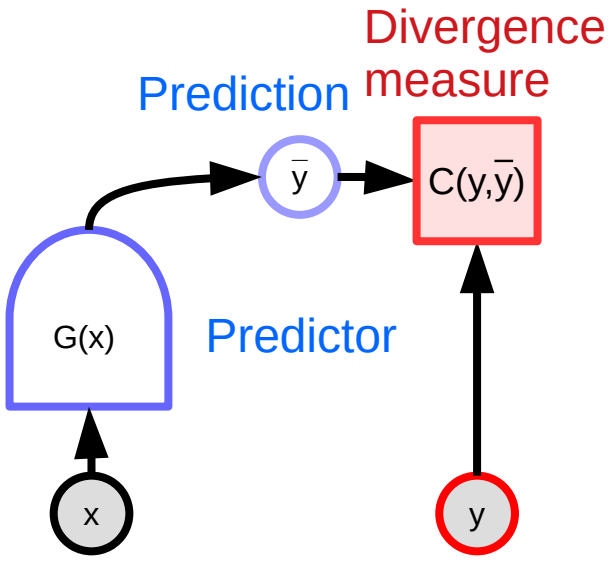
- **Example**
  - Blue dots are data points

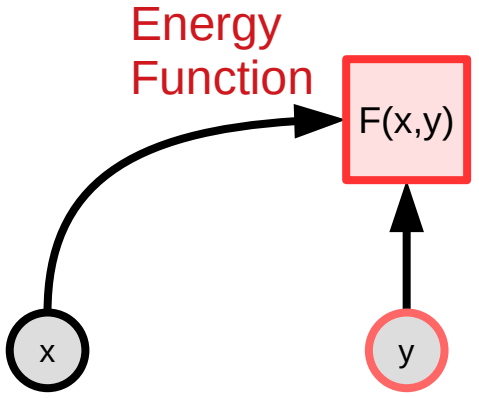


Energy-Based Model: implicit function

- **A feed-forward model is an explicit function that computes y from x.**
- **An EBM is an implicit function that captures the dependency between x and y**
- **Multiple y can be compatible with a single x**

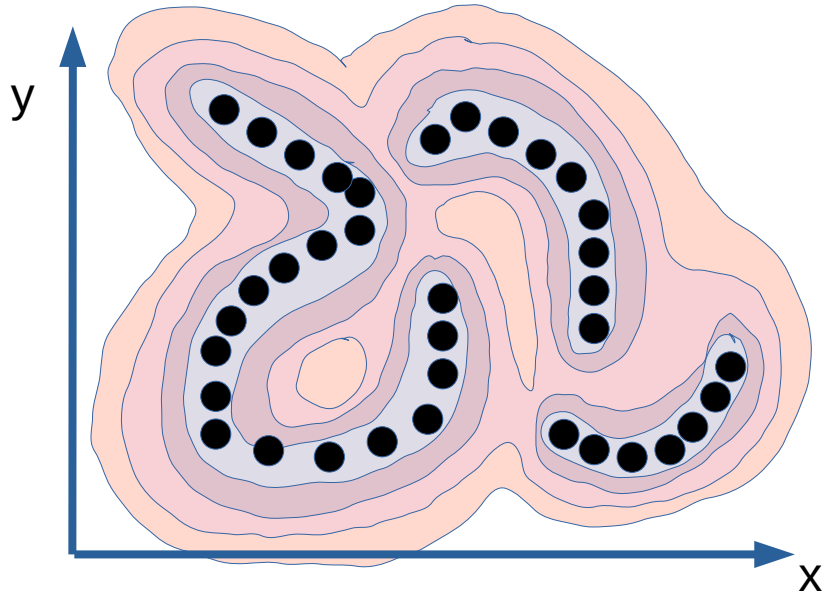




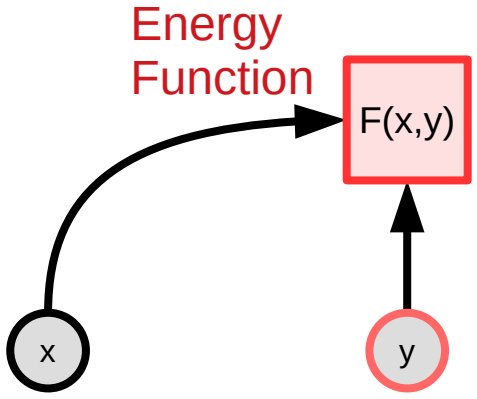


Energy-Based Model: implicit function

- **Energy function that captures the x,y dependencies:**
  - Low energy near the data points. Higher energy everywhere else.
  - If y is continuous, F should be smooth and differentiable, so we can use gradient-based inference algorithms.



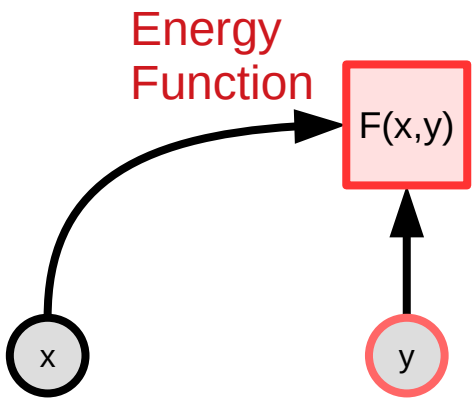
$$\check{y} = \text{argmin}_y F(x, y)$$

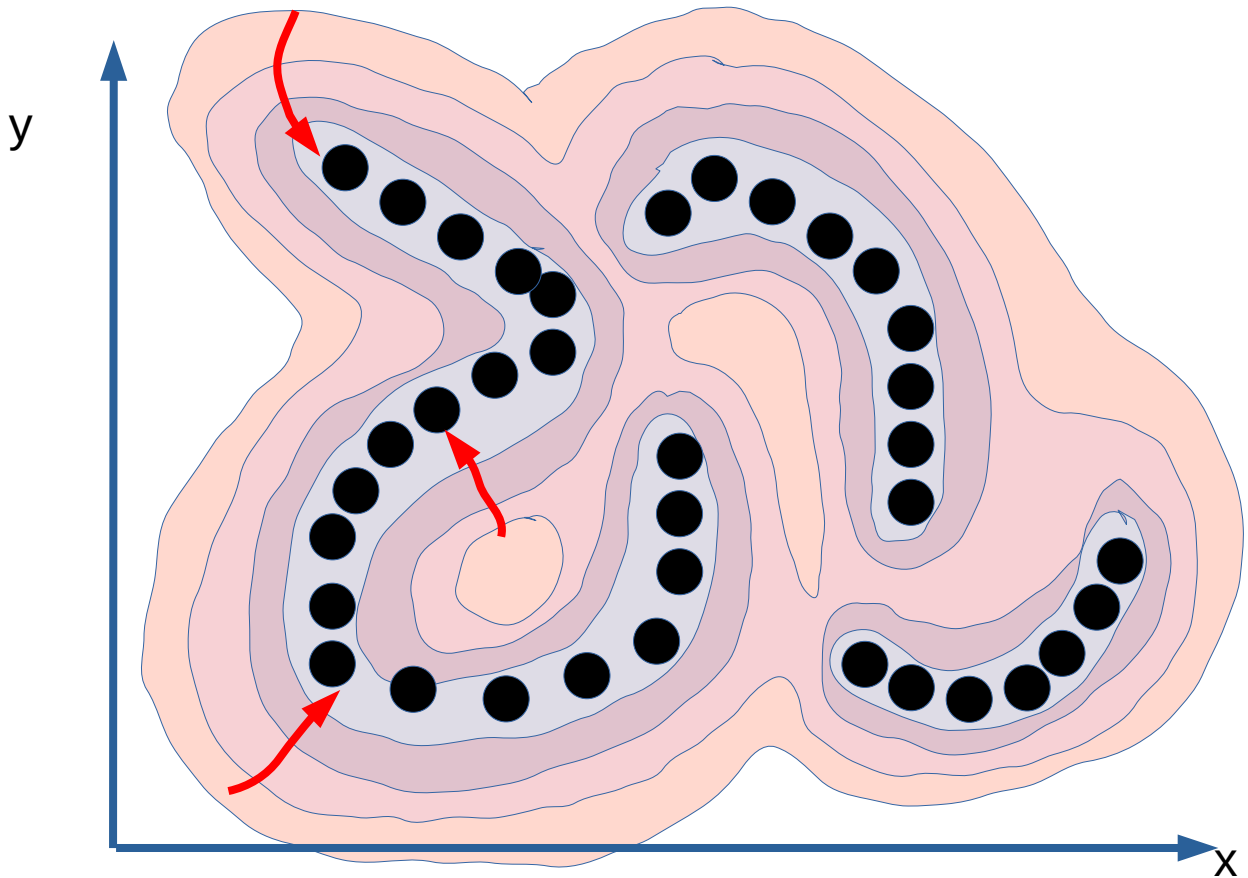


Energy-Based Model: gradient-based inference

- **If y is continuous**
  - We can use a gradient-based method for inference.

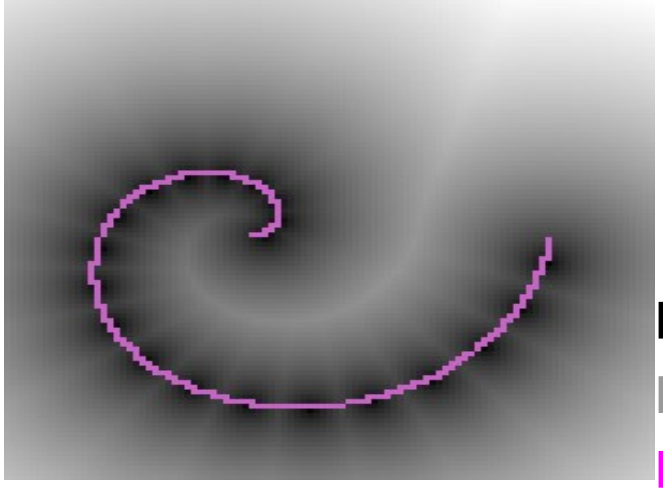
$$\check{y} = \text{argmin}_y F(x, y)$$





Conditional and Unconditional Energy-Based Models

- **Conditional EBM: F(x,y)**
- **Unconditional EBM: F(y)**
  - measures the compatibility between the components of y
  - If we don't know in advance which part of y is known and which part is unknown

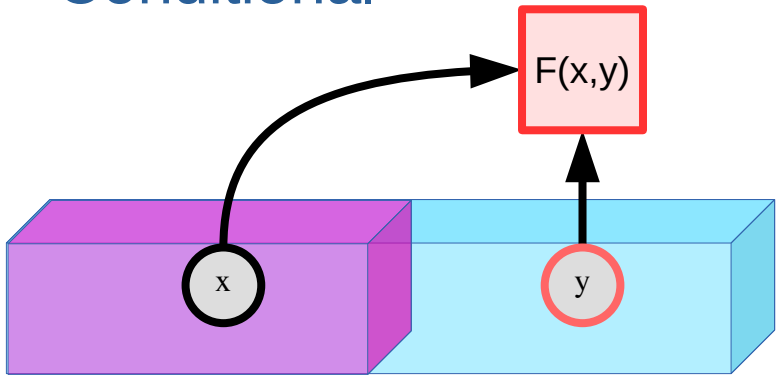


Dark = low energy (good)

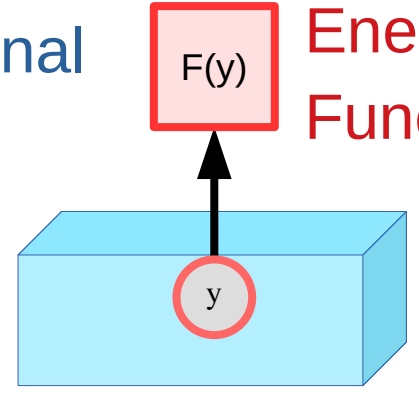
Bright = high energy (bad)

Purple = data manifold

Conditional Energy Function

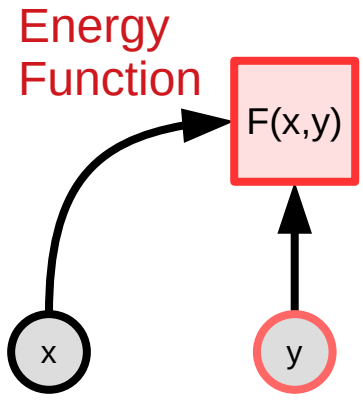


Unconditional Energy Function



Energy-Based Models vs Probabilistic Models

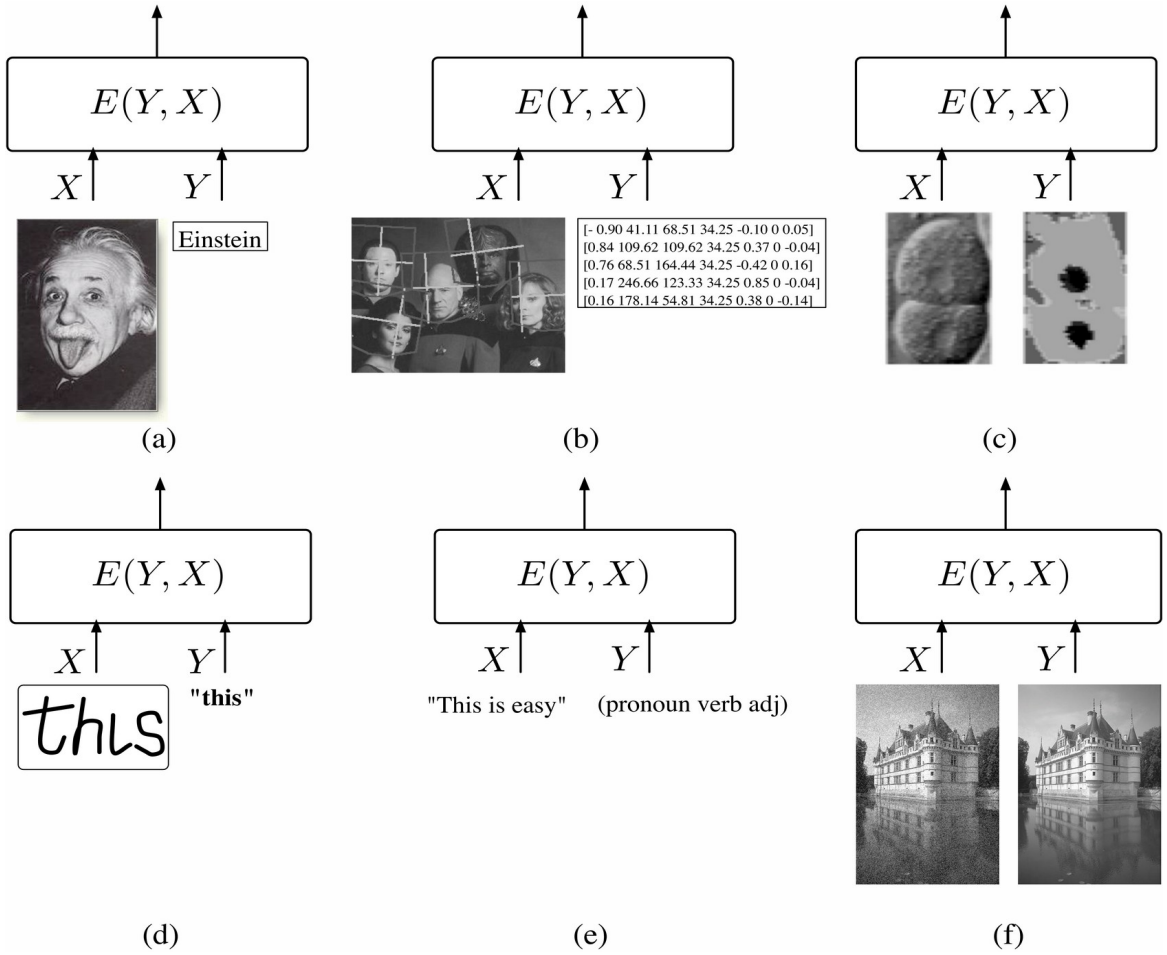
- **Probabilistic models are a special case of EBM**
  - Energies are like un-normalized negative log probabilities
- **Why use EBM instead of probabilistic models?**
  - EBM gives more flexibility in the choice of the scoring function.
  - More flexibility in the choice of objective function for learning
- **From energy to probability: Gibbs-Boltzmann distribution**
  - Beta is a positive constant



$$P(y|x) = \frac{e^{-\beta F(x,y)}}{\int_{y'} e^{-\beta F(x,y')}}$$

When inference is hard

- **Cases where inference is hard:**
  - Output is a high-dimensional object with structure:
    - Sequence, image, video,…
  - Output has compositional structure:
    - Text, action sequence,…
  - Output results from a long chain of reasoning
    - That can be reduced to an optimization problem

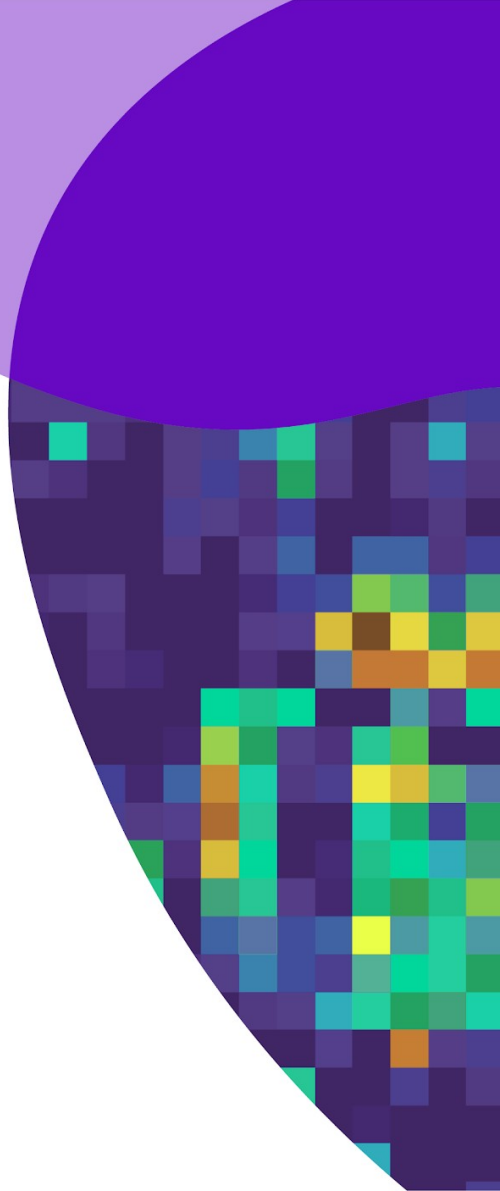


FACEBOOK AI

EBM Architectures

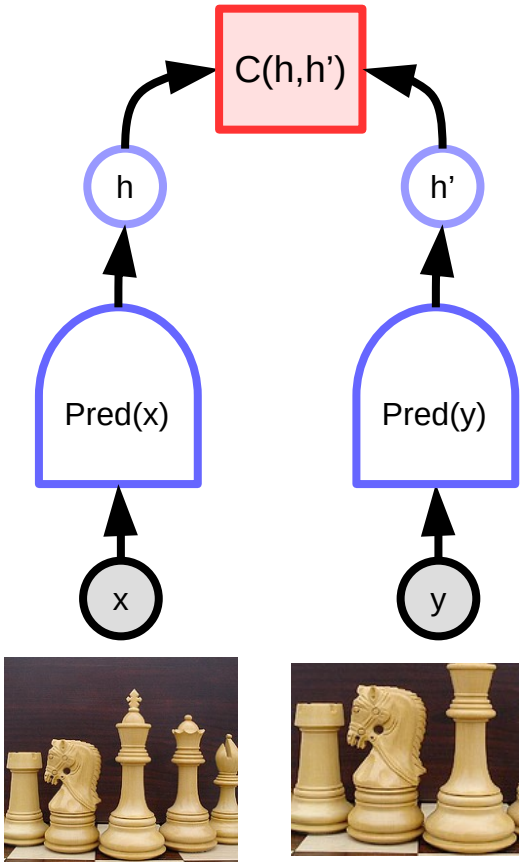
for multimodal prediction

Joint embedding architectures
Latent variable models



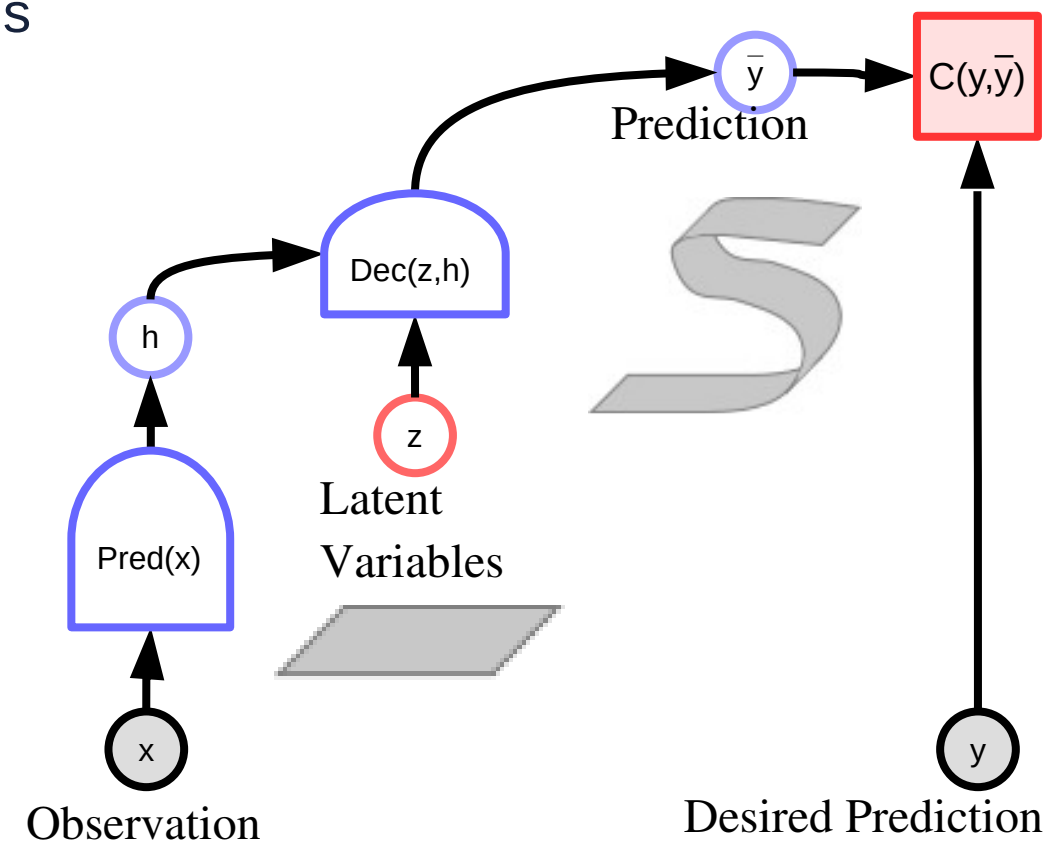
Joint Embedding

- **Distance measured in feature space**
- **Multiple “predictions” through feature invariance**
- **Siamese nets, metric learning**
  - [Bromley NIPS’93] [Chopra CVPR’05] [Hadsell CVPR’06]
- **Advantage: no pixel-level reconstruction**
- **Difficulty: <in a few slides>**
- **Many successful examples for image recognition:**
  - DeepFace [Taigman et al. CVPR 2014]
  - PIRL [Misra et al. Arxiv:1912.01991]
  - MoCo [He et al. Arxiv:1911.05722]
  - SimCLR [Chen et al. Arxiv:2002.05709]
  - …..



Latent-Variable Predictive EBM

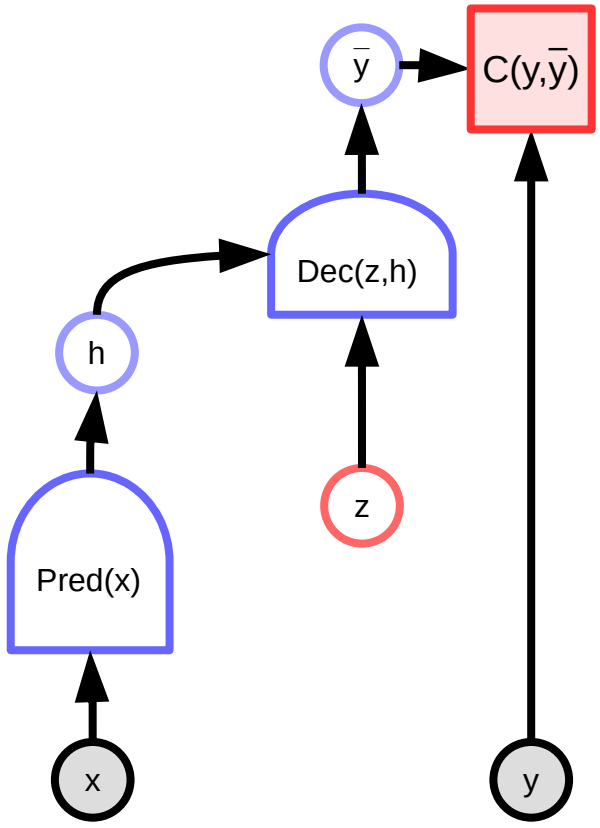
- **Latent variables:**
  - parameterize the set of predictions
- **Ideally, the latent variable represents independent explanatory factors of variation of the prediction.**
- **The information capacity of the latent variable must be minimized.**
  - Otherwise all the information for the prediction will go into it.



When inference involves latent variables

- **Latent variables are variables whose value is never given to us.**
  - Examples: to read a handwritten word, it helps to know where the characters are

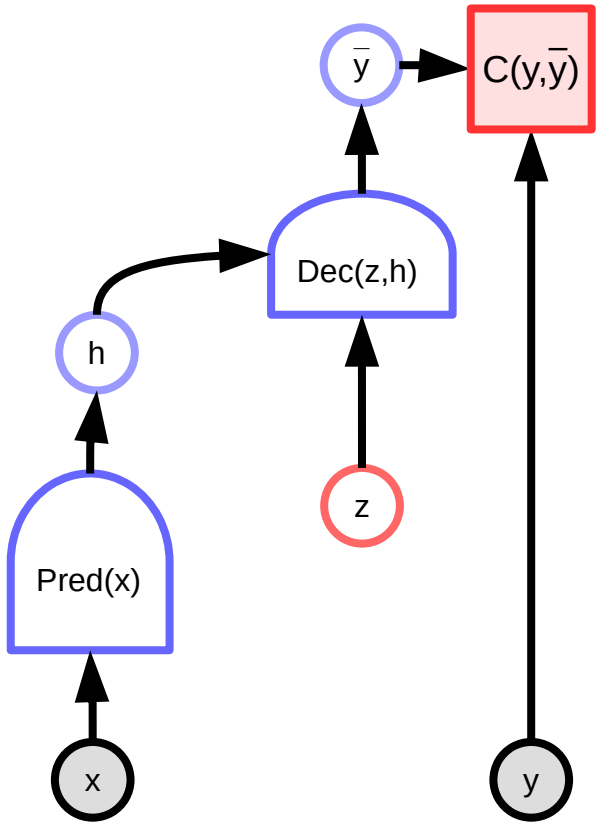
  - To recognize speech, it helps to know where the words and phonemes are
    - Youcantreadthisifyoudontunderstandenglish
    - Vousnepouvezpaslirececisivousneparlezpasfrançais



When inference involves latent variables

- **Latent variables are variables whose value is never given to us.**
  - Examples: to read a handwritten word, it helps to know where the characters are

  - To recognize speech, it helps to know where the words and phonemes are
    - You can't read this if you don't understand english
    - Vous ne pouvez pas lire ceci si vous ne parlez pas français



Latent-Variable EBM: inference

- **Simultaneous minimization with respect to y and z**

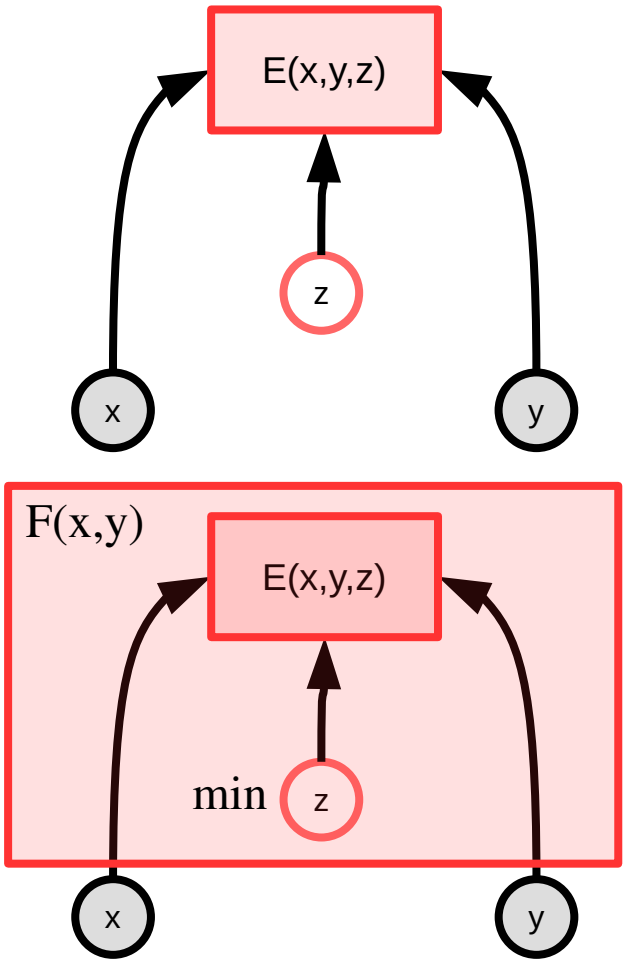
$$\check{y}, \check{z} = \text{argmin}_{y,z} E(x, y, z)$$

- **Redefinition of F(x,y)**

$$F_\infty(x, y) = \min_z E(x, y, z)$$

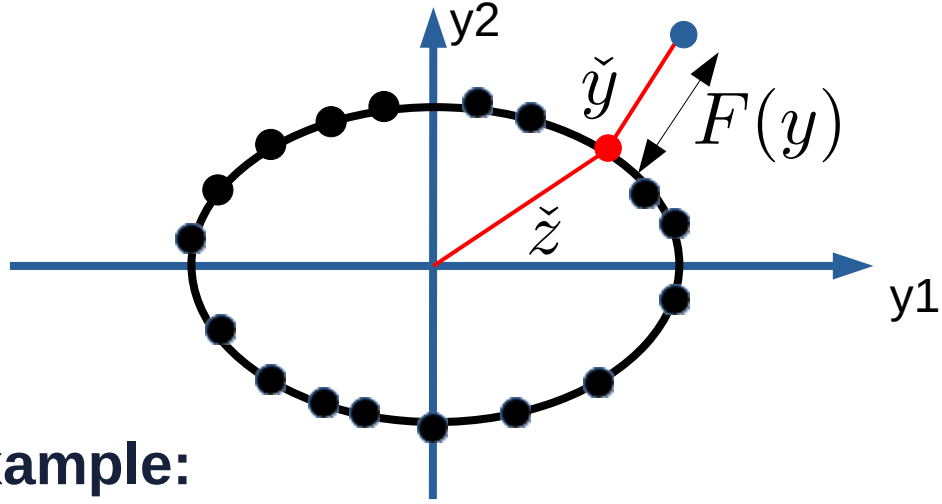
$$F_\beta(x, y) = -\frac{1}{\beta} \log \int_z e^{-\beta E(x,y,z)}$$

$$\check{y} = \text{argmin}_y F(x, y)$$



Inference with Latent Variable EBMs

- **The latent variable parameterizes the data manifold(s).**
- **The energy computes a distance to the learned manifold(s).**
- **The gradient of the energy points to the closest point on the data manifold(s).**



- **Example:**
  - learned manifold = ellipse
  - Latent variable = angle
  - Energy = distance of data point to ellipse

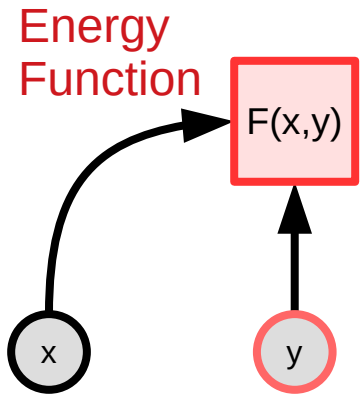
- **Model:**

$$E(y,z) = (y_1 - r_1 \sin(z))^2 + (y_2 - r_2 cos(z))^2$$

$$F(y) = \min_z (y_1 - r_1 \sin(z))^2 + (y_2 - r_2 cos(z))^2$$

Turning Energies to Probabilities

- **From energy to probability: Gibbs-Boltzmann distribution**
  - Beta is a positive constant
- **This is not always possible, not desirable.**



$$P(y|x) = \frac{e^{-\beta F(x,y)}}{\int_{y'} e^{-\beta F(x,y')}}$$

Marginalizing over a latent variable

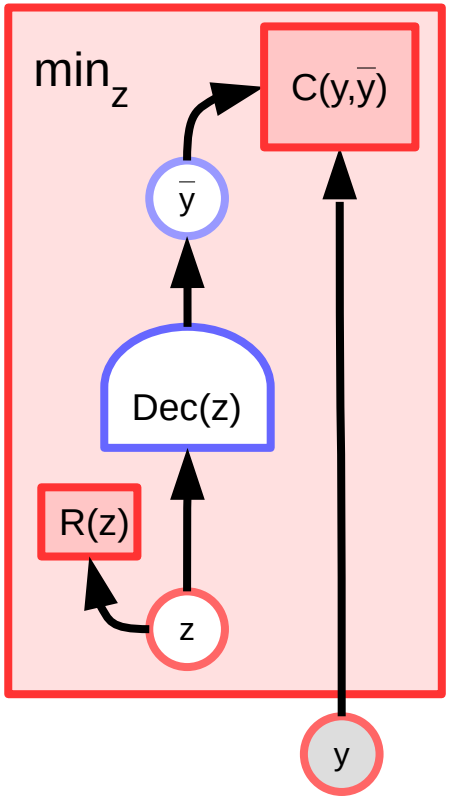
$$P(y,z|x) = \frac{e^{-\beta E(x,y,z)}}{\int_y \int_z e^{-\beta E(x,y,z)}} \qquad P(y|x) = \int_z P(y,z|x)$$

$$P(y|x) = \frac{\int_z e^{-\beta E(x,y,z)}}{\int_y \int_z e^{-\beta E(x,y,z)}} = \frac{e^{-\beta\left[-\frac{1}{\beta}\log \int_z e^{-\beta E(x,y,z)}\right]}}{\int_y e^{-\beta\left[-\frac{1}{\beta}\log \int_z e^{-\beta E(x,y,z)}\right]}} = \frac{e^{-\beta F_\beta(x,y)}}{\int_y e^{\beta F_\beta(x,y)}}$$

- **Free energy F(x,y)** $F_\beta(x,y) = -\frac{1}{\beta}\log \int_z e^{-\beta E(x,y,z)}$

Example: Unconditional Latent-Variable EBM

- **Basic idea: limiting the information capacity of the representation**
- **Examples: K-Means, sparse coding**



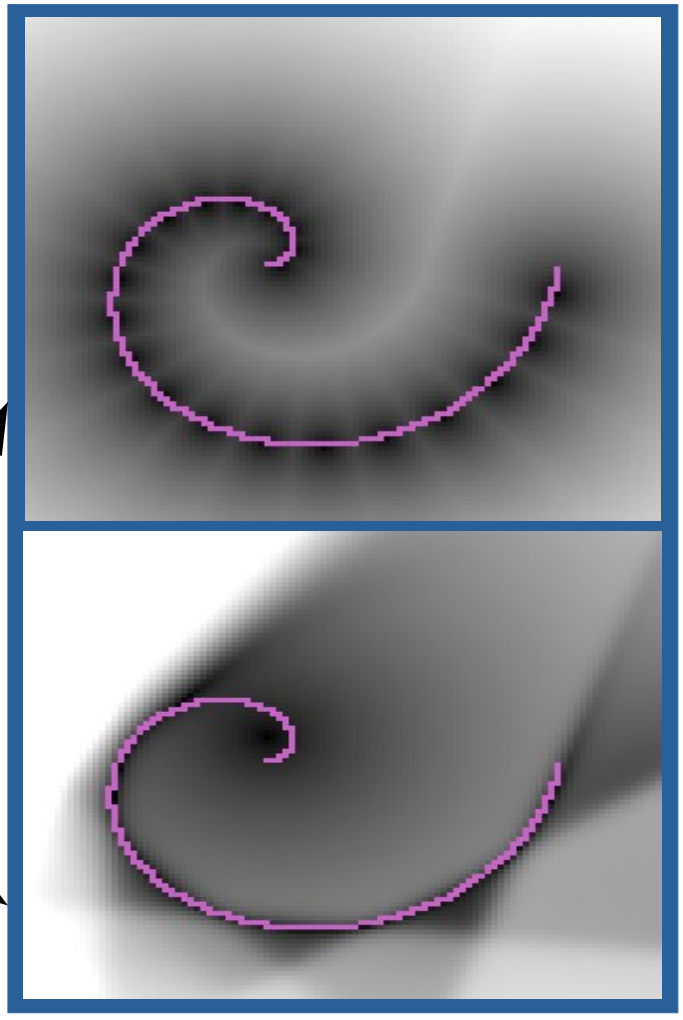
$$E(y,z) = C(y, \mathrm{Dec}(z)) + R(z)$$

$$F_\infty(x,y) = \min_z E(x,y,z)$$

$$\check{y}, \check{z} = \mathrm{argmin}_{y,z} E(x,y,z)$$

$$E(y,z) = \|y - Wz\|^2 \quad z \in 1\,hot$$

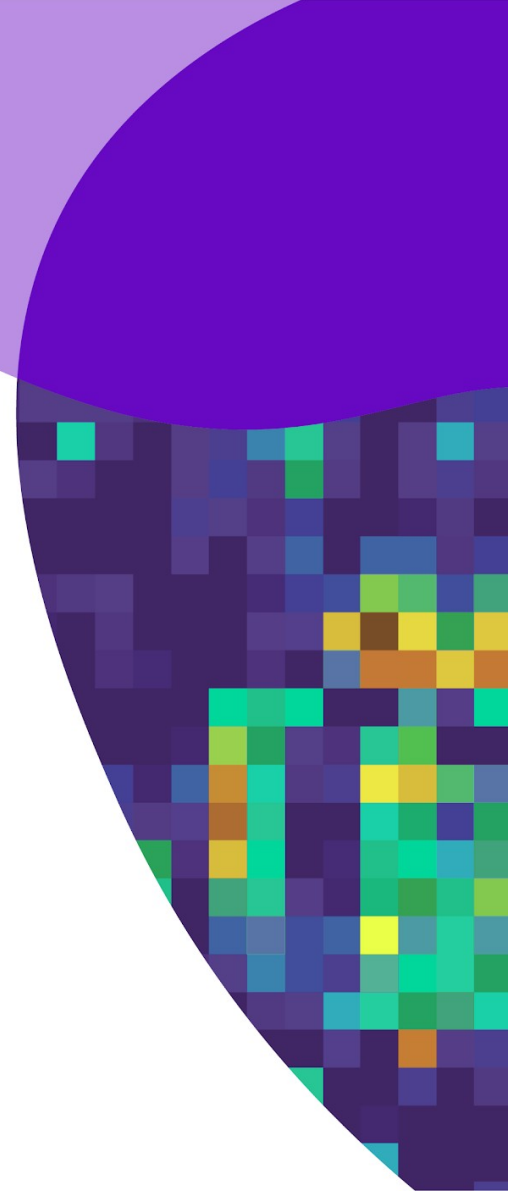
$$E(y,z) = ||y - wz||^2 + \lambda |z|_{L1|}$$



FACEBOOK AI

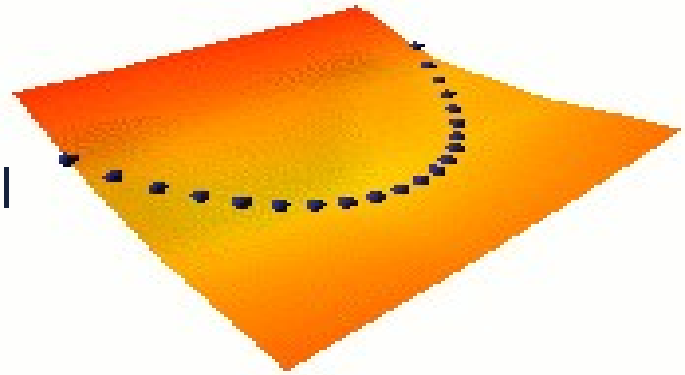
Training EBMs

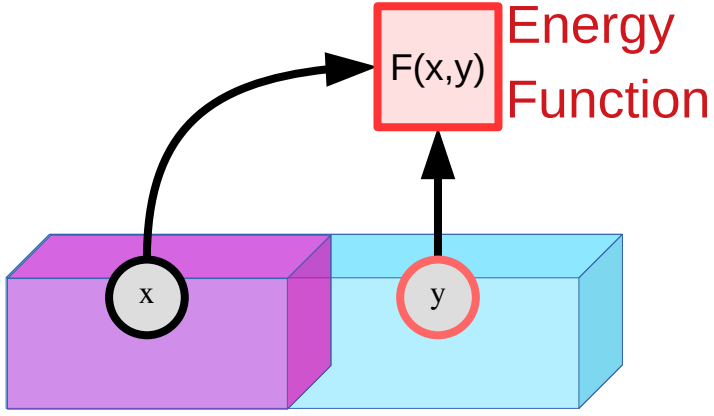
Push down on the energy of data points
Make sure the energy is higher elsewhere



Training an Energy-Based Model

- **Parameterize F(x,y)**
- **Training samples: x[i], y[i]**
- **Shape F(x,y) so that:**
  - F(x[i], y[i]) is strictly smaller than F(x[i], y) for all y different from y[i]
  - Keep F smooth
    - Max-likelihood probabilistic methods break that!
- **Two classes of learning methods:**
  - 1. **Contrastive methods:** push down on F(x[i], y[i]), push up on other points F(x[i], y')
  - 2. **Regularized/Architectural Methods:** build F(x,y) so that the volume of low energy regions is limited or minimized through regularization





Contrastive Methods vs Regularized/Architectural Methods

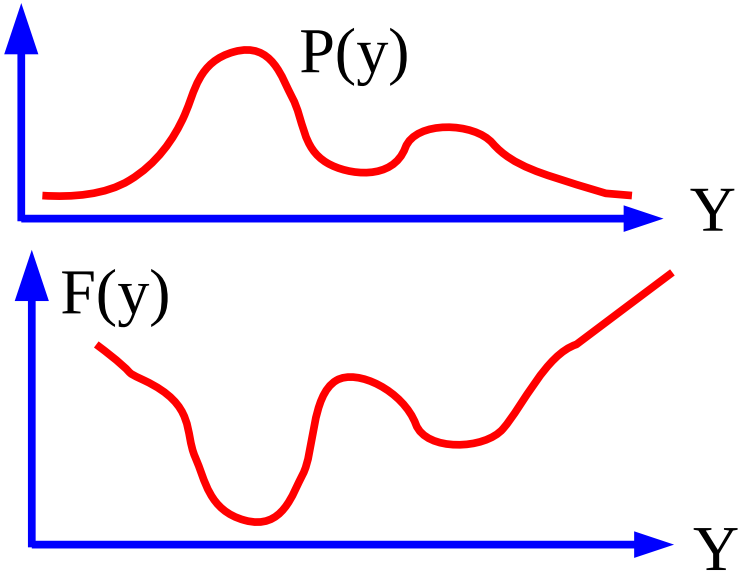
- **Contrastive: [they all are different ways to pick which points to push up]**
  - C1: push down of the energy of data points, push up everywhere else: Max likelihood (needs tractable partition function or variational approximation)
  - C2: push down of the energy of data points, push up on chosen locations: max likelihood with MC/MMC/HMC, Contrastive divergence, Metric learning/Siamese nets, Ratio Matching, Noise Contrastive Estimation, Min Probability Flow, adversarial generator/GANs
  - C3: train a function that maps points off the data manifold to points on the data manifold: denoising auto-encoder, masked auto-encoder (e.g. BERT)
- **Regularized/Architectural: [Different ways to limit the information capacity of the latent representation]**
  - A1: build the machine so that the volume of low energy space is bounded: PCA, K-means, Gaussian Mixture Model, Square ICA, normalizing flows…
  - A2: use a regularization term that measures the volume of space that has low energy: Sparse coding, sparse auto-encoder, LISTA, Variational Auto-Encoders, discretization/VQ/VQVAE.
  - A3: F(x,y) = C(y, G(x,y)), make G(x,y) as "constant" as possible with respect to y: Contracting auto-encoder, saturating auto-encoder
  - A4: minimize the gradient and maximize the curvature around data points: score matching

Contrastive Methods: Max likelihood / Probabilistic Methods

- **The energy can be interpreted as an unnormalized negative log density**
- **Gibbs distribution: Probability proportional to exp(-energy)**
  - Beta parameter is akin to an inverse temperature
- **Don't compute probabilities unless you absolutely have to**
  - Because the denominator is often intractable

$$P(y) = -\frac{\exp[-\beta F(y)]}{\int_{y'} \exp[-\beta F(y')]}$$

$$P(y|x) = -\frac{\exp[-\beta F(x,y)]}{\int_{y'} \exp[-\beta F(x,y')]}$$



Contrastive Methods: Max likelihood / Probabilistic Methods

- **Push down on data points, push up of other points**
  - well chosen contrastive points
- **Max likelihood / probabilistic models**

$$P_w(y|x) = \frac{e^{-\beta F_w(x,y)}}{\int_{y'} e^{-\beta F_w(x,y')}}$$

- Loss: $$\mathcal{L}(x,y,w) = F_w(x,y) + \frac{1}{\beta}\log\int_{y'} e^{-\beta F_w(x,y')}$$
- Gradient: $$\frac{\partial \mathcal{L}(x,y,w)}{\partial w} = \frac{\partial F_w(x,y)}{\partial w} - \int_{y'} P_w(y'|x)\frac{\partial F_w(x,y')}{\partial w}$$
- MC/MCMC/HMC/CD: $\hat{y}$ sampled from $P_w(y|x)$

$$\frac{\partial \mathcal{L}(x,y,w)}{\partial w} = \frac{\partial F_w(x,y)}{\partial w} - \frac{\partial F_w(x,\hat{y})}{\partial w}$$

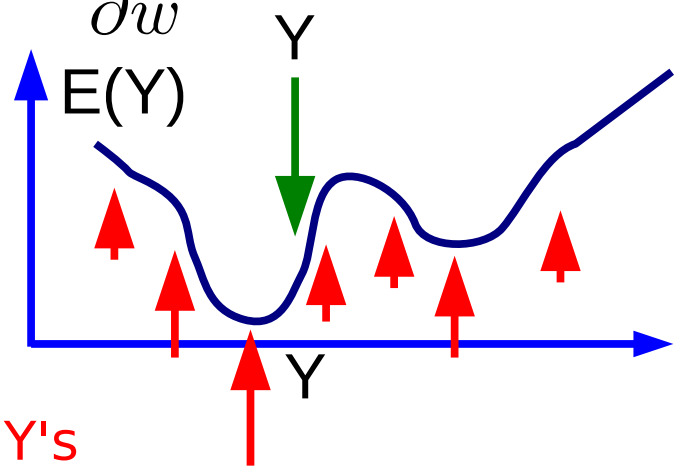
push down of the energy of data points, push up everywhere else

Gradient of the negative log-likelihood loss for one sample Y:

$$\frac{\partial \mathcal{L}(x,y,w)}{\partial w} = \frac{\partial F_w(x,y)}{\partial w} - \int_{y'} P_w(y'|x) \frac{\partial F_w(x,y')}{\partial w}$$

Gradient descent:

$$w \leftarrow w - \eta \frac{\partial \mathcal{L}(x,y,w)}{\partial w}$$



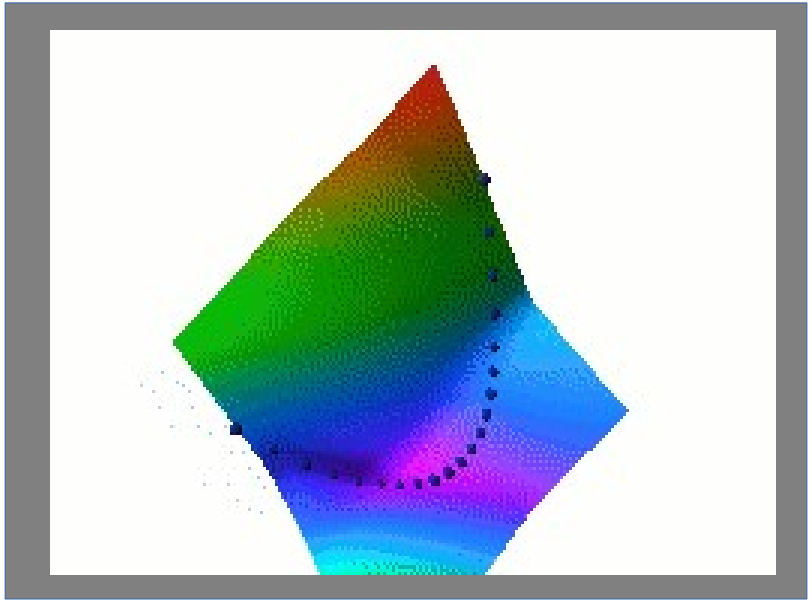
Pushes down on the energy of the samples

Pulls up on the energy of low-energy Y's

$$w \leftarrow w - \eta \frac{\partial F_w(x,y)}{\partial w} + \eta \int_{y'} P_w(y'|x) \frac{\partial F_w(x,y')}{\partial w}$$

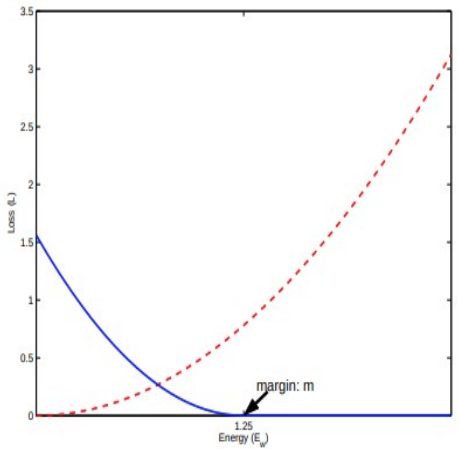
Problem with Max Likelihood / Probabilistic Methods

- **It wants to make the difference between the energy on the data manifold and the energy just outside of it infinitely large!**
- **It wants to make the data manifold an infinitely deep and infinitely narrow canyon.**
- **The loss must be regularized to keep the energy smooth**
  - e.g. à la Wassertstein GAN.
  - So that gradient-based inference works
  - Equivalent to a prior
  - But then, why use a probabilistic model?



Contrastive Methods: other losses

- **Push down on data points, push up of other points**
  - well chosen contrastive points
  - General margin loss: $\mathcal{L}(x, y, \hat{y}, w) = H(F_w(x, y), F_w(x, \hat{y}), m(y, \hat{y}))$
    - Where H(F^+,F^-,m) is a strictly increasing function of F^+ and a strictly decreasing function of F^- , at least whenever F^- - F^+ < m.
  - Examples:
    - Simple [Bromley 1993]:
      $\mathcal{L}(x, y, \hat{y}, w) = [F_w(x, y)]^+ + [m(y, \hat{y}) - F_w(x, \hat{y})]^+$
    - Hinge pair loss [Altun 2003], Ranking loss [Weston 2010]:
      $\mathcal{L}(x, y, \hat{y}, w) = [F_w(x, y) - F_w(x, \hat{y}) + m(y, \hat{y})]^+$
    - Square-Square: [Chopra CVPR 2005] [Hadsell CVPR 2006]:
      $\mathcal{L}(x, y, \hat{y}, w) = \left([F_w(x, y)]^+\right)^2 + \left([m(y, \hat{y}) - F_w(x, \hat{y})]^+\right)^2$



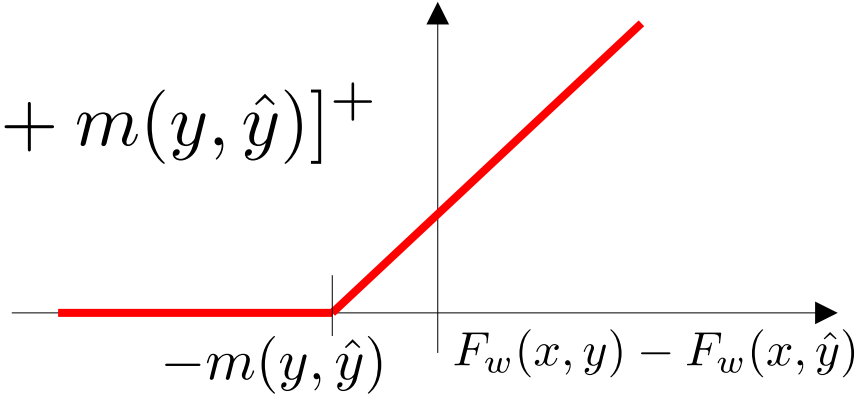
General margin loss

- **Considers all possible outputs**

$$\mathcal{L}(x, y, w) = \sum_{\hat{y} \in \mathcal{Y}} H(F_w(x, y), F_w(x, \hat{y}), m(y, \hat{y}))$$

- **Hinge loss that makes F(x,y) lower than F(x,y') by a quantity (margin) that depends on the distance between y and y'**
- **Example:**

$$\mathcal{L}(x, y, w) = \sum_{\hat{y} \in \mathcal{Y}} [F_w(x, y) - F_w(x, \hat{y}) + m(y, \hat{y})]^+$$



Plenty of Contrastive Loss Functions to Choose From

Good and bad loss functions: good ones have non-zero margin

Loss	Formula	Margin
energy loss	$F(x,y)$	0
perceptron	$F(x,y) - \min_{\check{y}\in} F(x,\check{y})$	0
hinge	$\max(0, m + F(x,y) - F(x,\hat{y}))$	m
log	$\log\left(1 + e^{F(x,y)-F(x,\hat{y})}\right)$	∞
LVQ2	$\min(M, \max(0, F(x,y) - F(x,\hat{y}))$	0
MCE	$\left(1 + e^{-(F(x,y)-F(x,\hat{y}))}\right)^{-1}$	∞
square-square	$F(x,y)^2 - (\max(0, m(y,\hat{y}) - F(x,\hat{y})))^2$	m
square-exp	$F(x,y)^2 + \beta e^{-F(x,\hat{y})}$	∞
NLL/MMI	$F(x,y) + \frac{1}{\beta}\log\int_{\hat{y}\in} e^{-\beta E(x,\hat{y})}$	∞
MEE	$1 - e^{-\beta F(x,y)} / \int_{\hat{y}\in} e^{-\beta F(x,\hat{y})}$	∞

Contrastive Methods: group losses

- **Push down on a group of data points, push up on a group of contrastive points**
  - General group loss on p^+ data points and p^- contrastive points:

$$\mathcal{L}(x_1 \dots x_{p^+}, y_1 \dots y_{p^+}, \hat{y}_1 \dots \hat{y}_{p^-}, w) = H\left(F(x_1, y_1), \dots F(x_{p^+}, y_{p^+}), F(x_1, \hat{y_1}), \dots F(x_{p^+}, \hat{y_{p^+}}), M(Y_{1\dots p^+}, \hat{Y}_{1\dots p^-})\right)$$

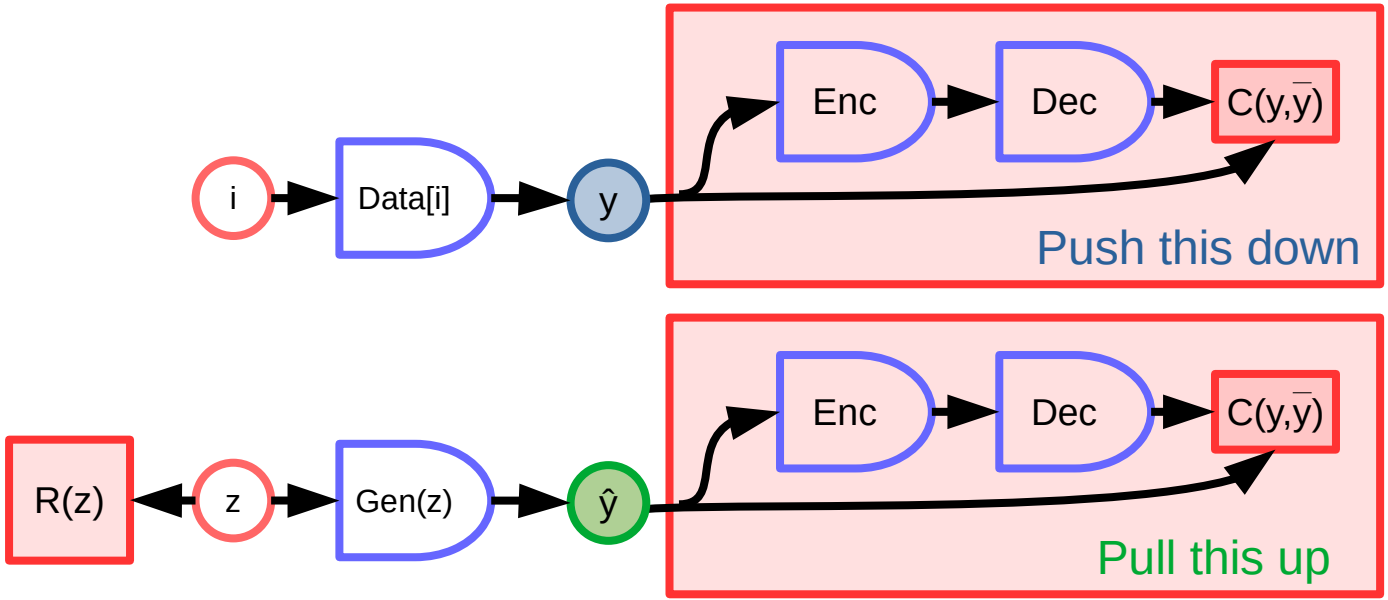
    - Where H must be an increasing fn of the data energies and decreasing fn of the contrastive point energies within the margin.
    - M is a margin matrix for all pairs of y and ŷ in the group.
  - Example: Neighborhood Component Analysis, Noise Contrastive Estimation (implicit infinite margin) [Goldberger 2005] [Gutmann 2010]...[Misra 2019] [Chen 2020]

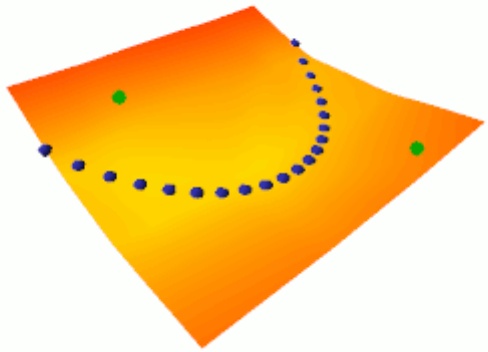
$$\mathcal{L}(x, y, \hat{y}_1, \dots \hat{y}_{p^-}, w) = -\log \frac{e^{-F_w(x,y)}}{e^{-F_w(x,y)} + \sum_{i=1}^{p^-} e^{-F_w(x,\hat{y}_i,w)}}$$

GANs are secretly a contrastive method for EBM

- **Energy-Based GAN** [Zhao 2016]**, Wasserstein GAN** [Arjovsky 2017]**,...**
  - GANs generate nice images
  - But learning representations of image has not been very successful.

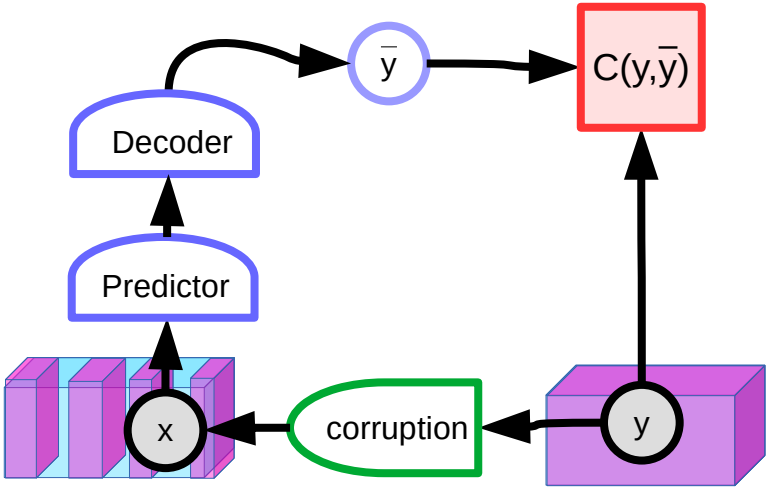
$$\mathcal{L}(x, y, \hat{y}, w) = H(F_w(x, y), F_w(x, \hat{y}), m(y, \hat{y}))$$





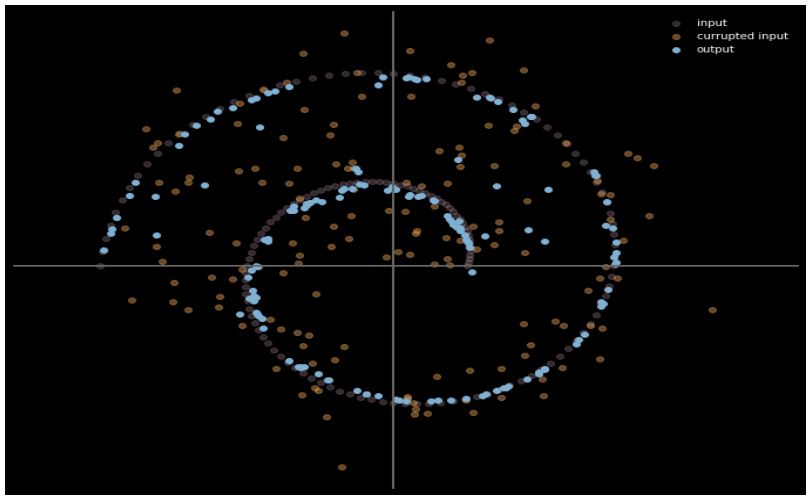
Contrastive Methods in NLP / Denoising AE / Masked AE

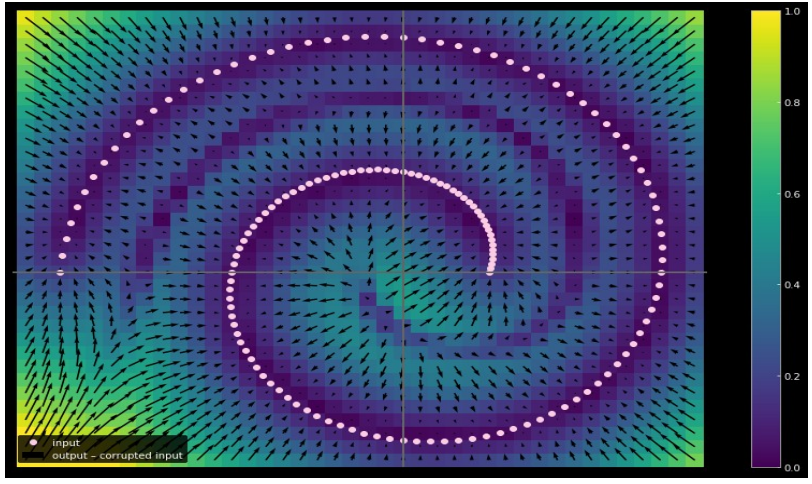
- **Contrastive method for NLP**
  - [Collobert-Weston 2011]
- **Denoising AE** [Vincent 2008]
- **Masked AE: Learning text representations**
  - BERT [Devlin 2018], RoBERTa [Ott 2019]



This is a [...] of text extracted [...] a large set of [...] articles

This is a piece of text extracted from a large set of news articles

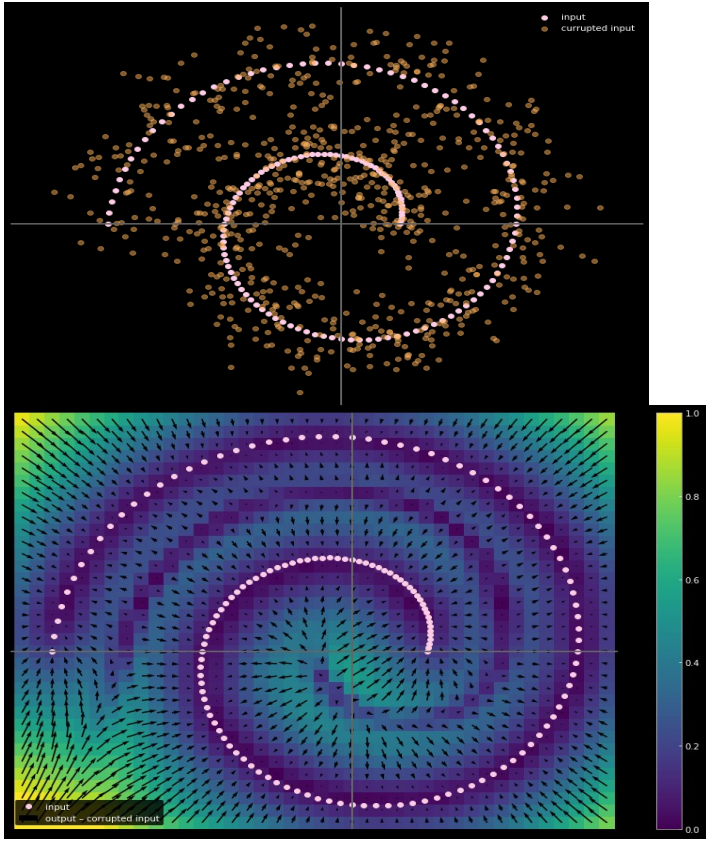


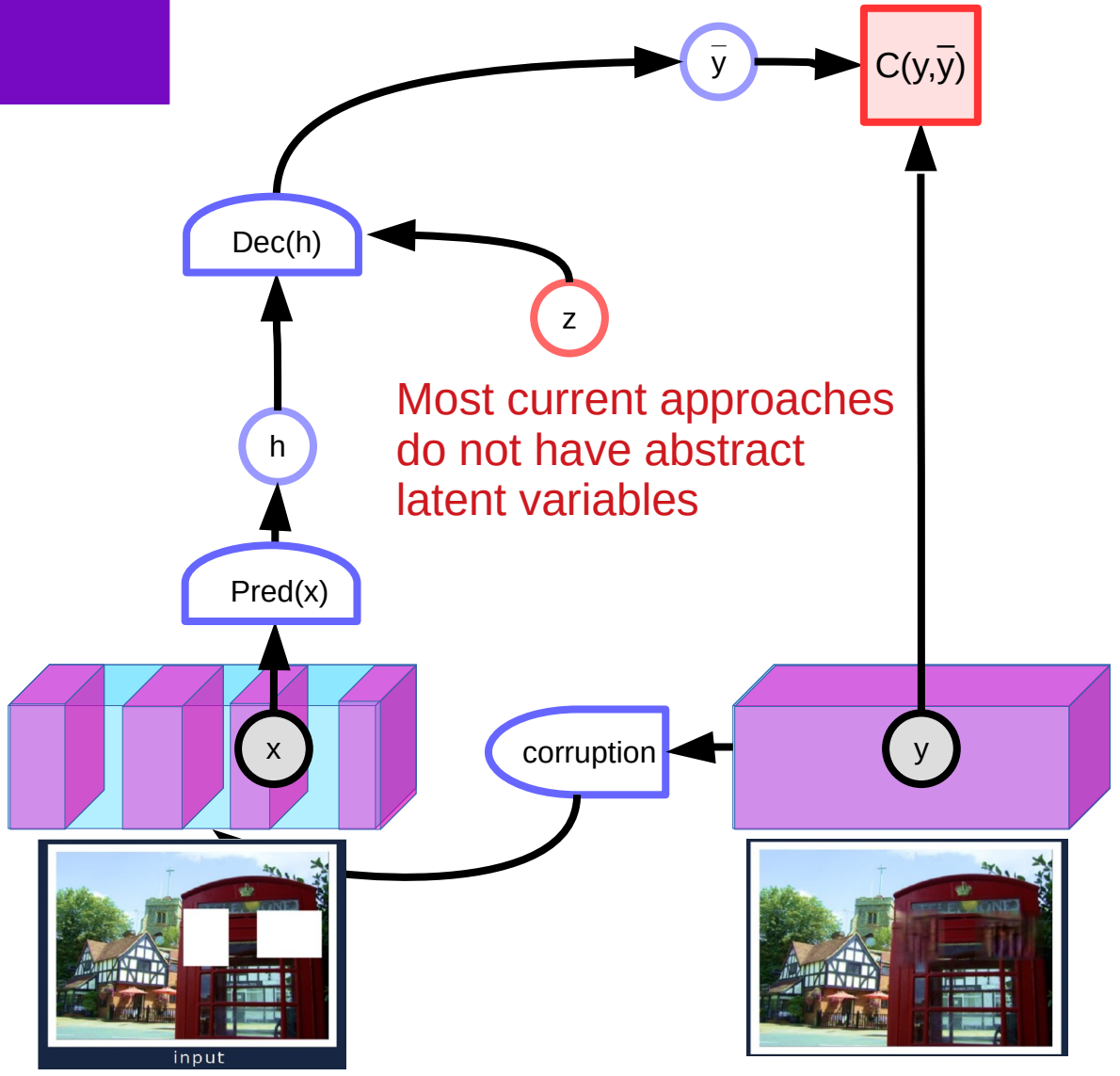


Figures: Alfredo Canziani

Denoising AE in continuous domains?

- **Image inpainting** [Pathak 17]
- Latent variables? GAN?





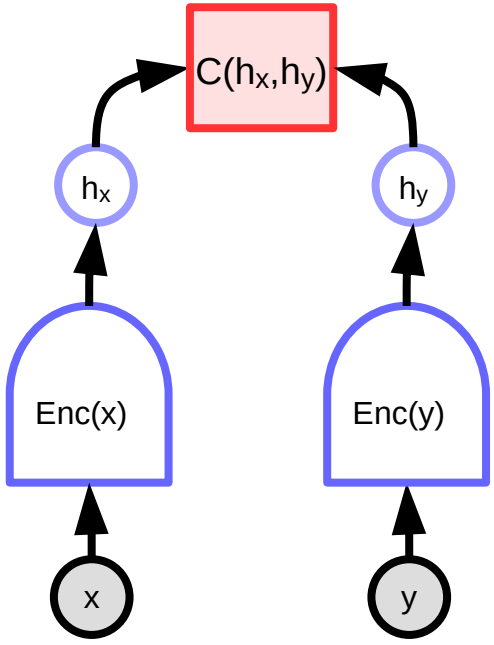
Most current approaches do not have abstract latent variables

Reconstructing Images is Hard

- **Representing uncertainty in the prediction**
  - Easy for discrete object, hard for continuous ones
- **Predicting missing words is easy**
  - Words are a discrete set
  - We can represent distributions over discrete sets (softmax)
- **Predicting missing images is hard**
  - Images are high-dimensional and continuous
  - We don’t have good ways of representing distributions over images
- **Solution: no reconstruction, joint embedding**

Contrastive Joint Embedding

- **Siamese nets, metric learning**
- **Two identical networks with shared weights**
  - Signature verification: [Bromley NIPS'93],
  - Face verification [Chopra CVPR'05]
  - Face reco, DeepFace [Taigman et al. CVPR 2014]
  - Video feature learning [Taylor CVPR 2011]
  - Use square-square or square-exp loss
- **Advantages:**
  - no pixel-level reconstruction
  - Learns a similarity metric
  - Multimodality through encoder invariance

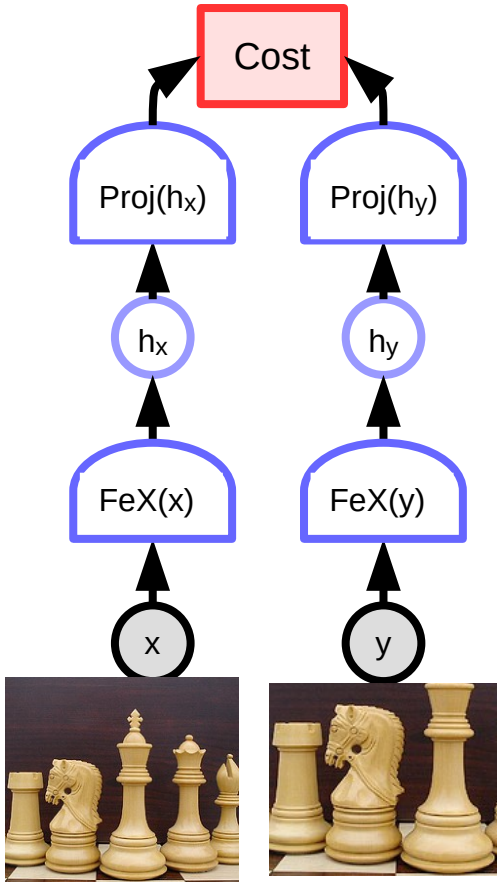


Positive pair:
Make F small

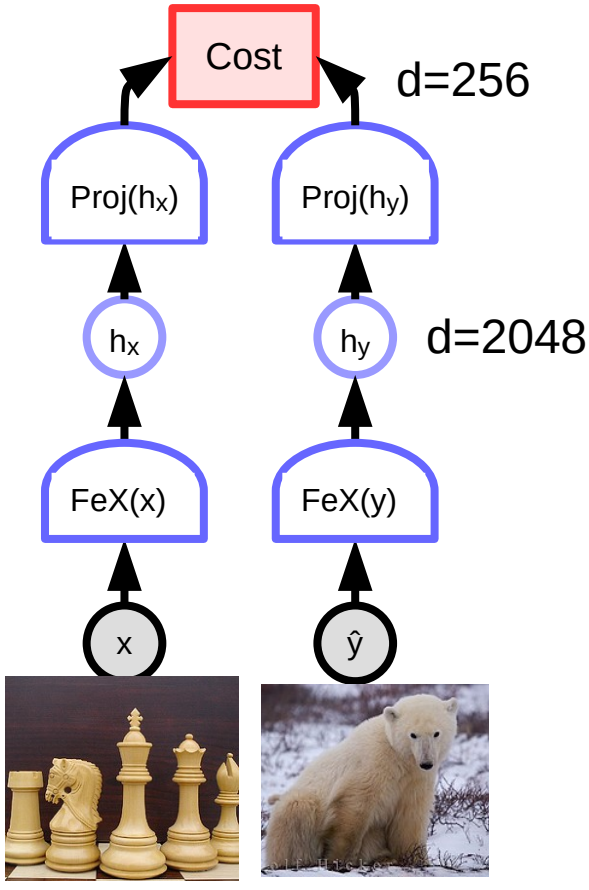
Negative pair:
Make F large

Contrastive Joint Embedding

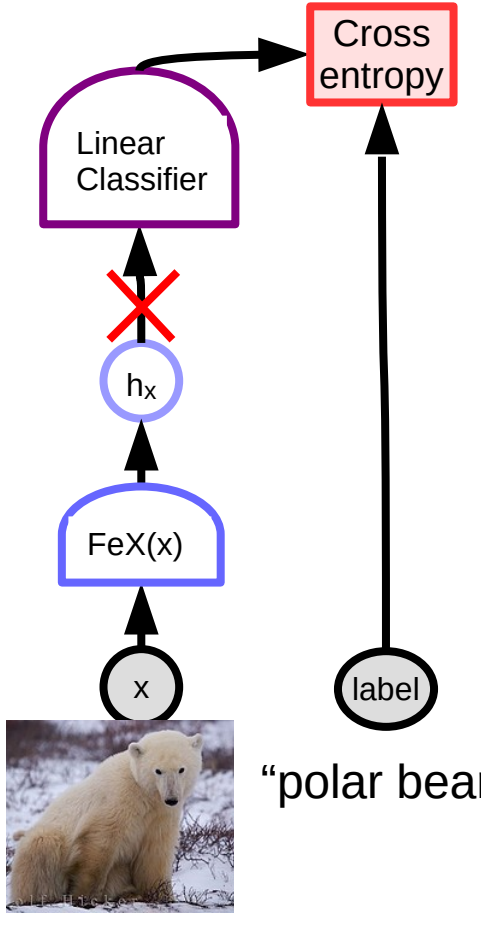
Make F(x,y) small



Make F(x,ŷ) large



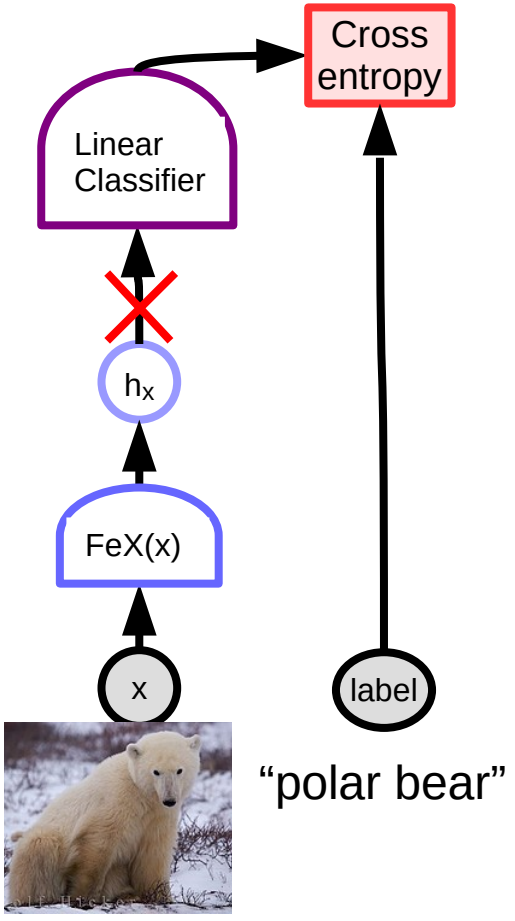
Training a supervised linear head



“polar bear”

Contrastive Joint Embedding

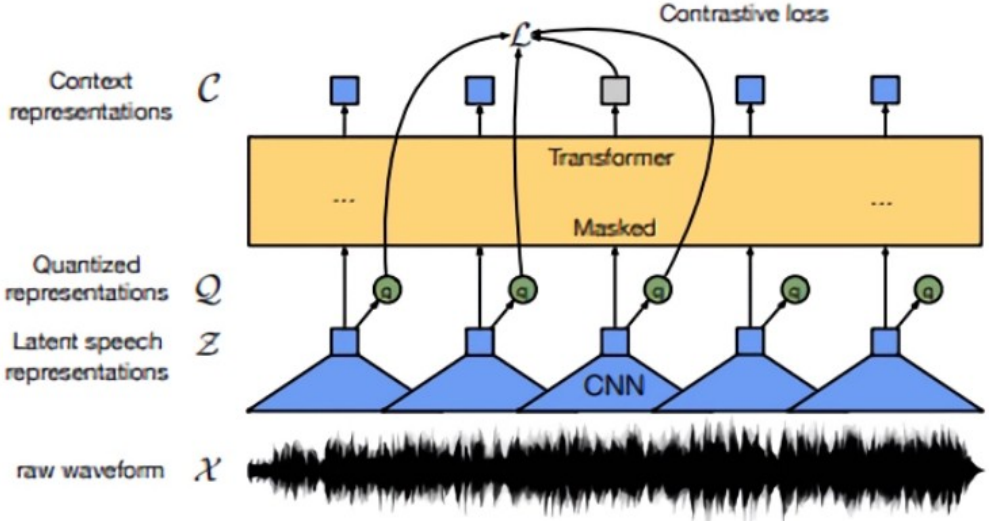
- **Issues:**
  - Hard negative mining
  - Expensive computationally
  - Only works for small dimension of embeddings (256)
- **Successful examples for image recognition:**
  - PIRL [Misra et al. Arxiv:1912.01991]
  - MoCo [He et al. Arxiv:1911.05722]
  - SimCLR [Chen et al. Arxiv:2002.05709]
- **Use InfoNCE group loss**

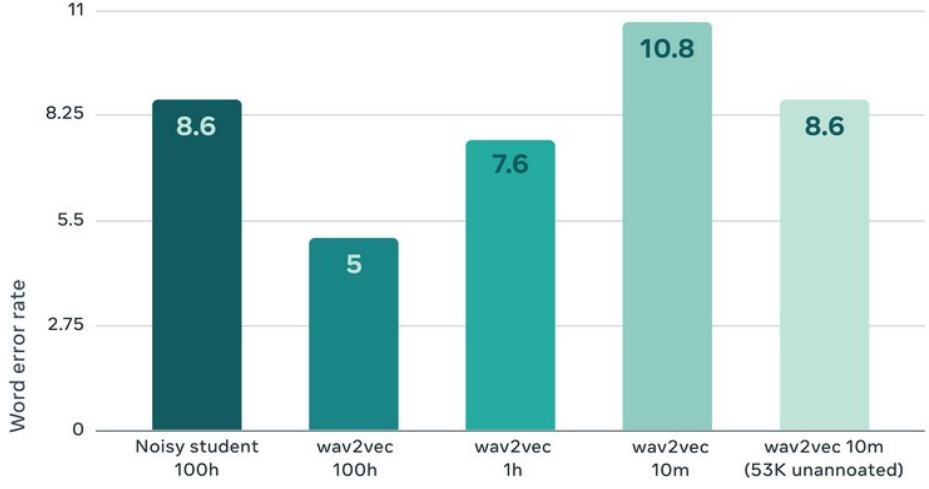


$$\mathcal{L}(x, y, \hat{y_1}, \ldots \hat{y}_q, w) = F_w(x, y) + \log \left[e^{-F_w(x,y)} + \sum_{i=1}^{q} e^{-F_w(x,\hat{y}_i,w)} \right]$$

Wav2Vec 2.0: SSL for speech recognition

- **Pre-train on 960h of unlabeled speech,**
- **then train with 10 minutes, 1h or 100h of labeled speech**
- **Results on LibriSpeech**
  - Wav2vec on 10 minutes = Same WER as previous SOTA on 100h
  - Papers: [Baevski et al. NeurIPS 2020] [Xu et al. ArXiv:2010.11430]
  - Code: Github: PyTorch/fairseq

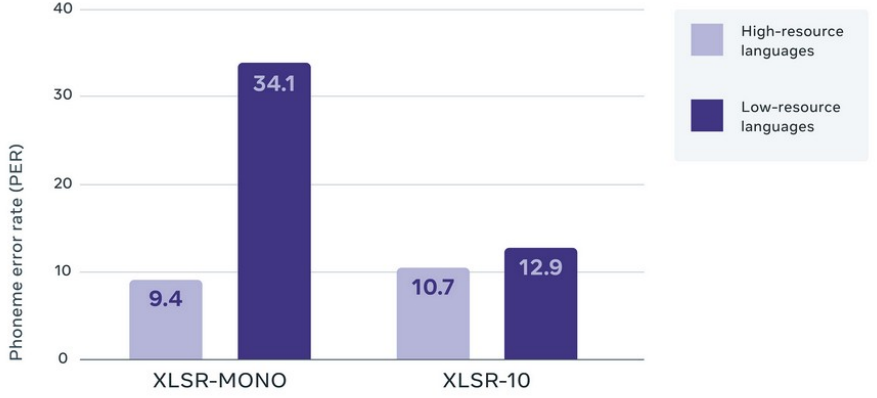




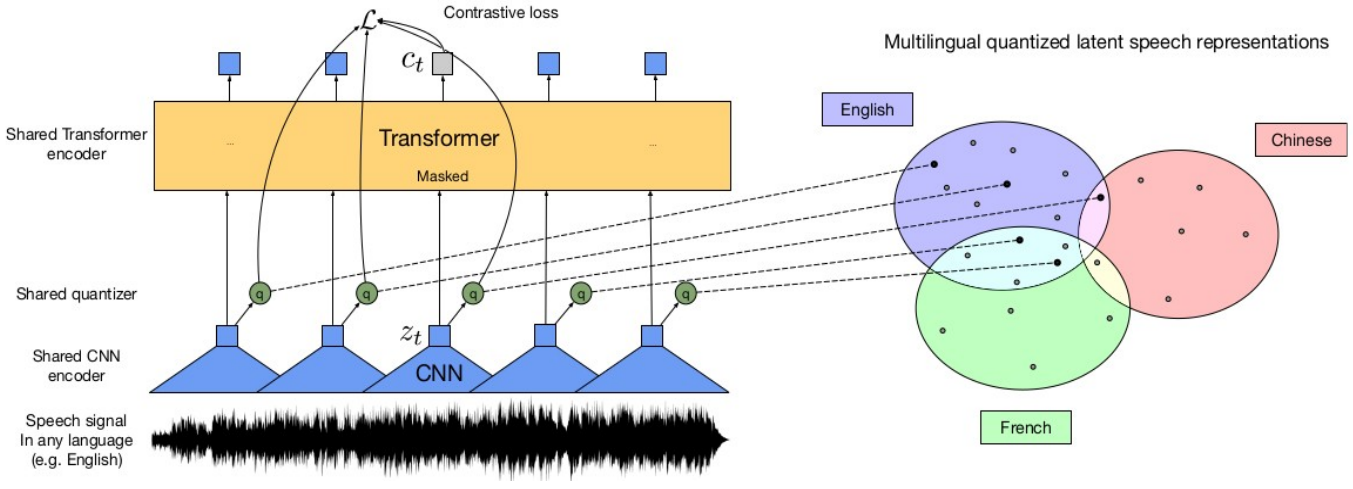
WER for Noisy Student self-training with 100 hours of labeled data. Wav2vec 2.0 with 100 hours, 1 hour, and only 10 minutes of labeled data. All models use the remainder of the LibriSpeech corpus (total 960 hours) as unannotated data, except for the last result, which uses 53K hours from LibriVox.

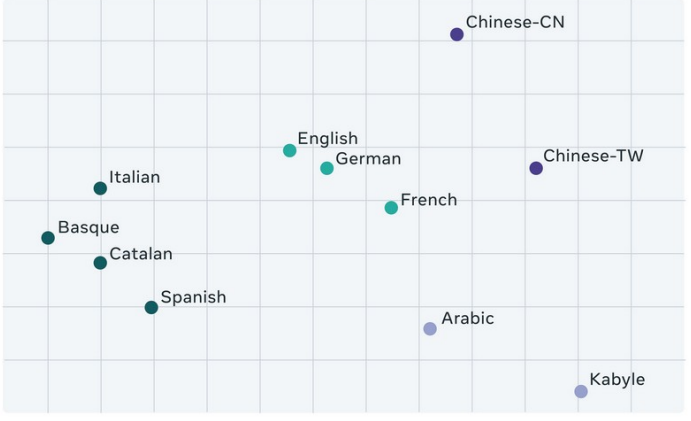
XLSR: multilingual speech recognition

- **Multilingual self-supervised ASR**
  - [Conneau arXiv:2006.13979]
  - Raw audio → ConvNet → Transformer
  - CommonVoice: 72% reduction of PER
  - BABEL: 16% reduction of WER



Results on the Common Voice benchmark in terms of phoneme error rate (PER), comparing training on each language individually (XLSR-Mono) with training on all 10 languages simultaneously (XLSR-10).

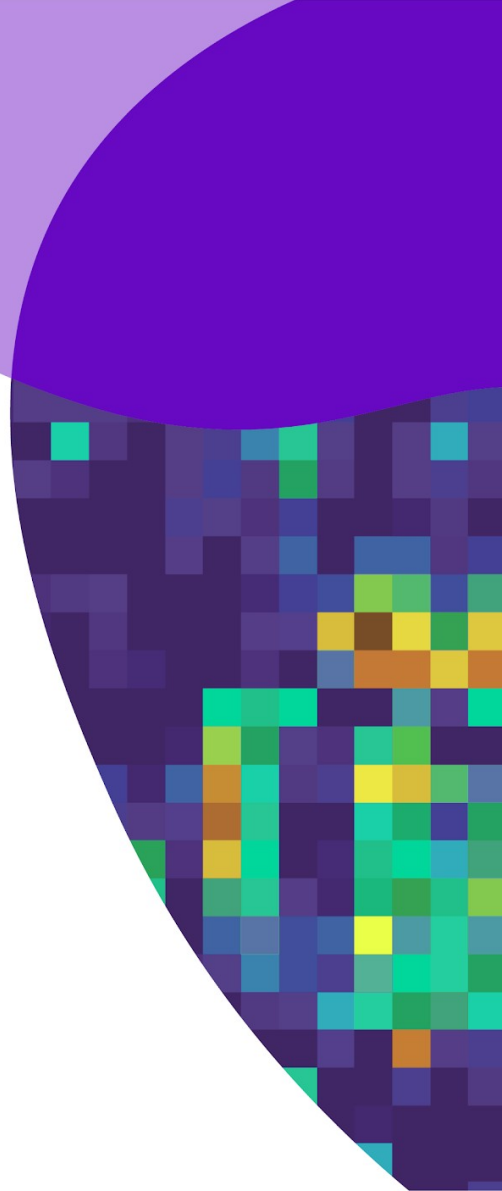




Visualization of how the learned units are used across languages. Graph shows a 2D PCA plot of how units are used in each language. Languages closer to each other, like English and German or Basque and Catalan, tend to use similar units.

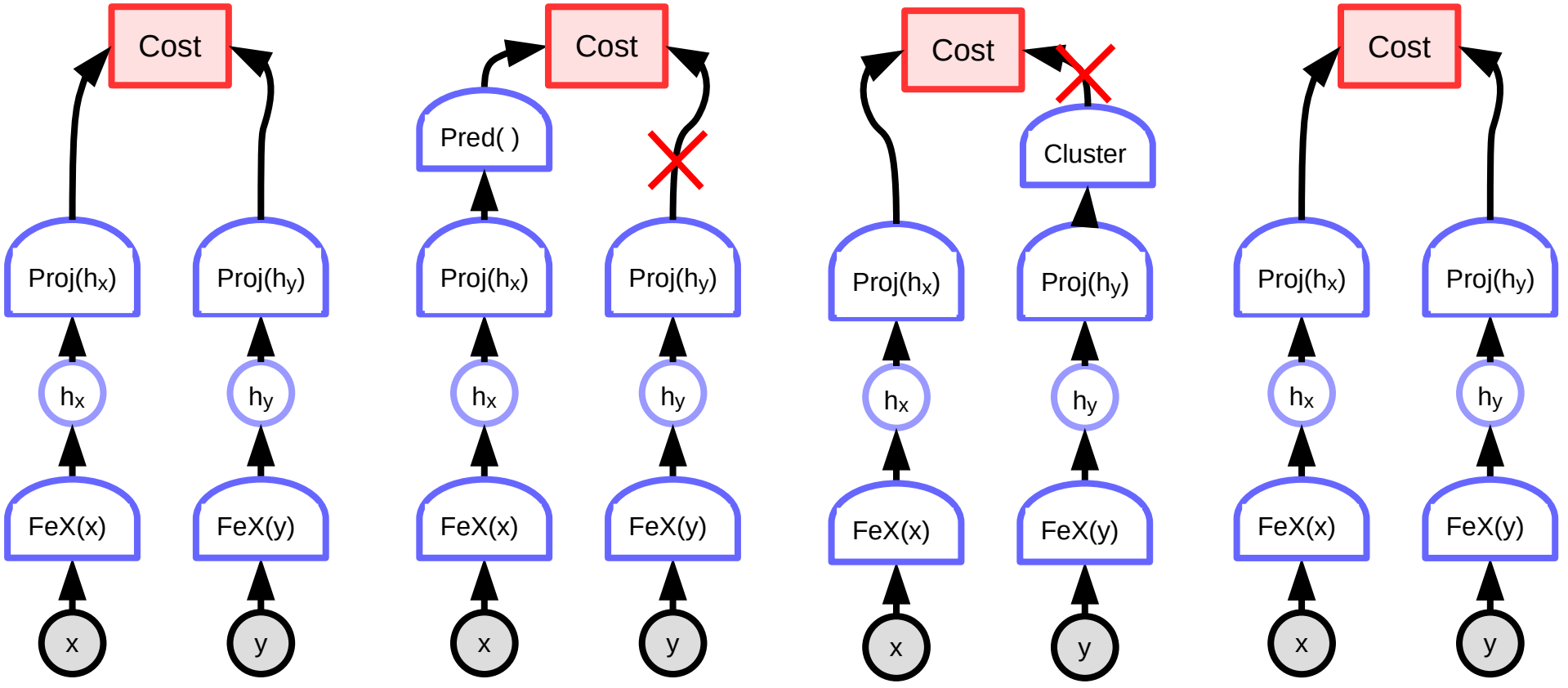
FACEBOOK AI

Non-Contrastive EBM Training



Push down on the energy of data points,
Minimize the volume of low-energy space.

Joint Embedding Architectures & Methods to prevent collapse.



Contrastive
DrLIM, PIRL,
MoCo,SimCLR,

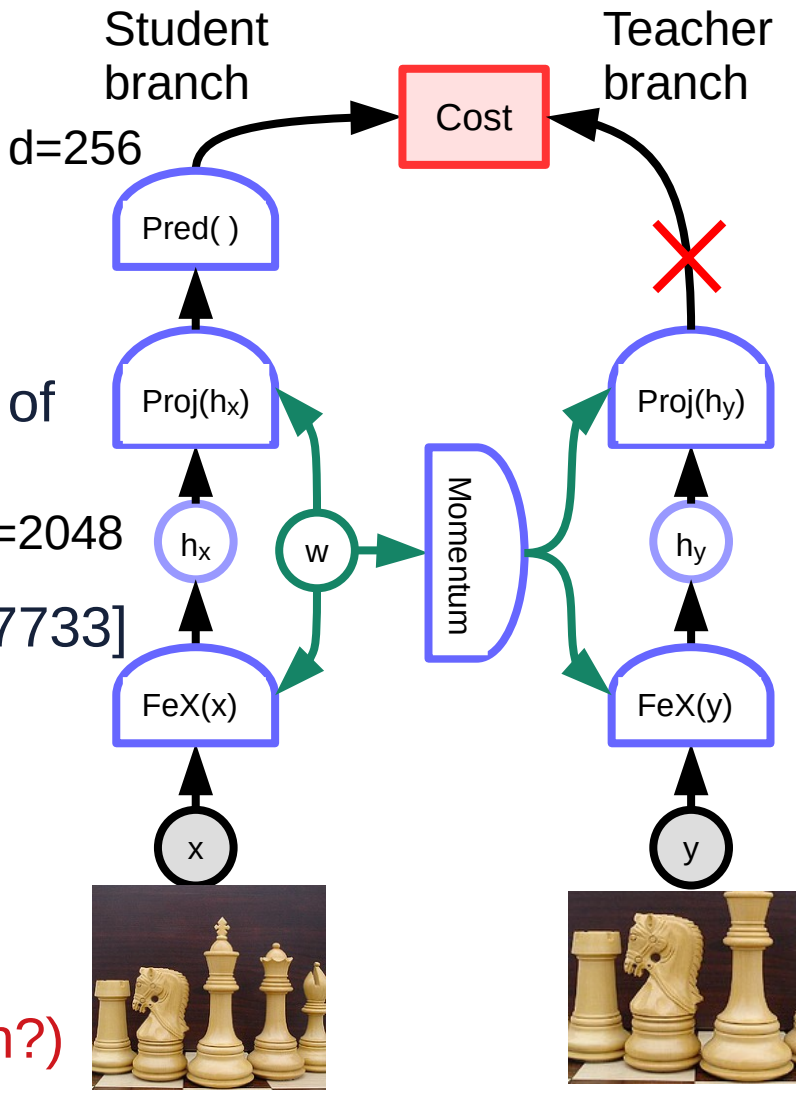
Distillation
BYOL, SimSiam

Quantization
DeepCluster, SwAV

Information Max
Barlow Twins

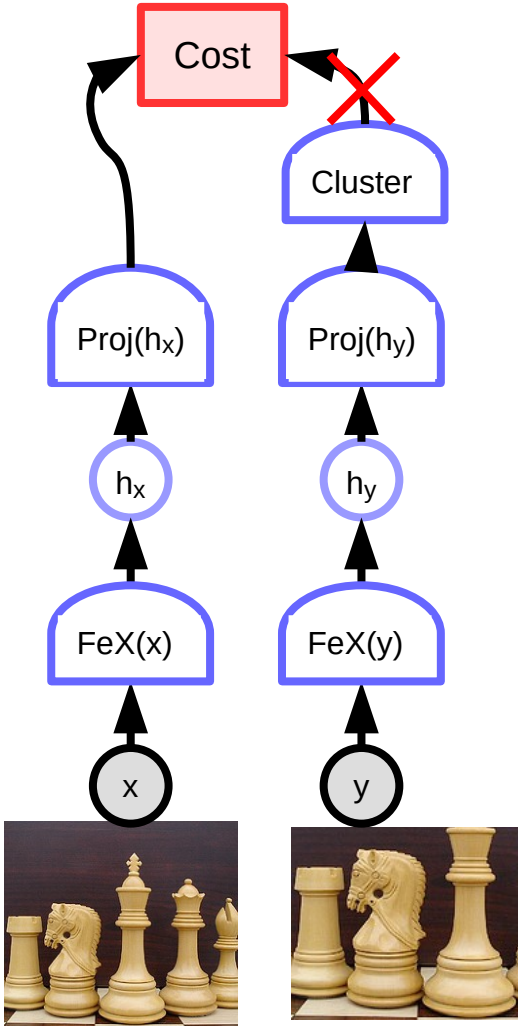
Distillation Methods

- **Modified Siamese nets**
  - Predictor head eliminates variation of representations due to distortions
  - BYOL: Teacher branch uses a moving-average of the parameters of the student branch
- **Examples:**
  - Bootstrap Your Own Latents [Grill arXiv:2006.07733]
  - SimSiam [Chen & He arXiv:2011.10566]
- **Advantages**
  - No negative samples
- **Issues**
  - Not clear why they don't collapse (normalization?)



Quantization Methods

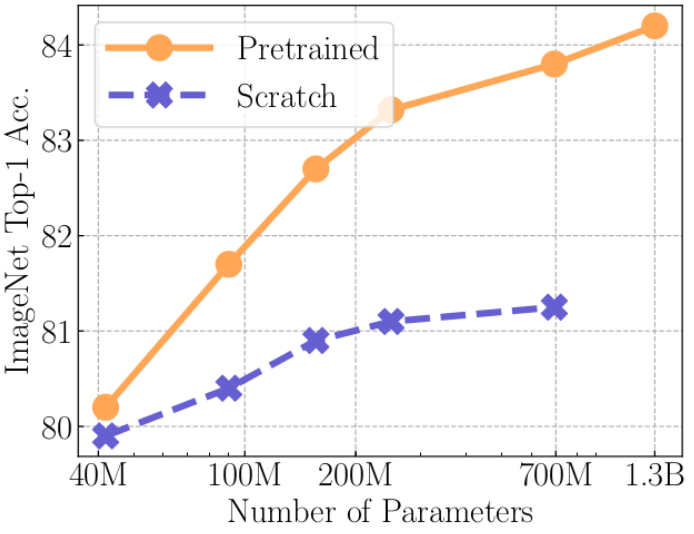
- **K-means clustering on embedding vectors**
  - Ensuring that all clusters are populated
    - Sinkhorn-Knapp procedure (information maximization)
  - Cluster centers used as targets for student branch
- **Examples**
  - DeepCluster [Caron arXiv:1807.05520]
  - SwAV [Caron arXiv:2006.09882]
- **Advantage:**
  - Works really well!
  - Uses large distortions (multicrop)
  - Scales to very large datasets

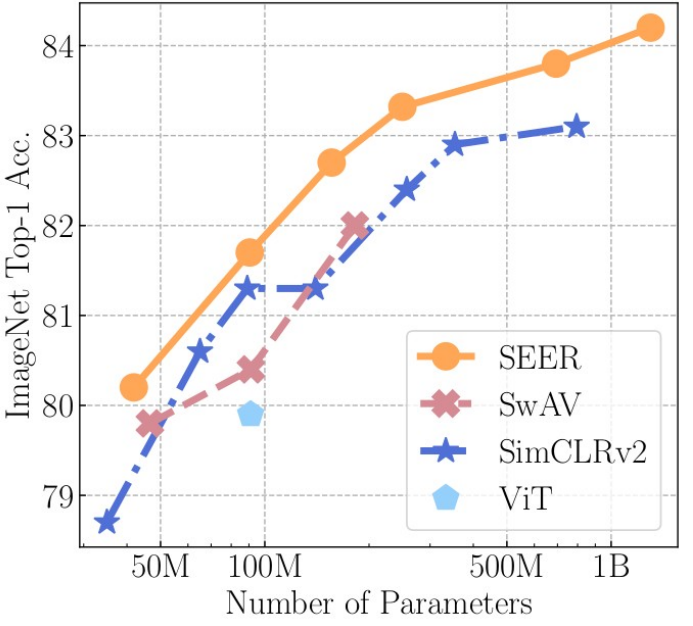


SEER [Goyal et al. ArXiv:2103.01988]

- **SwAV training on 1 billion random IG images**
- **RegNet architecture**
- **Fine-tuned on various datasets**
  - ImgNet full: 84.% top-1 correct
  - ImgNet 10%: 77.9%, ImgNet 1%: 60.5%
  - Inaturalist: 50.8%, Places205: 62.7%
  - Pascal VOC2007: 92.6%
- **Code: https://vissl.ai/**

Method	Data	#images	Arch.	#param.	Top-1
DeeperCluster [6]	YFCC100M	96M	VGG16	138M	74.9
ViT [14]	JFT	300M	ViT-B/16	91M	79.9
SwAV [7]	IG	1B	RX101-32x16d	182M	82.0
SimCLRv2 [9]	ImageNet	1.2M	RN152w3+SK	795M	83.1
SEER	IG	1B	RG128	693M	83.8
SEER	IG	1B	RG256	1.3B	**84.2**



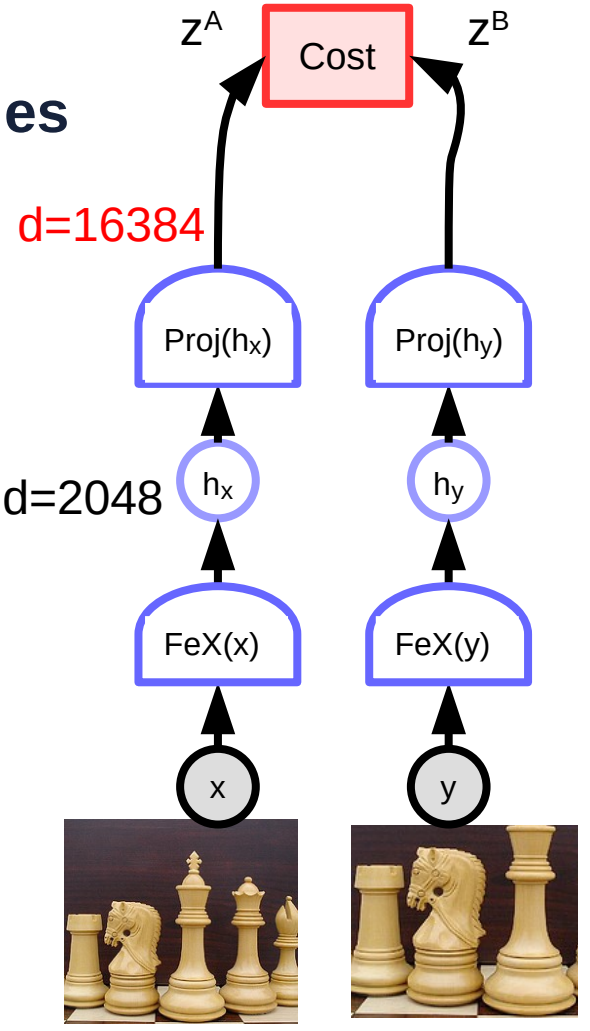


Information Maximization

- **Minimizes redundancy between embedding variables**
  - Maximizes information content of embedding vectors
- **Example: Barlow Twins**
  - [Zbontar et al. ArXiv:2103.03230]
  - Maximizes normalized correlation between the same variable in the two branches over a batch.
  - Minimizes normalized correlation between different variables in the two branches
  - Centered vectors z^A,z^B

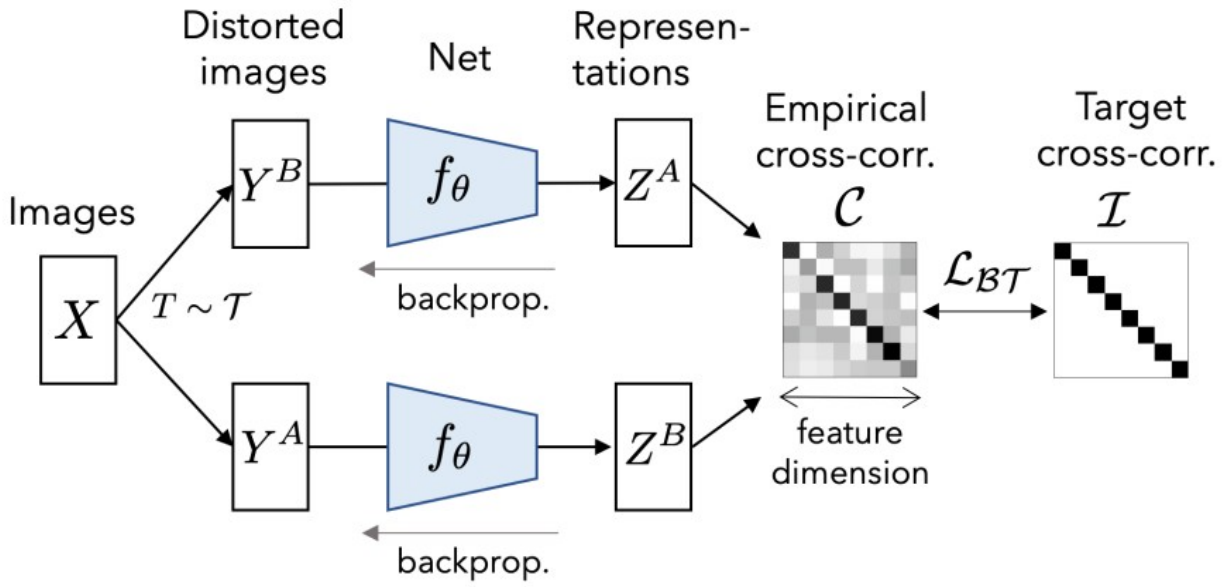
$$\mathcal{C}_{ij} \triangleq \frac{\sum_b z^A_{b,i} z^B_{b,j}}{\sqrt{\sum_b \left(z^A_{b,i}\right)^2} \sqrt{\sum_b \left(z^B_{b,j}\right)^2}}$$

$$\mathcal{L}_{\mathcal{BT}} \triangleq \underbrace{\sum_i (1 - \mathcal{C}_{ii})^2}_{\text{invariance term}} + \lambda \underbrace{\sum_i \sum_{j \neq i} \mathcal{C}_{ij}^2}_{\text{redundancy reduction term}}$$



Barlow Twins [Zbontar et al. ArXiv:2103.03230]

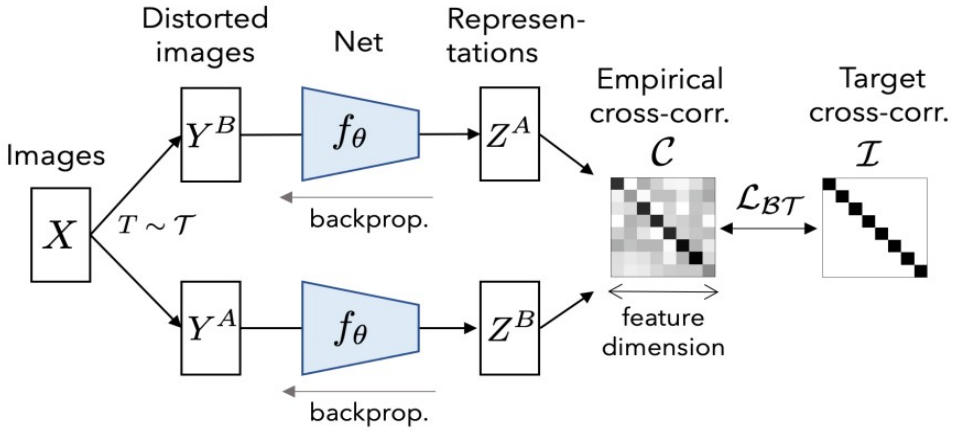
- Accuracy on ImageNet with linear classifier head
- Best accuracy for d=16,384 and batch-size=1024



Method	Top-1	Top-5
Supervised	76.5	
MoCo	60.6	
PIRL	63.6	-
SimCLR	69.3	89.0
MoCo v2	71.1	90.1
SimSiam	71.3	-
SwAV	71.8	-
BYOL	74.3	91.6
SwAV (w/ multi-crop)	75.3	-
Barlow Twins (ours)	73.2	91.0

Barlow Twins [Zbontar et al. ArXiv:2103.03230]

- Accuracy on ImageNet with linear classifier head



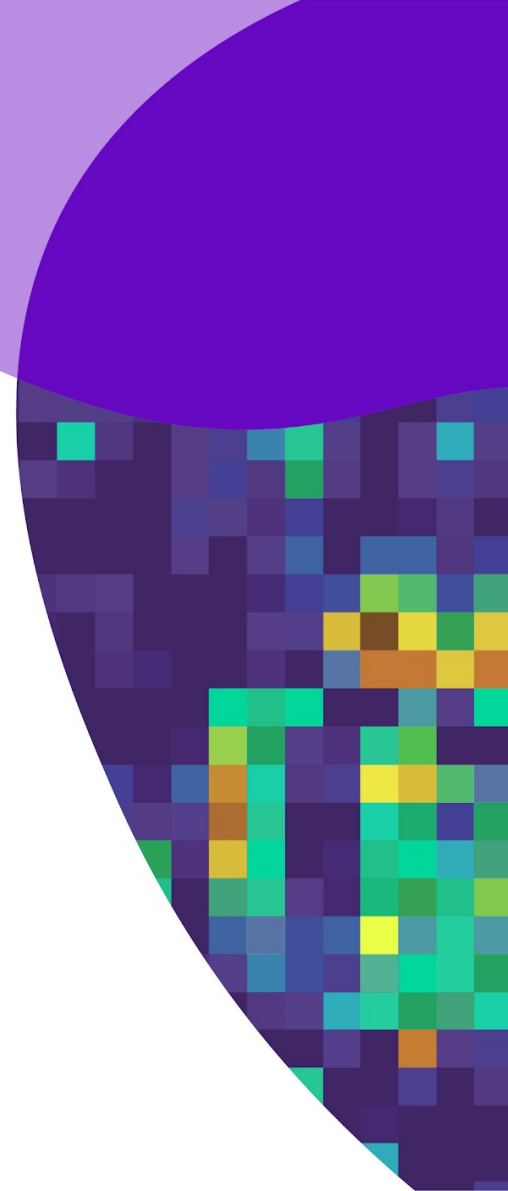
Method	Top-1		Top-5	
	1%	10%	1%	10%
Supervised	25.4	56.4	48.4	80.4
PIRL	-	-	57.2	83.8
SIMCLR	48.3	65.6	75.5	87.8
BYOL	53.2	68.8	78.4	89.0
SWAV (w/ multi-crop)	53.9	**70.2**	78.5	**89.9**
BARLOW TWINS (ours)	**55.0**	69.7	**79.2**	89.3

Method	VOC07+12 det			COCO det			COCO instance seg		
	AP_{all}	AP_{50}	AP_{75}	AP^{bb}	AP^{bb}_{50}	AP^{bb}_{75}	AP^{mk}	AP^{mk}_{50}	AP^{mk}_{75}
Sup.	53.5	81.3	58.8	38.2	58.2	41.2	33.3	54.7	35.2
MoCo-v2	**57.4**	82.5	**64.0**	**39.3**	58.9	**42.5**	**34.4**	55.8	36.5
SwAV	56.1	**82.6**	62.7	38.4	58.6	41.3	33.8	55.2	35.9
SimSiam	57	82.4	63.7	39.2	**59.3**	42.1	**34.4**	**56.0**	**36.7**
BT (ours)	56.8	**82.6**	63.4	39.2	59.0	**42.5**	34.3	**56.0**	36.5

FACEBOOK AI

Architectural EBM

Construct the machine so that the volume of low-energy space is fixed or limited.

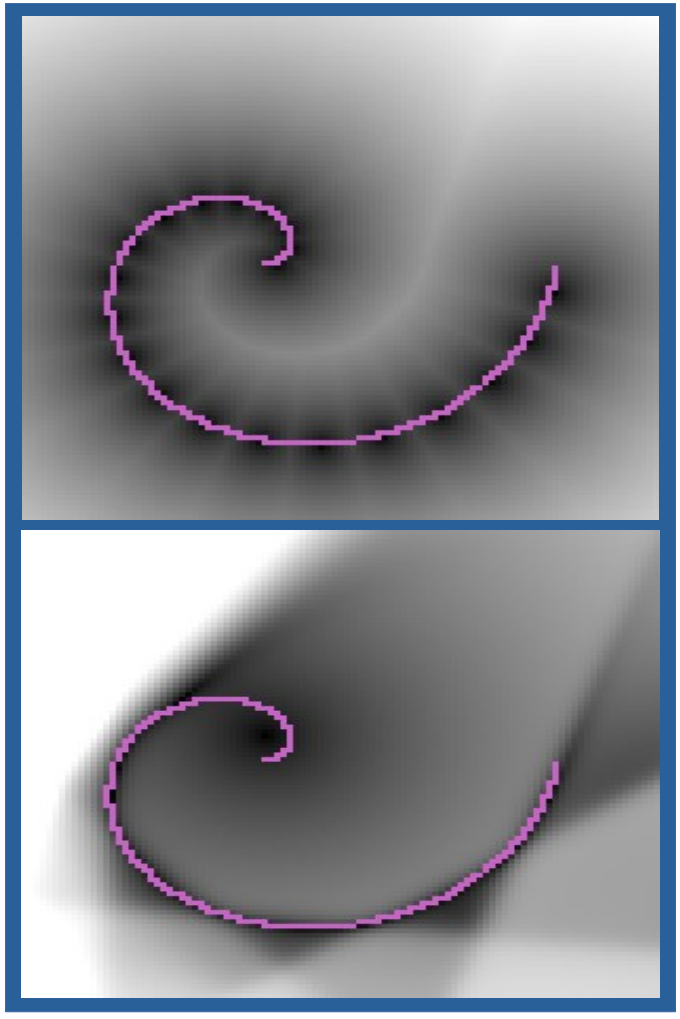


Architectural Methods & Regularized Methods

- **Basic ideas:**
  - Limiting the volume of low-energy space
  - limiting the information capacity of the representation

- **A1: build the machine so that the volume of the low energy regions is bounded:**
  - K-means, Gaussian Mixture Model, PCA, Bottleneck AE, Discretized AE (VQVAE),…

- **A2: regularize the volume of the low energy regions:**
  - Sparse coding, Sparse Auto-Encoder, LISTA, Variational Auto-Encoder.



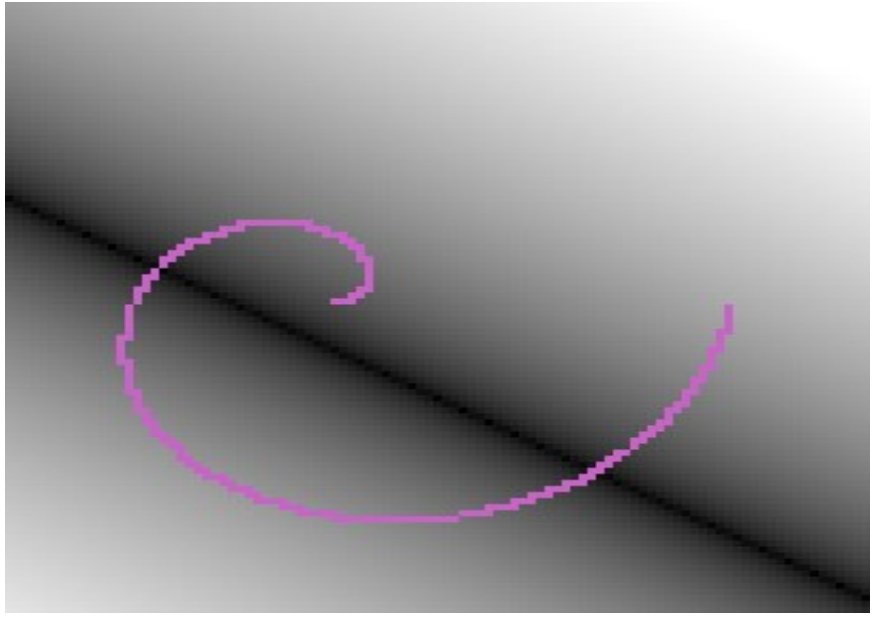
Architectural Methods

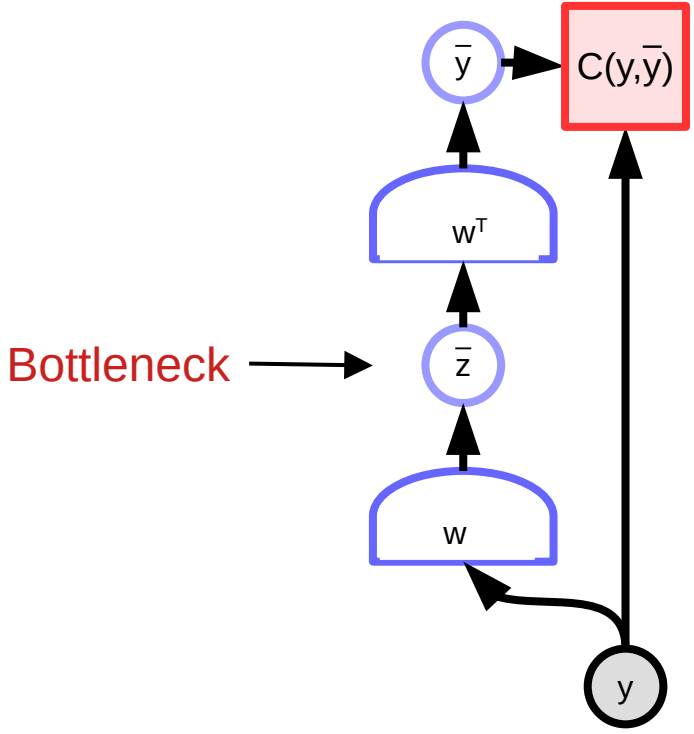
- **Architectural:** **[Different ways to limit the information capacity of the latent representation]**
  - A1: build the machine so that the volume of low energy space is bounded:
  - PCA: volume is dimension of principal subspace
  - K-means: volume limited by number of prototypes
  - Analytically normalized probabilistic models: volume is fixed

    Gaussian, and Gaussian Mixture Model (model is normalized)
  - Square Independent Component Analysis
  - Latent variable models with fixed latent distribution: volume is less than the "volume" (entropy) of the latent variable prior distribution.
    - Normalizing flows

Principal Component Analysis

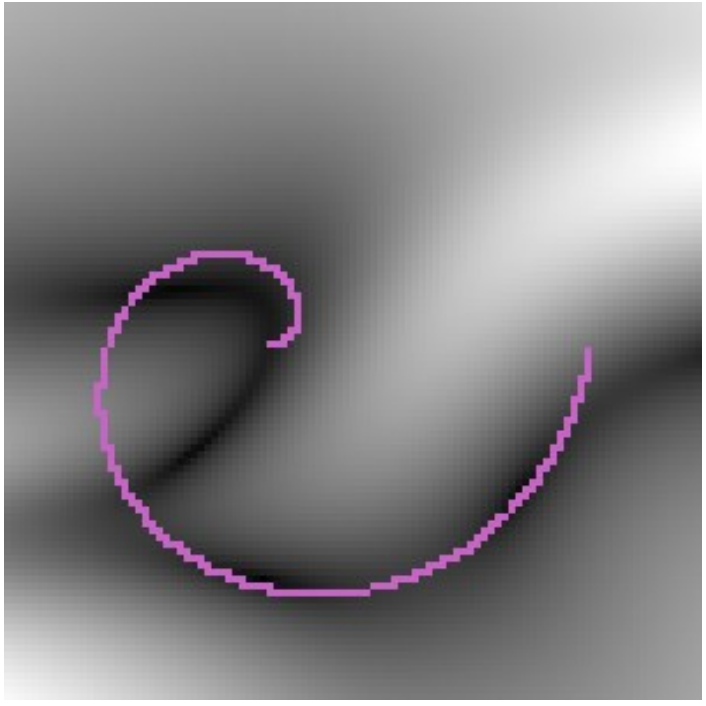
- **PCA is a 2-layer linear auto-encoder with a bottleneck.**
  - Energy: $F_w(y) = ||y - Dec(Enc(y))||^2 = ||y - w^T w||^2$
  - Loss $L(y, w) = F_w(y)$

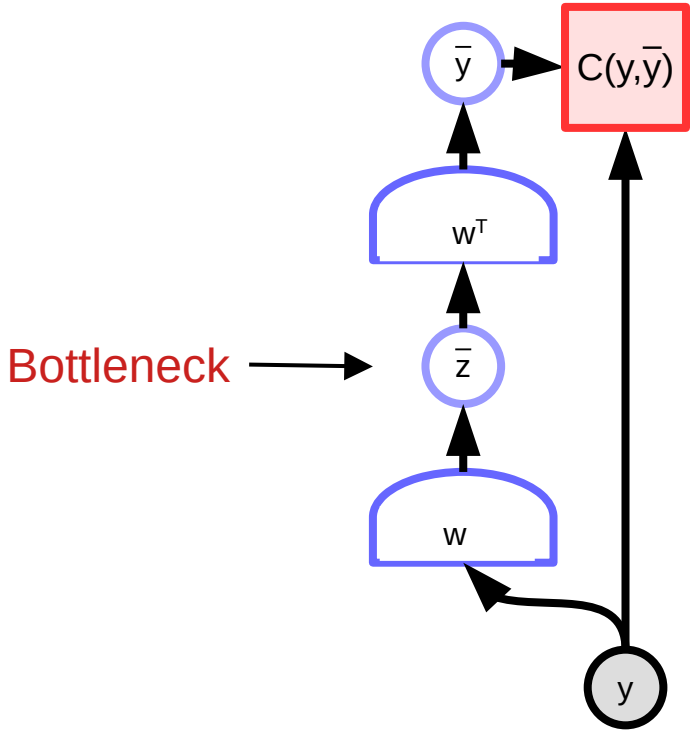




Auto-Encoder with Bottleneck

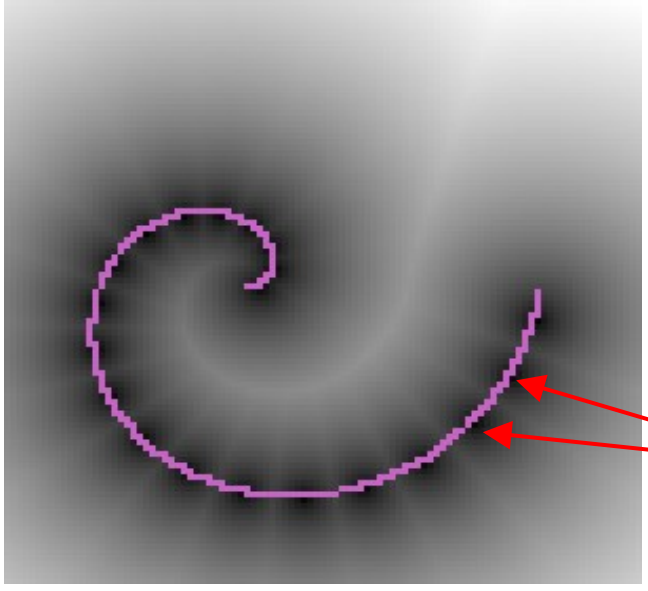
- **non-linear auto-encoder with a bottleneck.**
  - Energy: $F_w(y) = ||y - Dec(Enc(y))||^2$
  - Loss: $L(y, w) = F_w(y)$



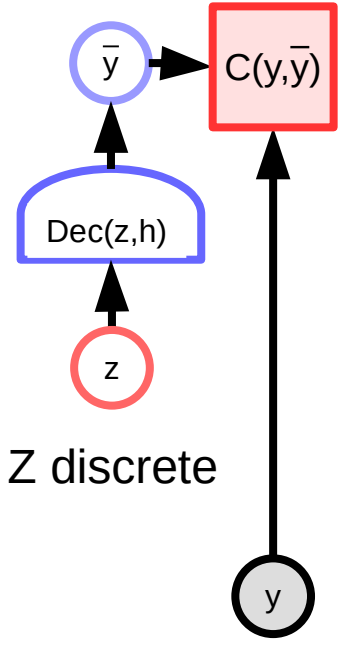


K-Means

- **Discrete latent-variable model with linear decoder**
  - Energy: $E(y,z) = ||y - Dec(z)||^2 = ||y - wz||^2$
  - Free Energy $F(y) = \min_{z \in \mathcal{Z}} E(y,z)$
  - Loss: $L(y,w) = F_w(y)$

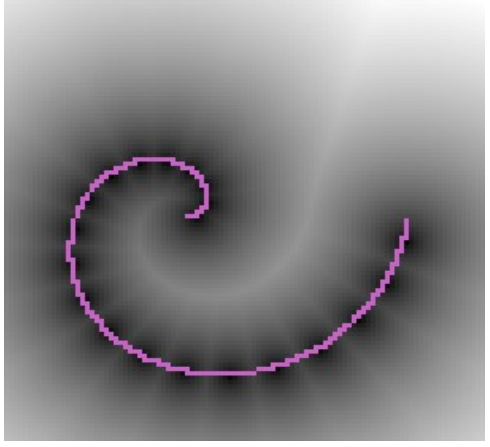


- Latent vector z is constrained to be a 1-hot vector: [0,0,..,01,0,..,0]
- 1 component selects a column of w
- F(y)=0 iff y is equal to a column of w.

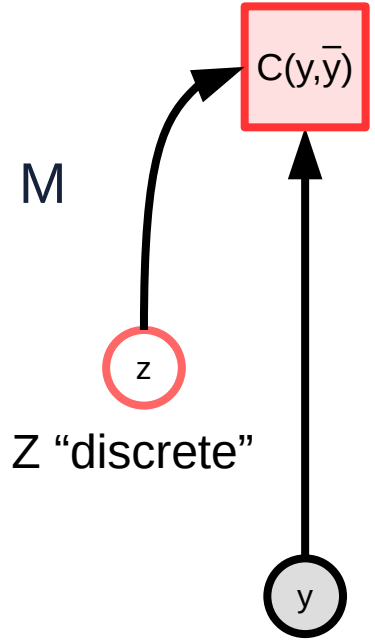


Gaussian Mixture Model

- **Similar to K-means with soft marginalization over latent.**
  - Energy: $E(y,z) = (y - wz)^T (Mz)(y - wz)$ $\quad (Mz)_{ij} = \sum_k M_{ijk} z_k$
  - Free Energy $\quad F(y) = -\frac{1}{\beta} \log \sum_{z \in \mathcal{Z}} e^{\beta E(y,z)}$
  - Loss: $L(y,w) = F_w(y)$ with normalization constraint on M



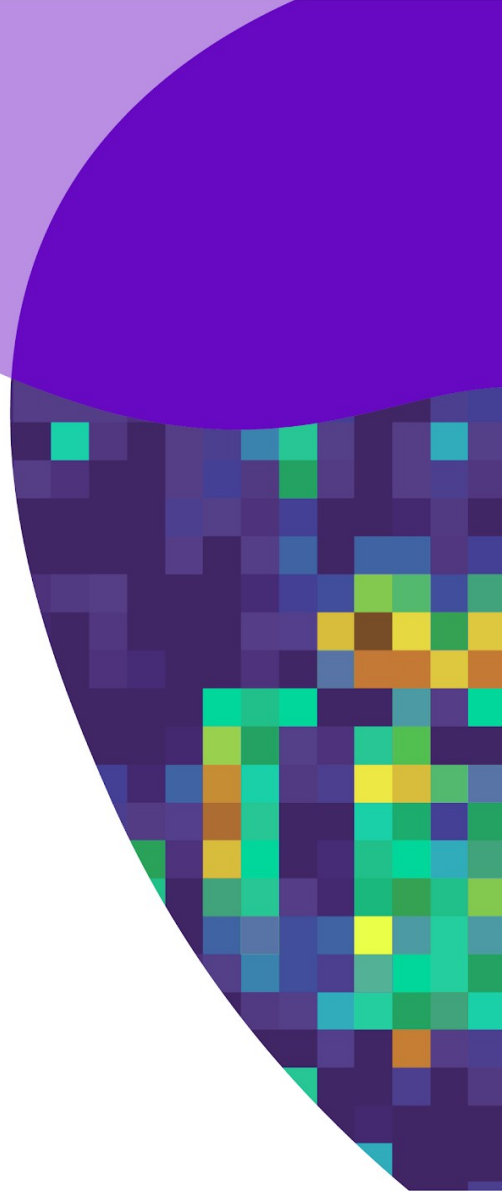
- Latent vector z is constrained to be a 1-hot vector: [0,0,..,01,0,..,0]
- But marginalization makes it “soft”



FACEBOOK AI

Generative Regularized Latent-Variable Architectures

1 predict y,
2 parameterize plausible y through a latent var z,
3 limit/regularize the information capacity of z

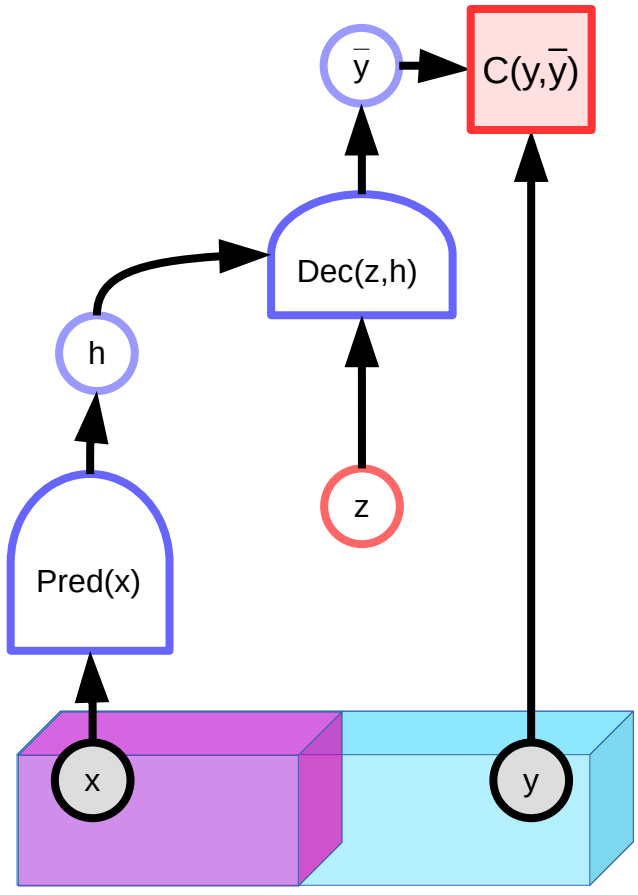


Prediction with Latent Variables

- **If the Latent has too much capacity...**
  - e.g. if it has the same dimension as y
- **... then the entire y space could be perfectly reconstructed**

$$E(x, y, z) = C(y, \mathrm{Dec}(\mathrm{Pred}(x), z))$$

- **For every y, there is always a z that will reconstruct it perfectly**
  - The energy function would be zero everywhere
  - This is no a good model….
- **Solution: limiting the information capacity of the latent variable z.**



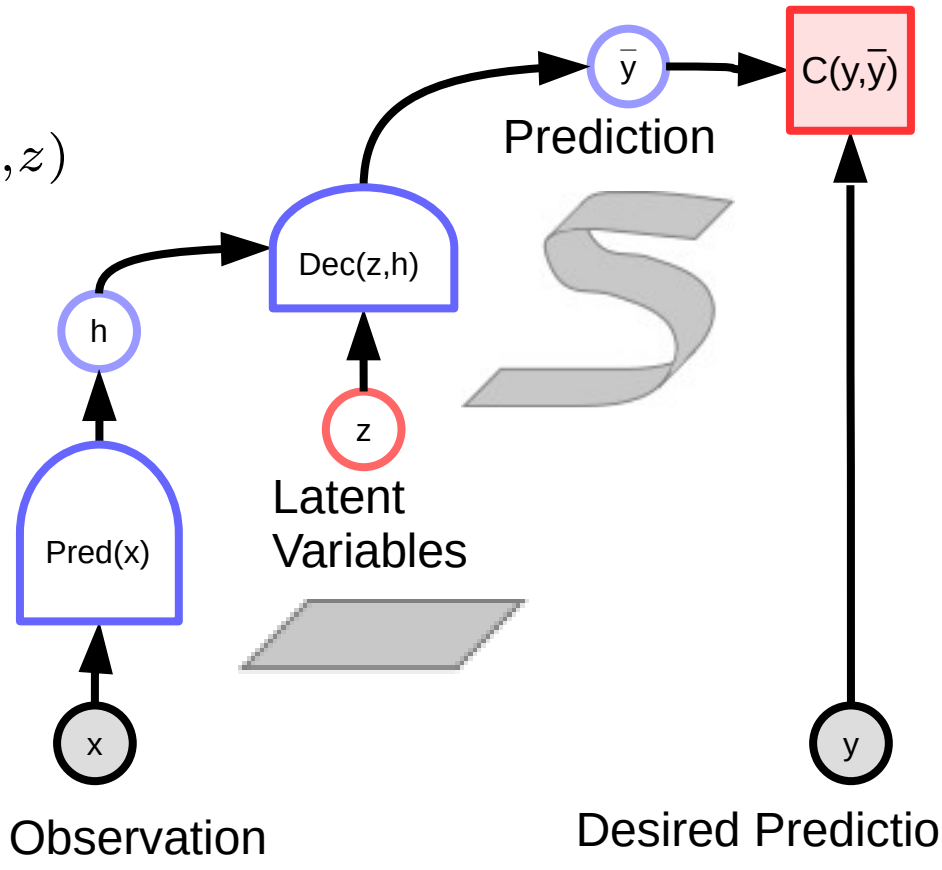
Architecture for Multimodal Output: latent variable EBM

- **Latent variables: parameterize the set of predictions**

$$F_\infty(x,y) = \text{argmin}_z E(x,y,z)$$

$$F_\beta(x,y) = -\frac{1}{\beta}\log\int_z e^{-\beta E(x,y,z)}$$

- **Ideally, the latent variable represents independent explanatory factors of variation of the prediction.**
- **The information capacity of the latent variable must be minimized.**
  - Otherwise all the information for the prediction will go into it.

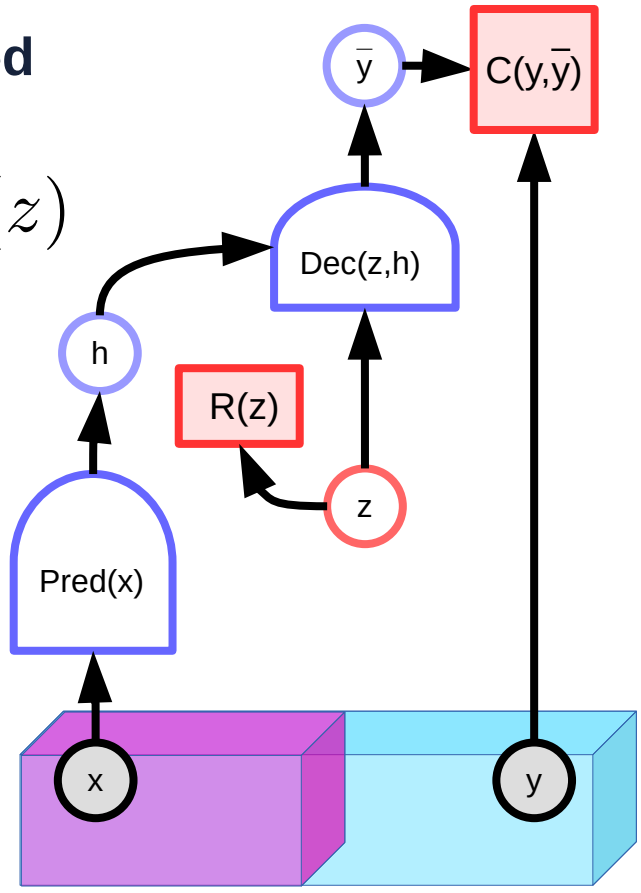


Regularized Latent Variable EBM

- **Regularizer R(z) limits the information capacity of z**
- **Without regularization, every y may be reconstructed exactly (flat energy surface)**

$$E(x, y, z) = C(y, \mathrm{Dec}(\mathrm{Pred}(x), z)) + \lambda R(z)$$

- **Examples of R(z):**
  - Effective dimension
  - Quantization / discretization
  - L0 norm (# of non-0 components)
  - L1 norm with decoder normalization
  - Maximize lateral inhibition / competition
  - Add noise to z while limiting its L2 norm (VAE)
  - <your_information_throttling_method_goes_here>

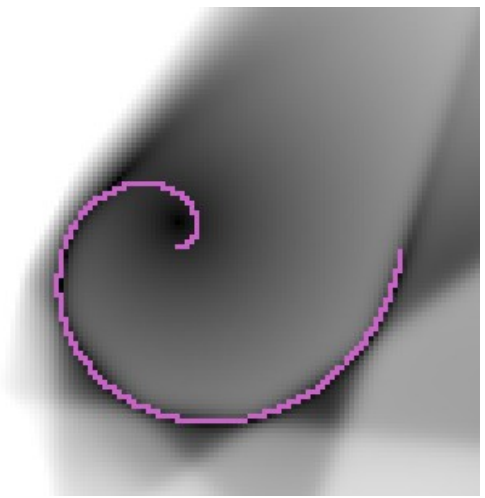


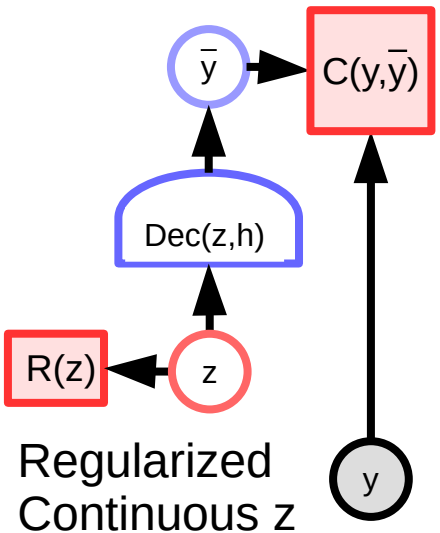
Regularized Latent Variable Methods: Sparse Coding

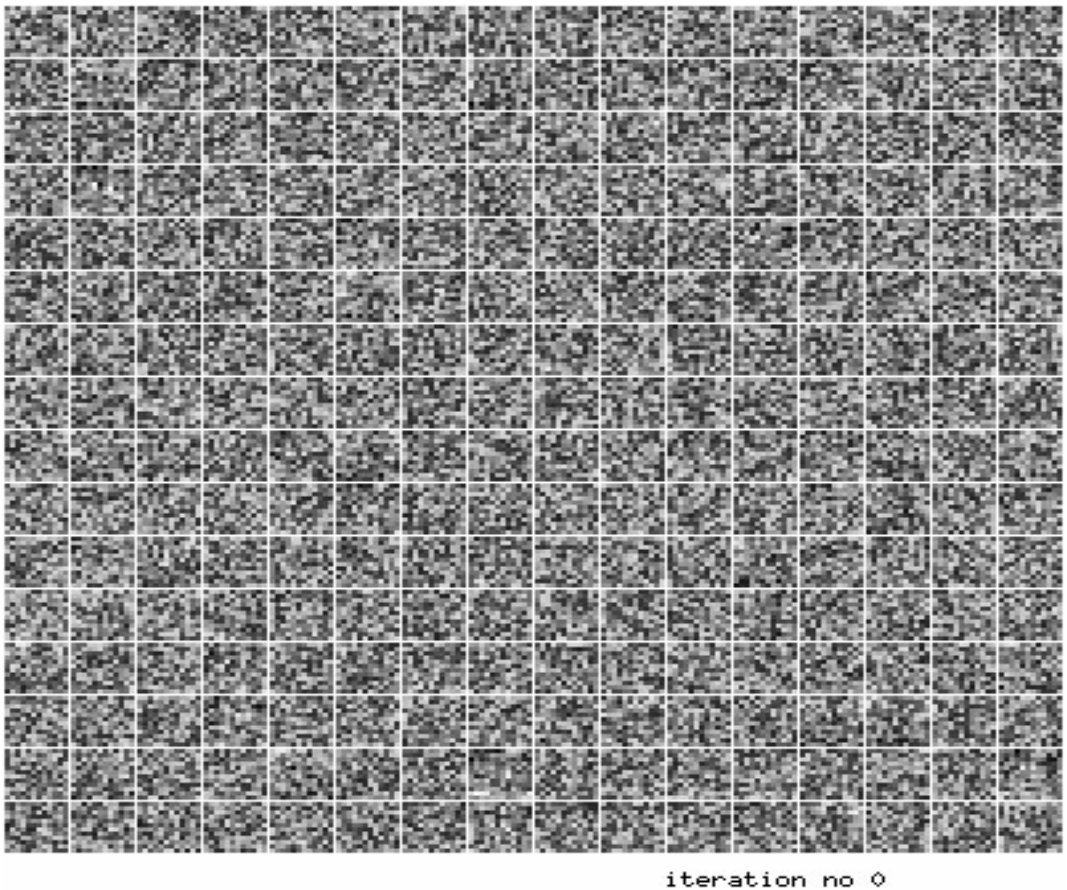
- **A2:** **regularize the volume of the low energy regions**

$$E(y,z) = ||y - wz||^2 + \lambda |z|_{L1|}$$

$$F(y) = \min_z E(y,z)$$

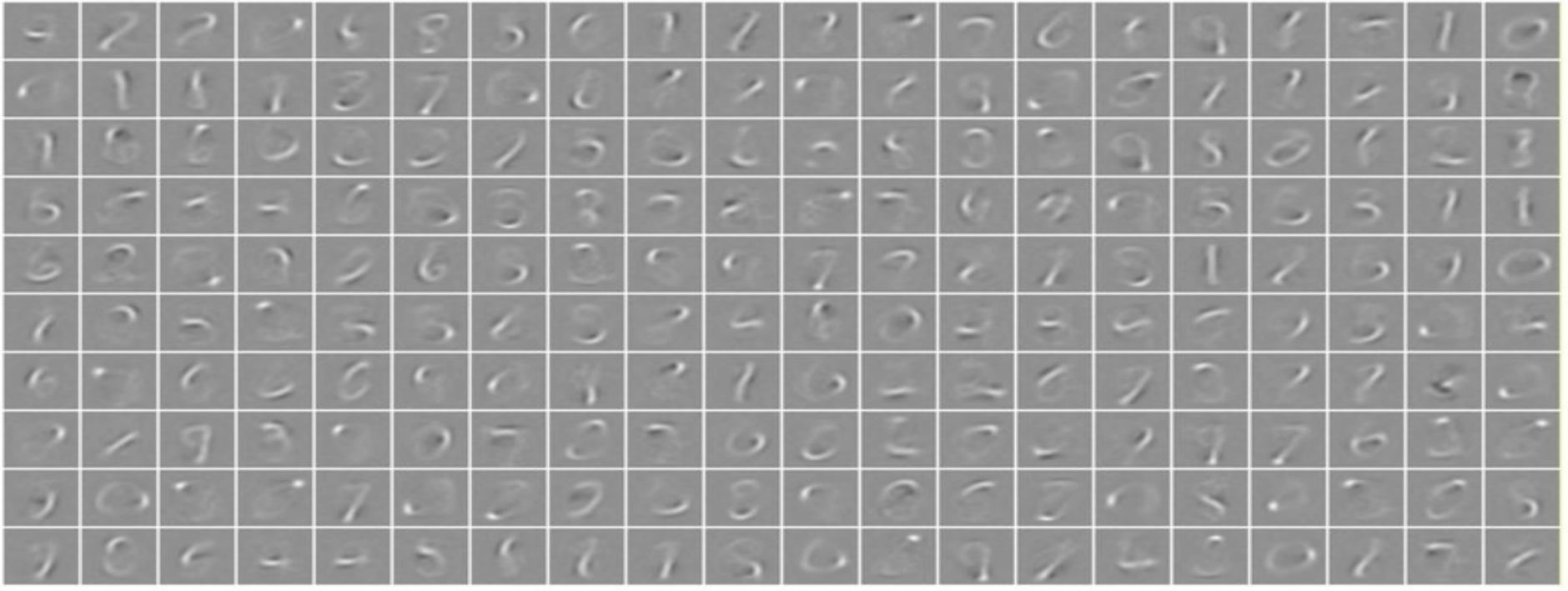






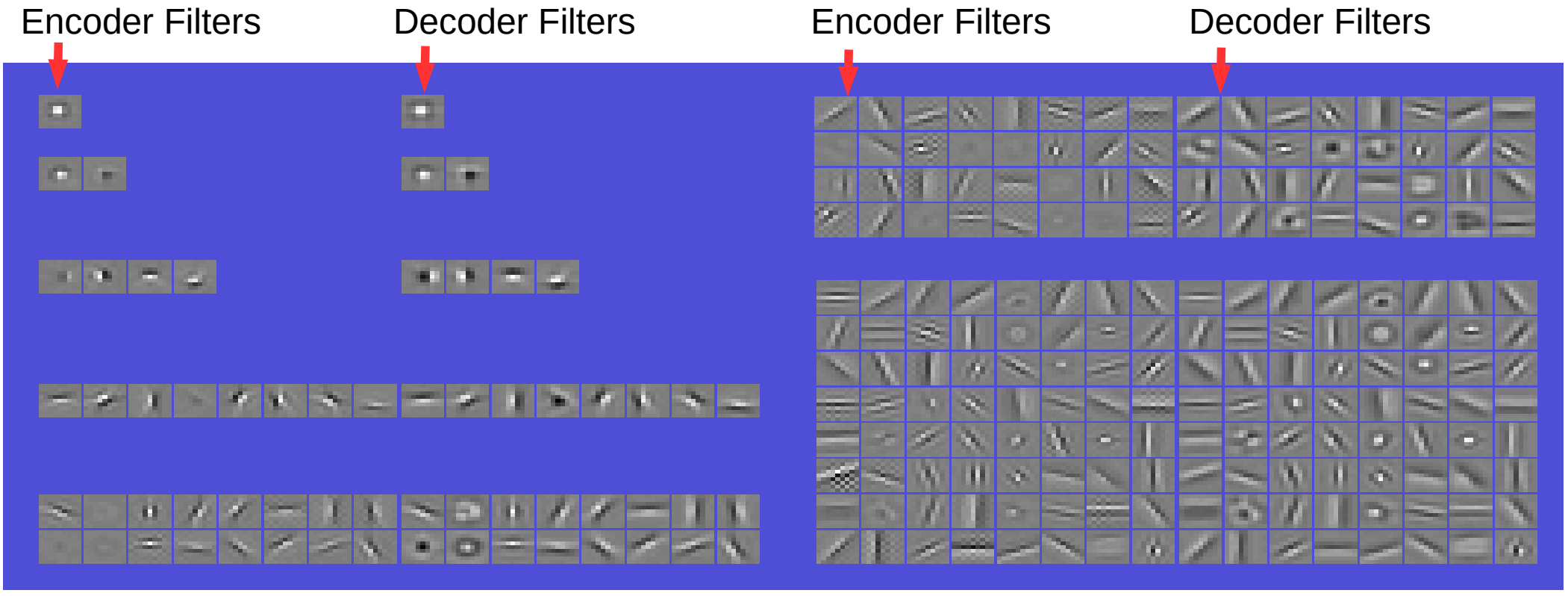
Sparse Modeling on handwritten digits (MNIST)

- **Basis functions (columns of decoder matrix) are digit parts**
- **All digits are a linear combination of a small number of these**



Convolutional Sparse Auto-Encoder on Natural Images

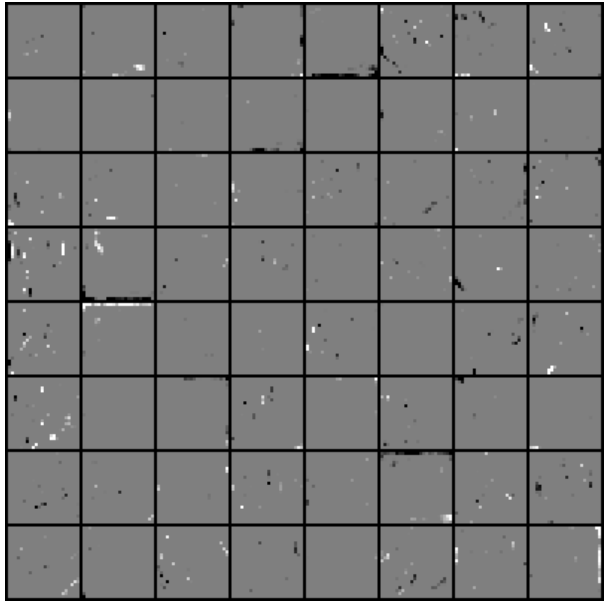
- **Filters and Basis Functions obtained. Linear decoder (conv)**
  - with 1, 2, 4, 8, 16, 32, and 64 filters [Kavukcuoglu NIPS 2010]



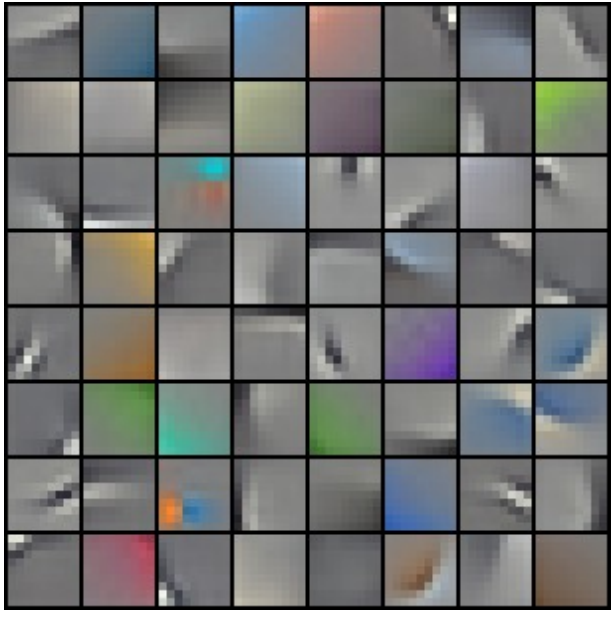
Convolutional Sparse Auto-Encoder on Natural Images

- **Trained on CIFAR 10 (32x32 color images)**
- **Architecture: Linear decoder, LISTA recurrent encoder**

sparse codes (z) from encoder



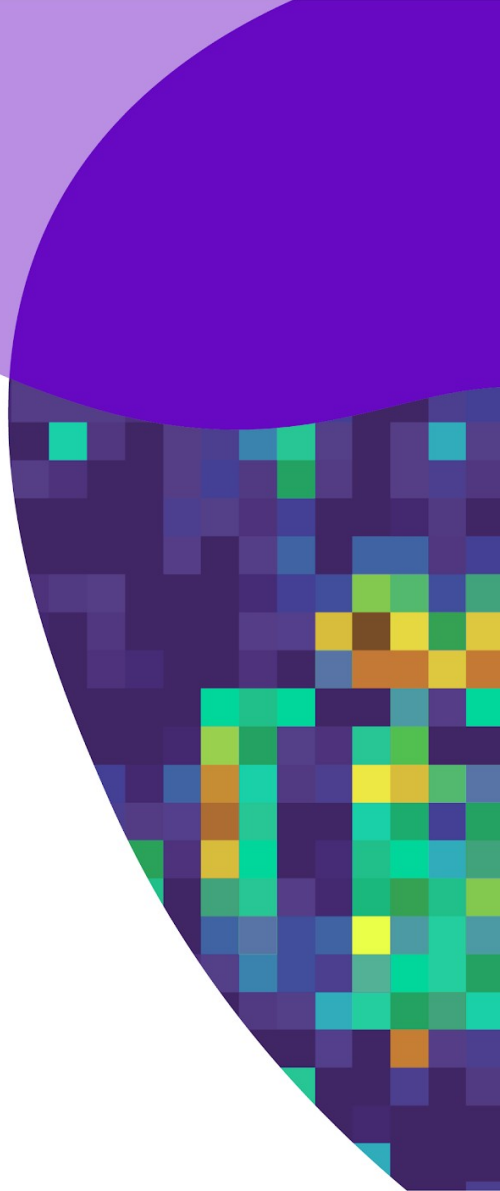
9x9 decoder kernels



FACEBOOK AI

Amortized Inference: Learning to predict the latent variable

Regularized auto-encoders:
Sparse AE
Variational AE



Amortized Inference

- **Training an encoder to give an approximate solution to the inference optimization problem**

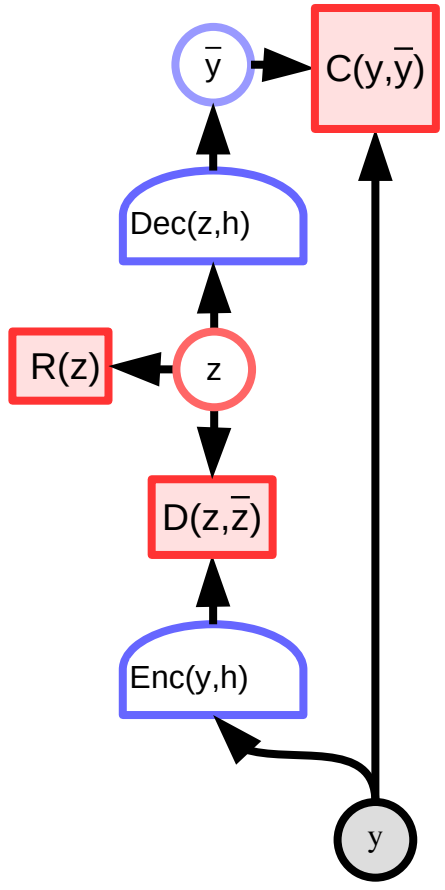
- **Regularized Auto-Encoder, Sparse AE, LISTA**

$$\mathrm{E(y,z)} = \mathrm{C(y,\ Dec((z))} + \mathrm{D(z,Enc(y))} + \lambda R(z)$$

$$F(y) = \min_z E(y,z)$$

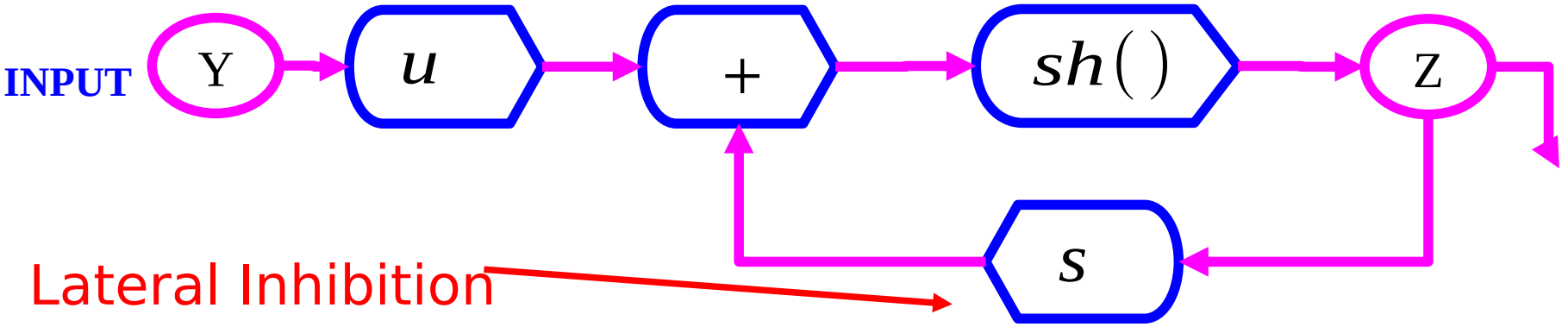
- **Variational AE**
  - Approximated by sampling and variational approximation

$$F(y) = -\log \int_z e^{-E(y,z)}$$



Giving the "right" structure to the encoder

- **ISTA/FISTA: iterative algorithm that converges to optimal sparse code**



$$z(t+1) = \text{Shrink}_{\alpha\eta}\left[z(t) - \eta w^t(wz(t) - y)\right]$$

- **ISTA/FastISTA reparameterized:**

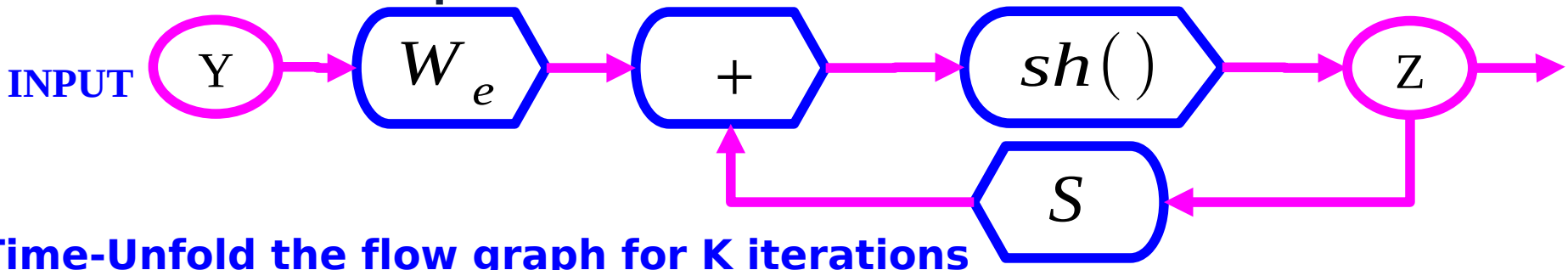
$$z(t+1) = \text{Shrink}_{\alpha\eta}\left[sz(t) + uy\right]; \quad u = \eta w; \quad s = I - \eta w^T w$$

- **LISTA (Learned ISTA): learn the We and S matrices to get fast solutions**

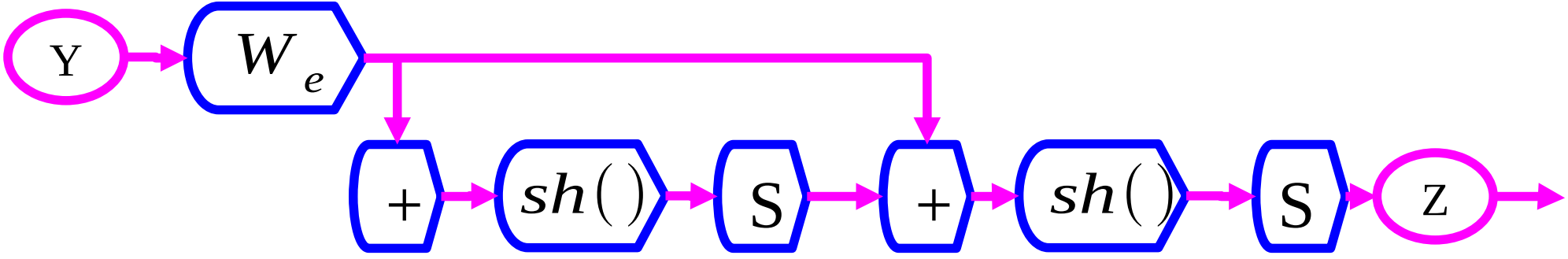
[Gregor & LeCun, ICML 2010], [Bronstein et al. ICML 2012], [Rolfe & LeCun ICLR 2013]

LISTA: Train We and S matrices to give a good approximation quickly

- **Think of the FISTA flow graph as a recurrent neural net where We and S are trainable parameters**



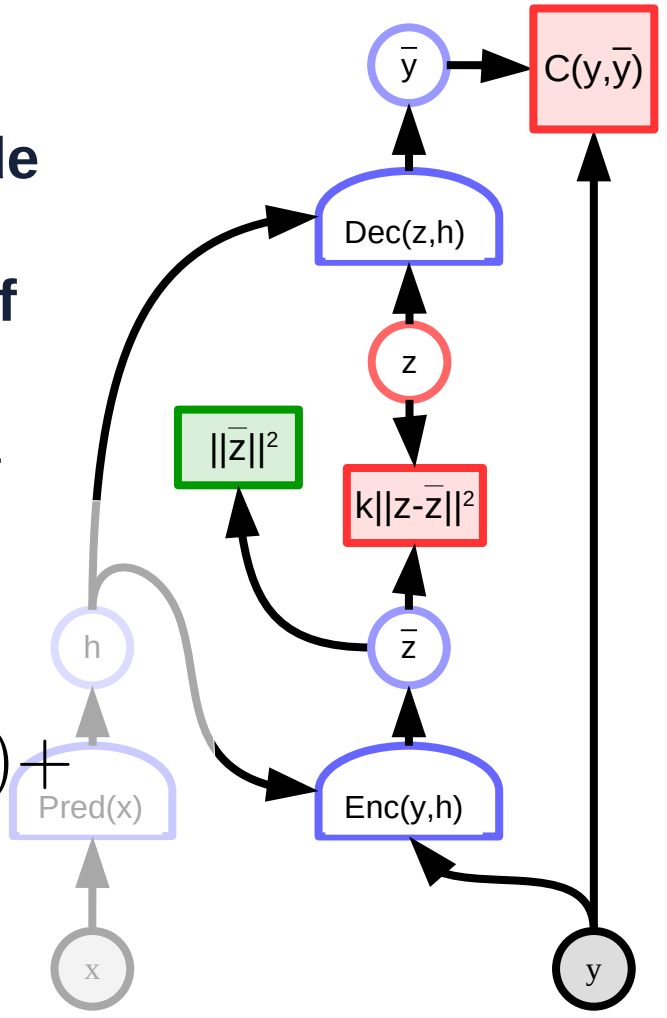
- **Time-Unfold the flow graph for K iterations**
- **Learn the We and S matrices with "backprop-through-time"**
- **Get the best approximate solution within K iterations**



Variational Auto-Encoder

- **Limiting the information capacity of the code by adding Gaussian noise**
- **The energy term $k||z-\bar{z}||^2$ is seen as the log of a prior from which to sample z**
- **The encoder output is regularized to have a mean and a variance close to zero.**

$$E(y,z) = C(y, Dec(z)) +$$
$$k(z - Enc(y))^T M(z - Enc(y)) +$$
$$\gamma ||Enc(y)||^2$$



Variational Auto-Encoder

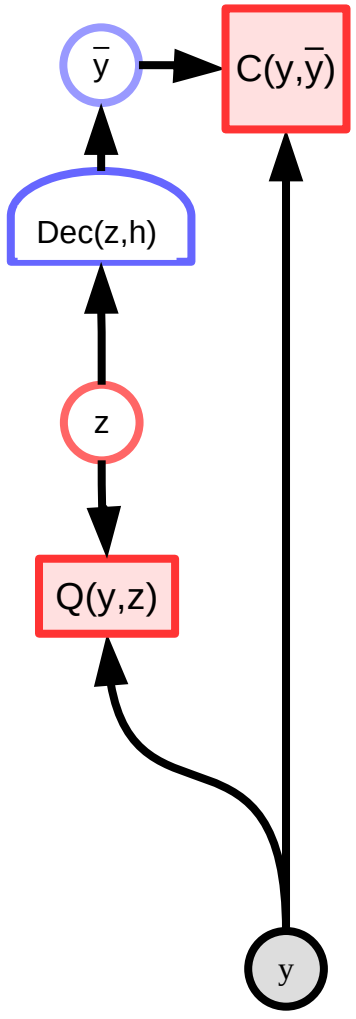
- **Variational approximation of marginalization over z**

$$E(y,z) = C(y, Dec(z))$$

$$F(y) = -\frac{1}{\beta}\log\int_z e^{-\beta E(y,z)}$$

$$F(y) = -\frac{1}{\beta}\log\int_z q(z|y)\left[\frac{e^{-\beta E(y,z)}}{q(z|y)}\right]$$

$$q(z|y) = \frac{e^{-\beta Q(y,z)}}{\int_{z'} e^{-\beta Q(y,z')}}$$



Variational Auto-Encoder

- **Variational approximation of marginalization over z**

$$F(y) = -\frac{1}{\beta} \log \int_z q(z|y) \frac{e^{-\beta E(y,z)}}{q(z|y)}$$

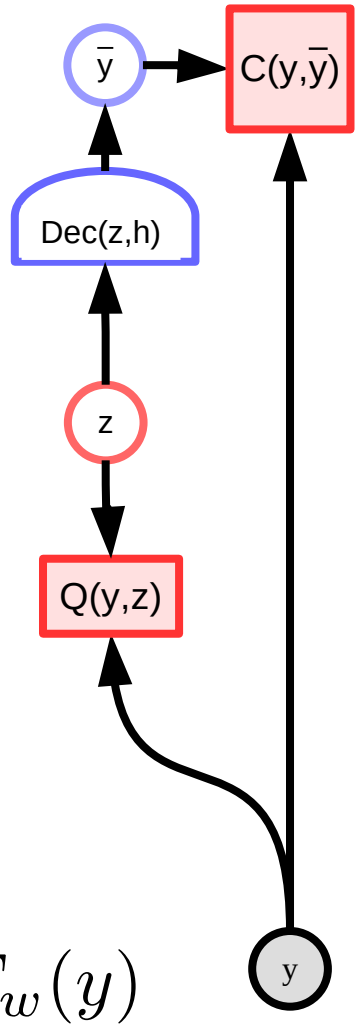
Jensen's inequality: log(average()) < average(log())

$$F(y) \leq \tilde{F}(y) = \int_z q(z|y) \left[-\frac{1}{\beta} \log \frac{e^{-\beta E(y,z)}}{q(z|y)} \right]$$

$$\tilde{F}(y) = \int_z q(z|y) E(y,z) + \frac{1}{\beta} \int_z q(z|y) \log(q(z|y))$$

$$F = \langle E \rangle - TS$$

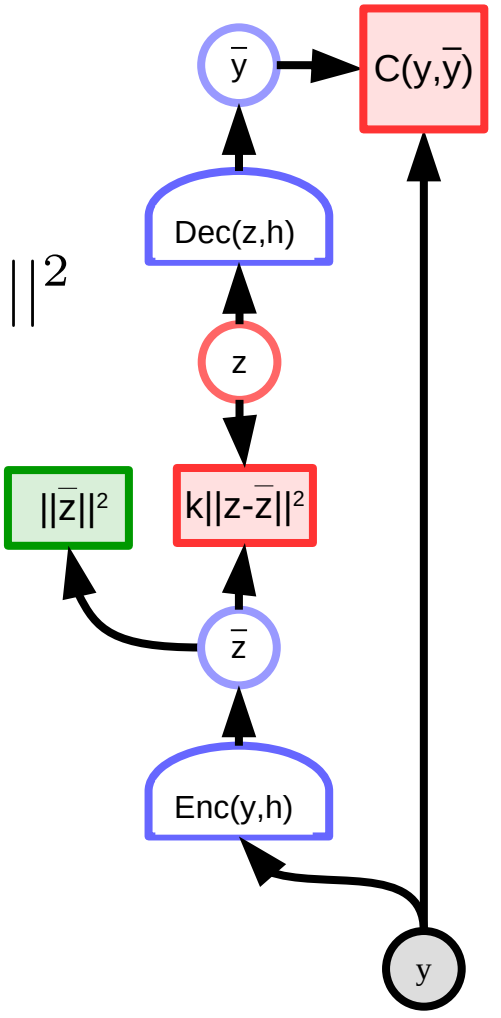
$$L(w) = F_w(y)$$



Variational Auto-Encoder

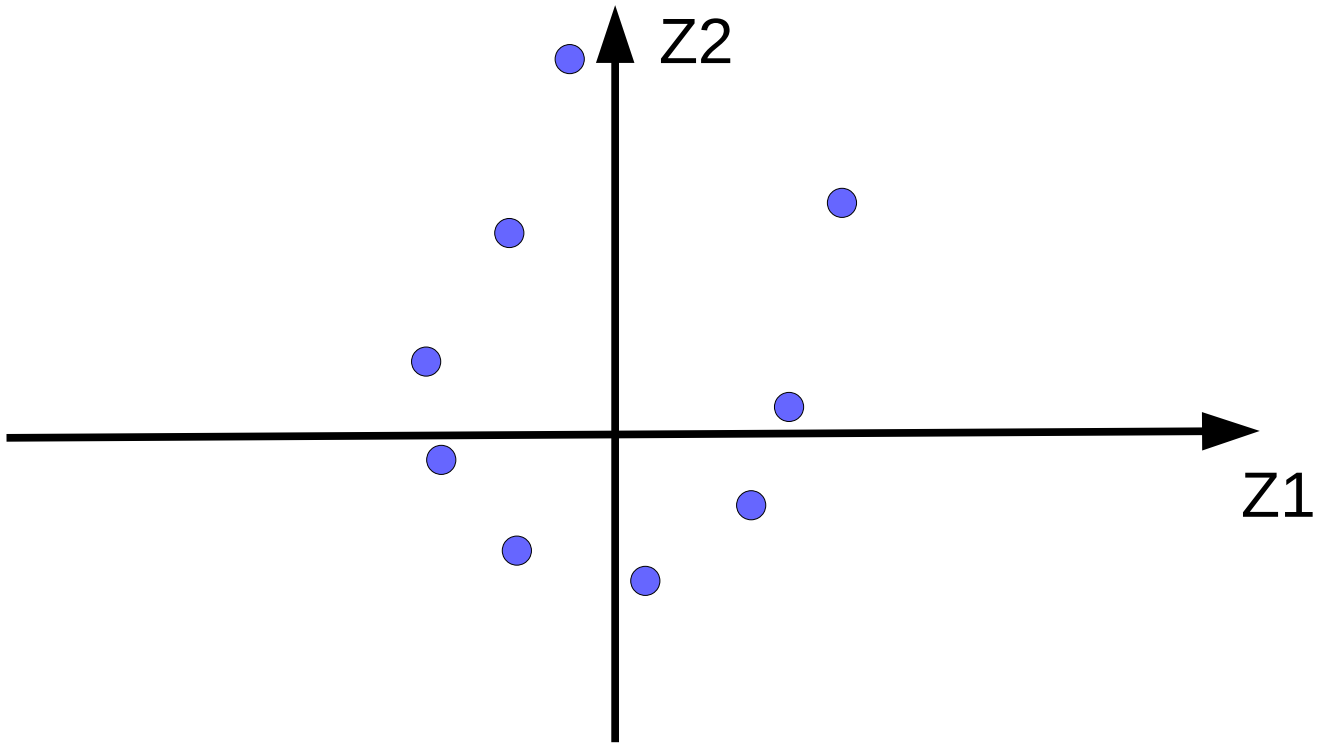
- **Q(y,z) is quadratic, q(z|y) is Gaussian.**

$$\mathrm{Q(y,z)} = (\mathrm{z\text{-}Enc(y)})^T M(z - Enc(y)) + \gamma||Enc(y)||^2$$



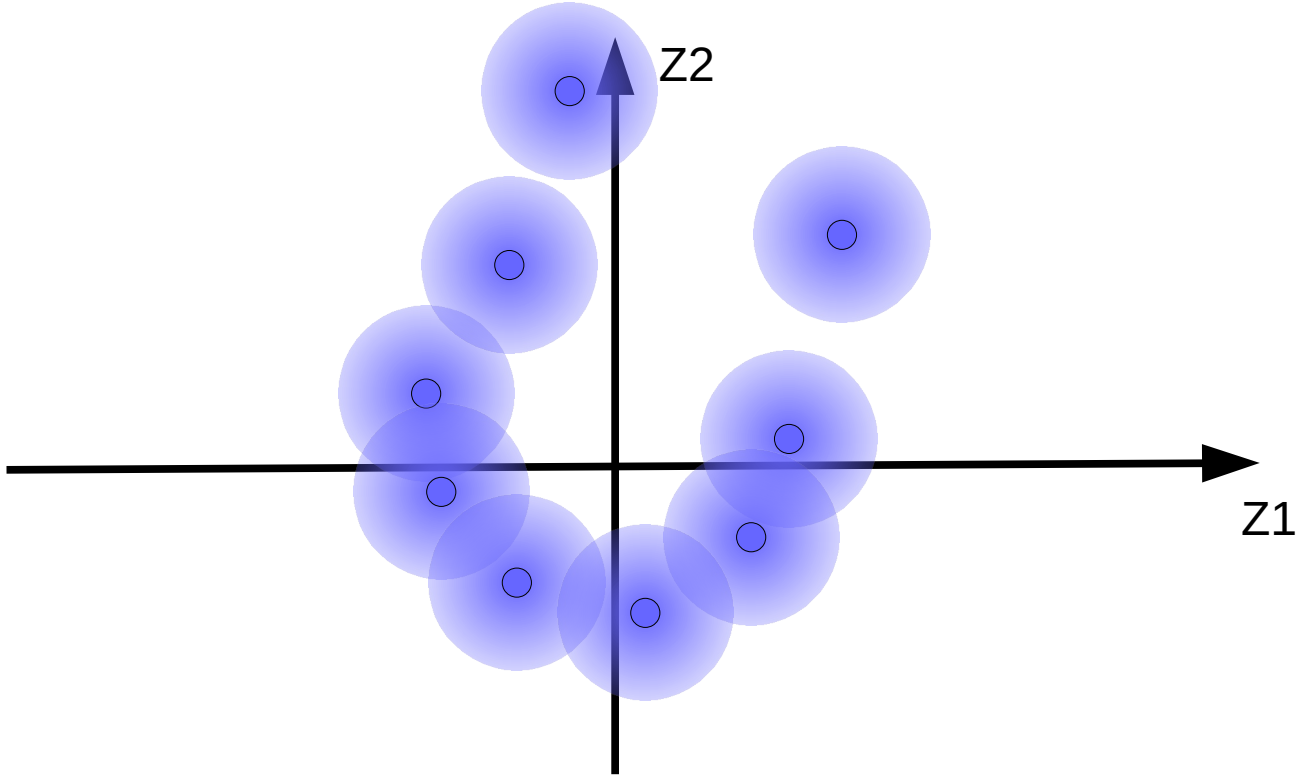
Variational Auto-Encoder

- **Code vectors for training samples**



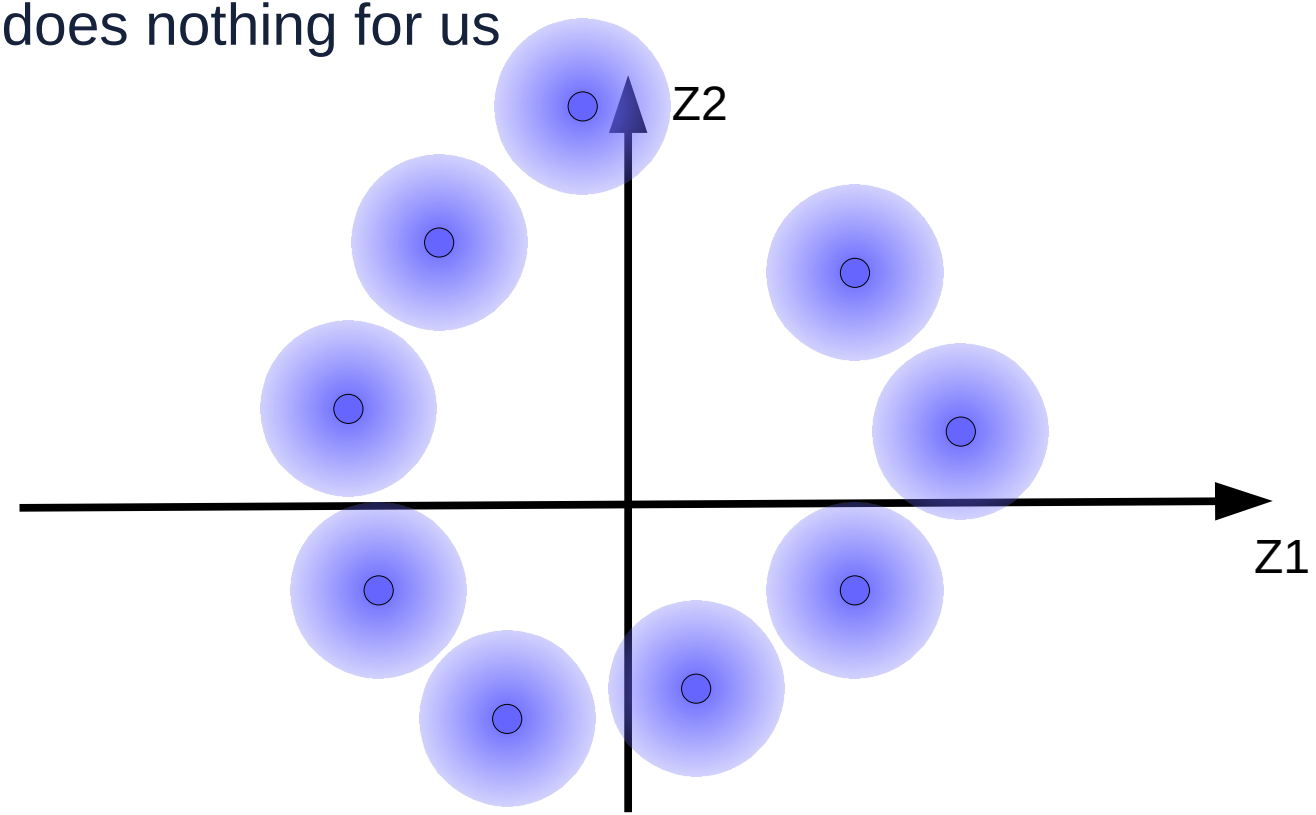
Variational Auto-Encoder

- **Code vectors for training sample with Gaussian noise**
  - Some fuzzy balls overlap, causing bad reconstructions



Variational Auto-Encoder

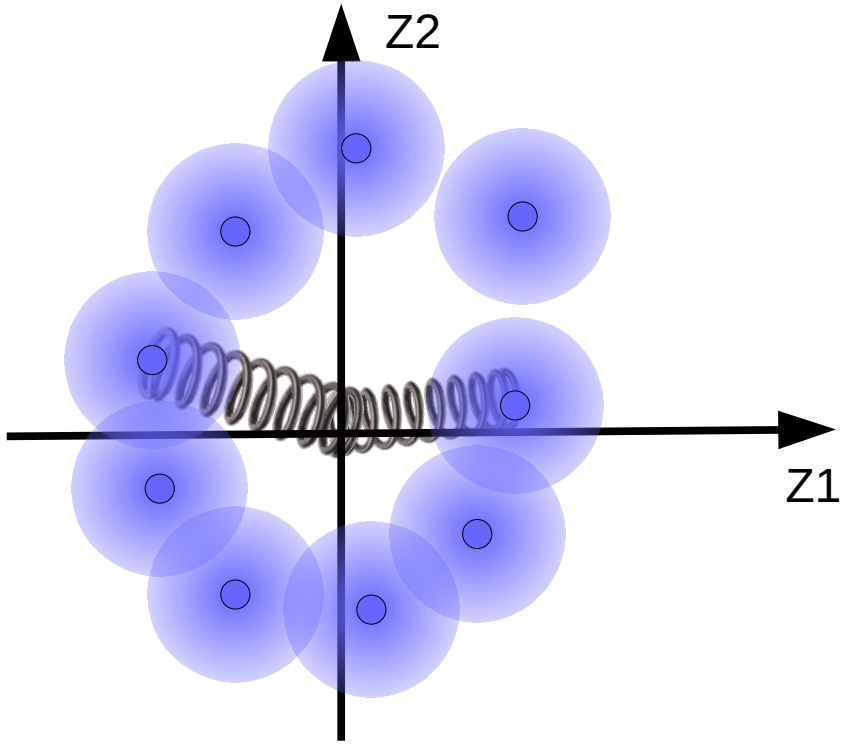
- **The code vectors want to move away from each other to minimize reconstruction error**
  - But that does nothing for us



Variational Auto-Encoder

- **Attach the balls to the center with a sping, so they don't fly away**
  - Minimize the square distances of the balls to the origin
- **Center the balls around the origin**
  - Make the center of mass zero
- **Make the sizes of the balls close to 1 in each dimension**
  - Through a so-called KL term

Talia Konkle

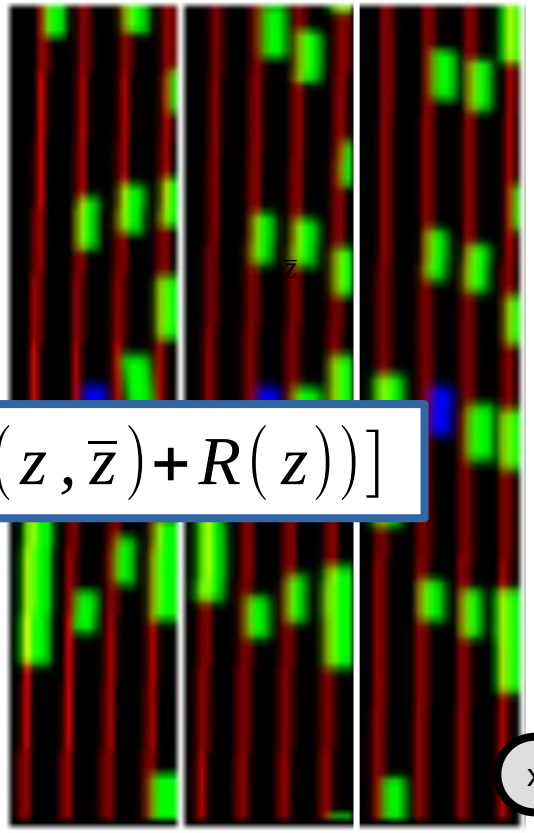


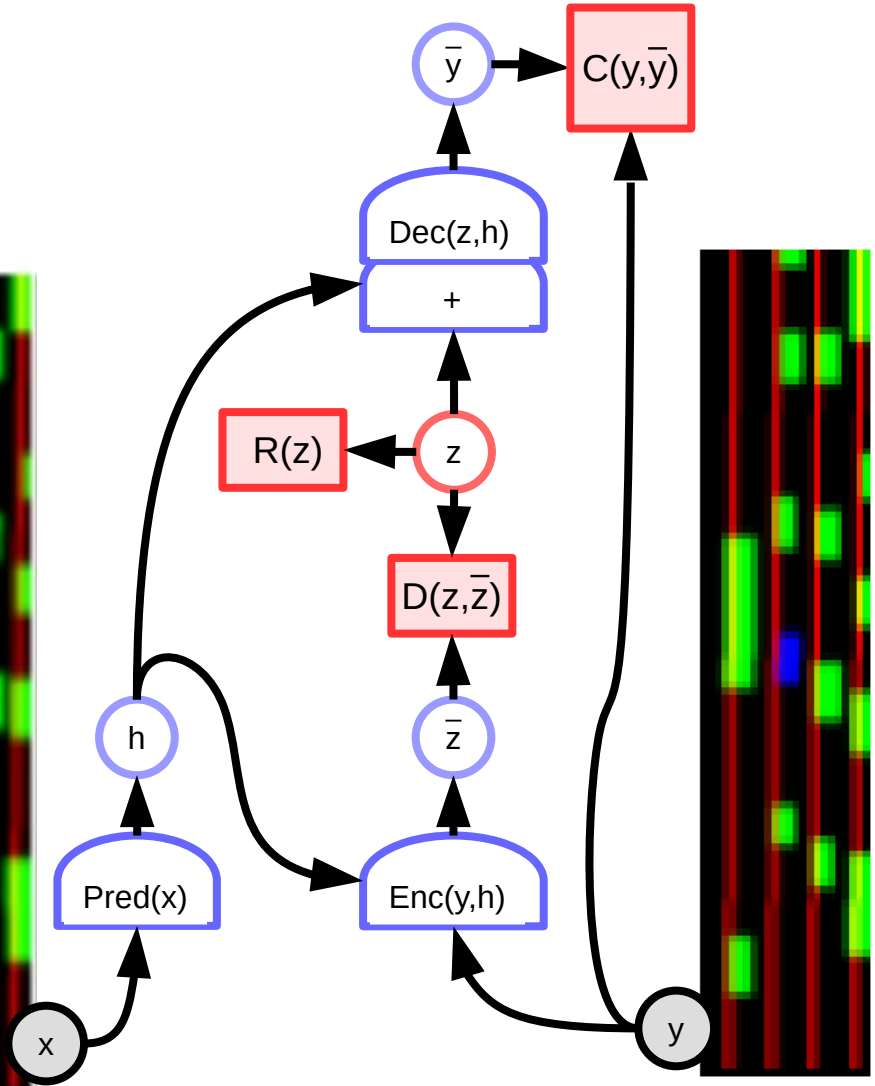
Conditional VAE + Drop Out

- **Training:**
  - Observe frames
  - Compute h
  - Predict $\bar{z}$ from encoder
  - Sample z, with:

$$P(z/\bar{z}) \propto \exp[-\beta(D(z,\bar{z})+R(z))]$$

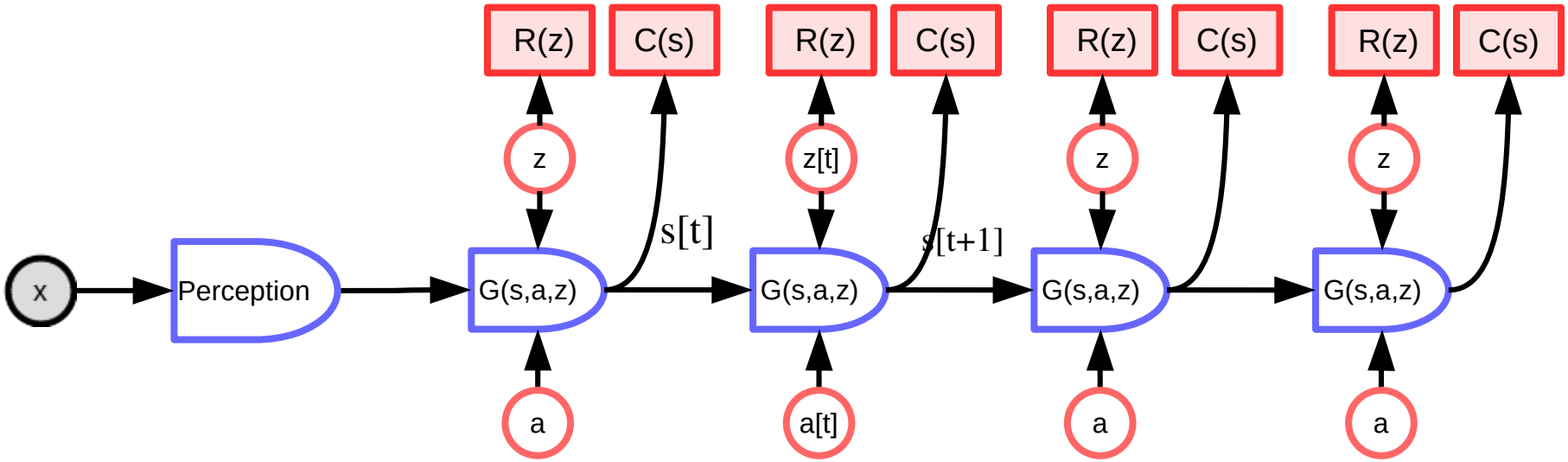
  - Half the time, set z=0
  - Predict next frame
  - backprop





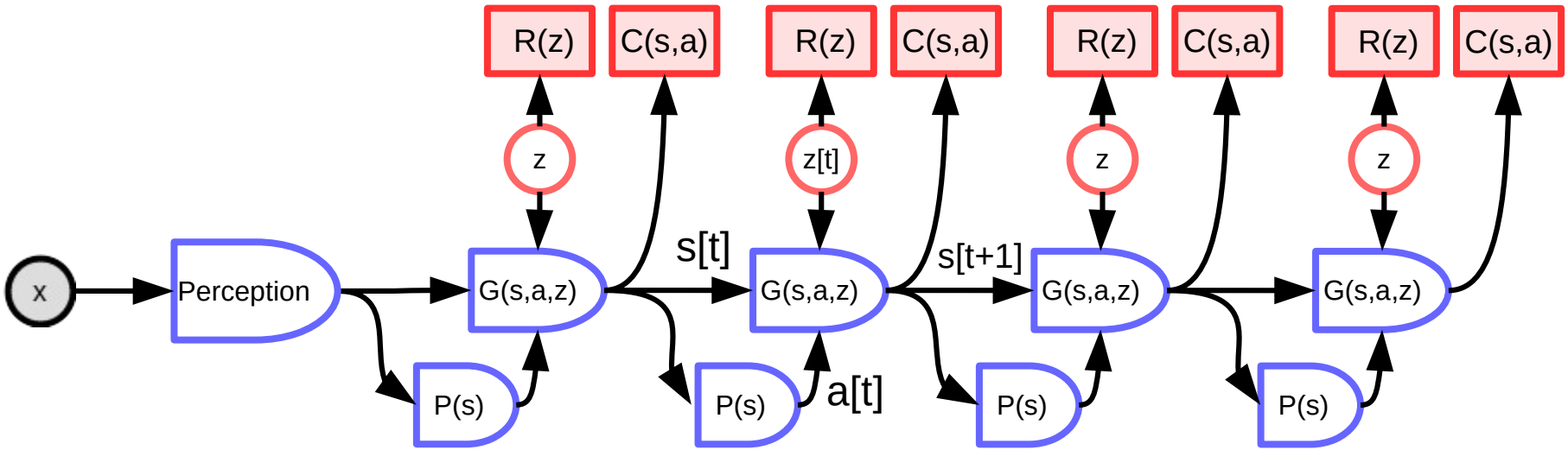
Forward Model for Model-Predictive Control

- **Forward model: s[t+1] = G(s[t], a[t], z[t])**
- **Cost/Energy: f[t] = C(s[t])**
- **Latent variable z sampled from q(z) proportional to exp(-R(z))**
- **Optimize (a[1],a[2]…,a[T]) = argmin Σ_t C(s[t])**
  through backprop (== Kelley-Bryson adjoint state method)



Forward Model for Gradient-Based Policy Learning

- **Forward model: s[t+1] = G(s[t], a[t], z[t])**
- **Cost/Energy: f[t] = C(s[t],a[t])**
- **Latent variable z sampled from q(z) proportional to exp(-R(z))**
- **Policy: a[t] = P(s[t])**
- **Learn P through backprop (== Kelley-Bryson adjoint state method)**



Conclusion

- **SSL is the future of representation learning**
  - Contrastive reconstruction-based SSL works very well in NLP
  - Contrastive prediction-based SSL works well in speech
  - Reconstruction/prediction does not work well for images
  - Joint embedding methods work better for images.
  - Contrastive joint embedding is too expensive
  - The most promising methods are non contrastive:
    - Distillation (BYOL, SimSiam), Clustering (SwAV), infomax (Barlow Twins)
- **SSL can be used to learn world models under uncertainty**
  - Regularized latent variable models (e.g VAE).

World models for autonomous AI systems

- **World Model: predicts future states**
- **Critic: predicts expected objective**
- **Cost: computes objective**
- **Perception: estimates world state**
- **Actor: computes action**

- **We only have one world model engine!**

- **Configurator: configures the world model engine for the situation at hand.**