Deep Learning

MLSS 2015
Austin, Texas

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Outline of the Tutorial

1. Representation Learning, motivations
2. Algorithms
   - Feedforward deep networks
   - Convolutional nets
   - Recurrent and recursive nets
   - Generative nets
3. Practical Considerations and Applications
4. Challenges

Upcoming book: "Deep Learning" http://www.iro.umontreal.ca/~bengioy/dlbook/ for draft chapters of the book and http://www.iro.umontreal.ca/~bengioy/talks/ for slides

Ultimate Goals

- **AI**
- Needs **knowledge**
- Needs **learning**
  (involves priors + ***optimization****/search*)
- Needs **generalization**
  (guessing where probability mass concentrates)
- Needs ways to fight the curse of dimensionality
  (exponentially many configurations of the variables to consider)
- Needs disentangling the underlying explanatory factors
  (making sense of the data)

Breakthrough

- **Deep Learning: machine learning algorithms inspired by brains, based on learning multiple levels of representation / abstraction.**

Impact

Deep learning has revolutionized

- **Speech recognition**
- **Object recognition**

More coming, including other areas of computer vision, NLP, dialogue, reinforcement learning…

Part 1

Motivations for Representation Learning and Deep Learning

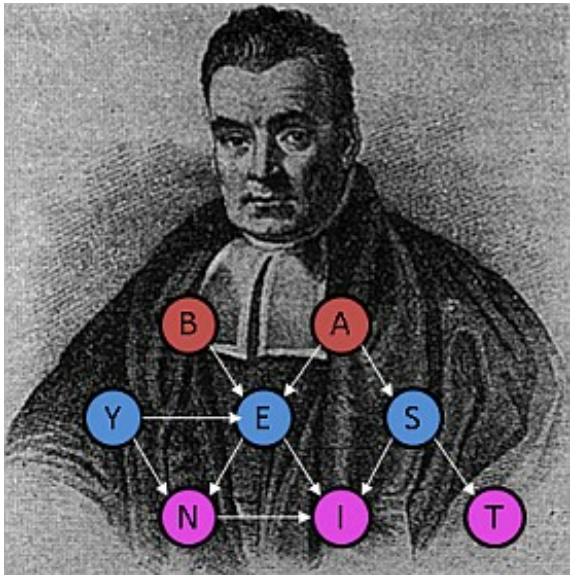
Representation Learning

- Good **features** essential for successful ML: 90% of effort

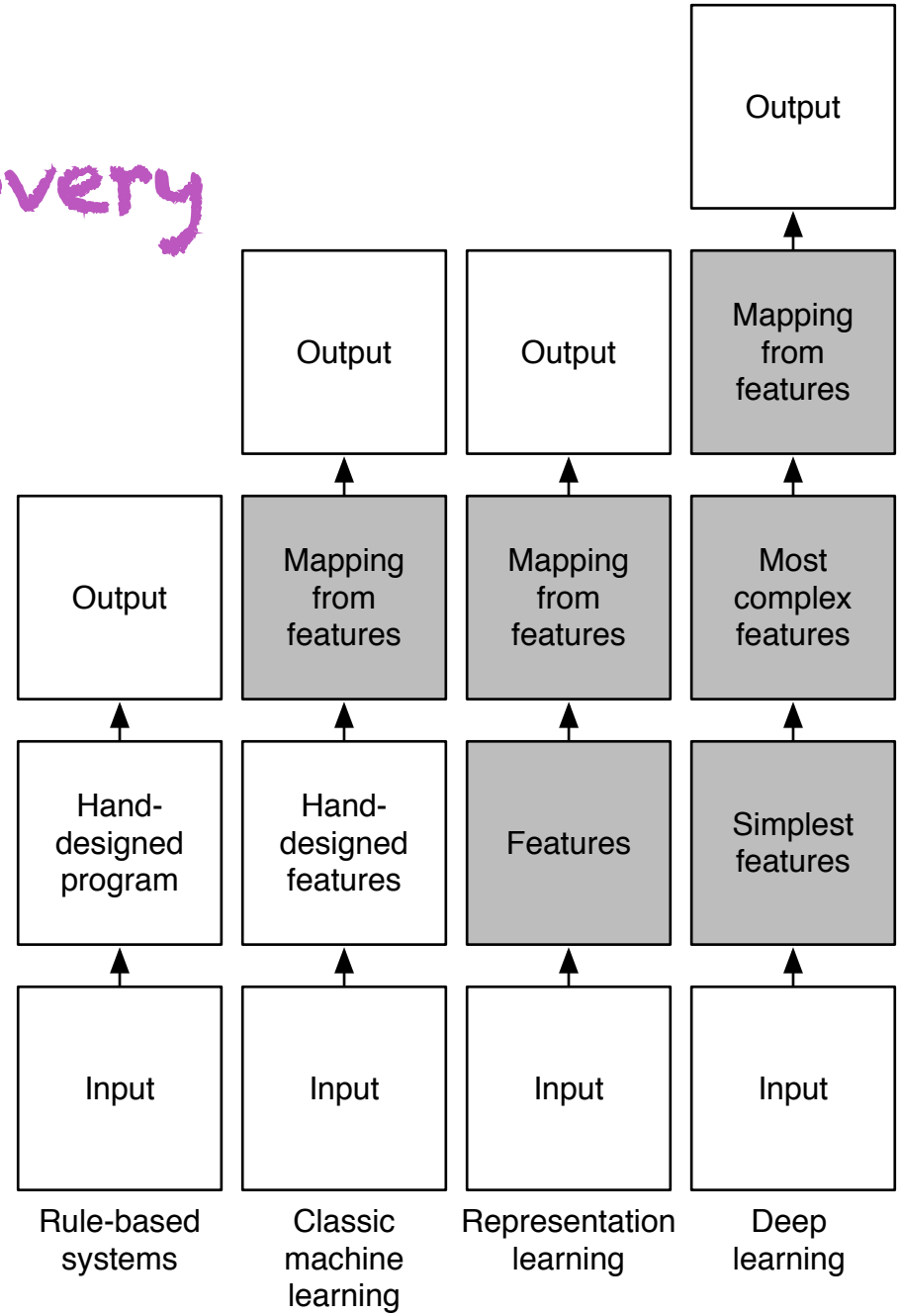
- Handcrafting features vs learning them

- Good representation?
- guesses

  the features / factors / causes



Automating Feature Discovery

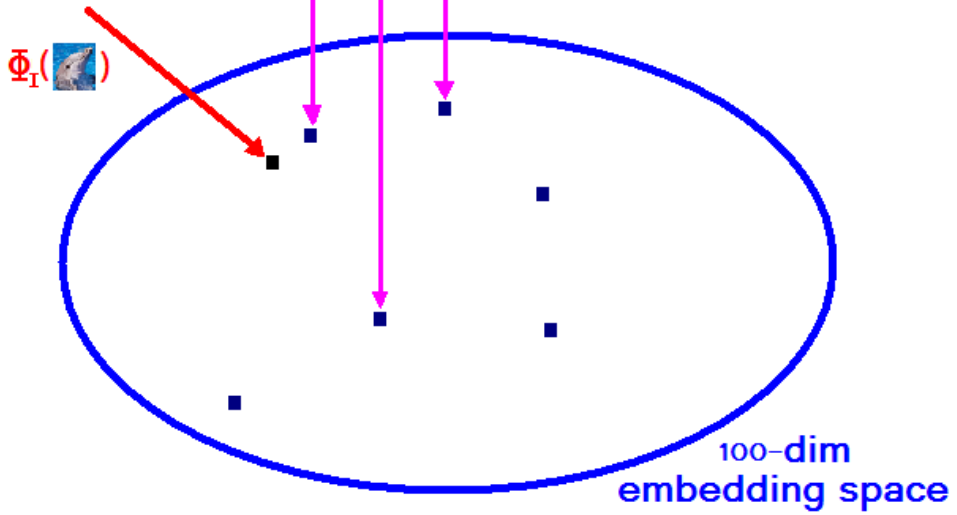


Google Image Search:
Different object types represented in the same space

Google:

S. Bengio, J. Weston & N. Usunier

(IJCAI 2011, NIPS'2010, JMLR 2010, MLJ 2010)

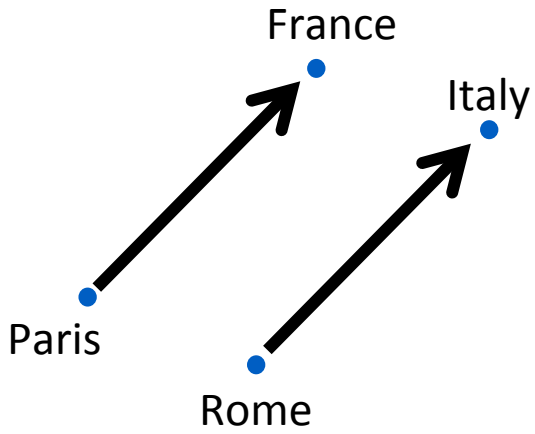


Learn $\Phi_I(\cdot)$ and $\Phi_W(\cdot)$ to optimize precision@k.

Following up on (Bengio et al NIPS'2000) Neural word embeddings - visualization

Analogical Representations for Free (Mikolov et al, ICLR 2013)

- Semantic relations appear as linear relationships in the space of learned representations
- King – Queen ≈ Man – Woman
- Paris – France + Italy ≈ Rome



Learning multiple levels of representation

There is theoretical and empirical evidence in favor of multiple levels of representation

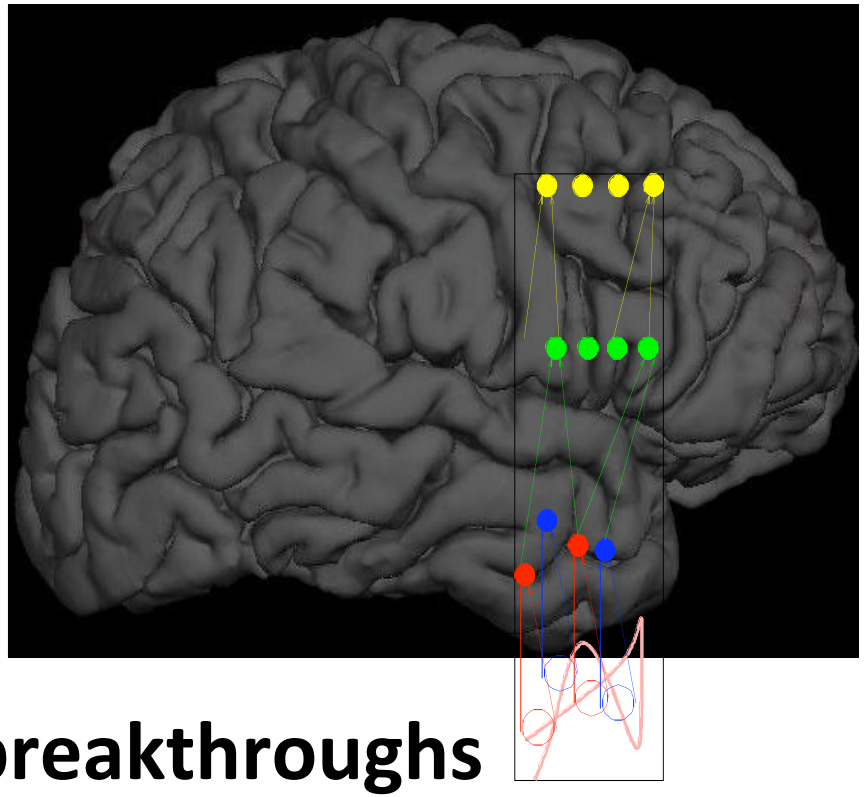
Exponential gain for some families of functions

Biologically inspired learning

Brain has a deep architecture

Cortex seems to have a generic learning algorithm

Humans first learn simpler concepts and compose them



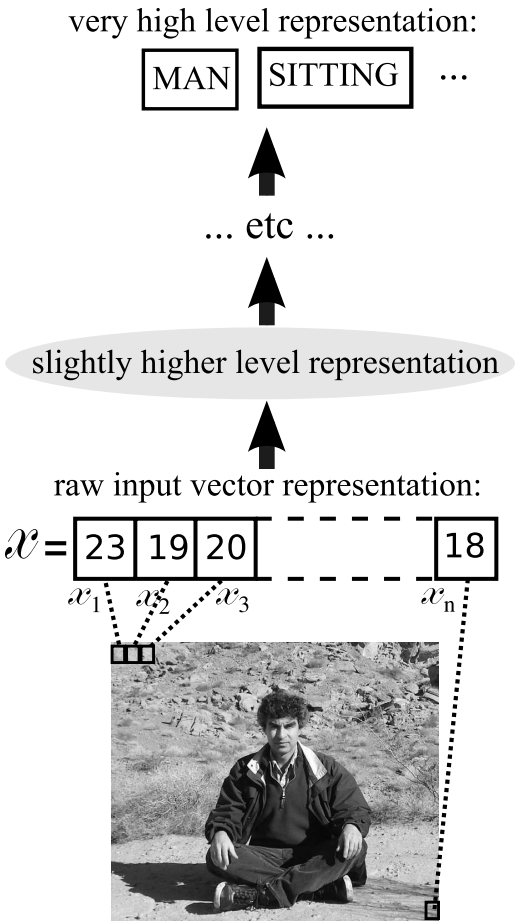
It works! Speech + vision breakthroughs

Deep Architecture in our Mind

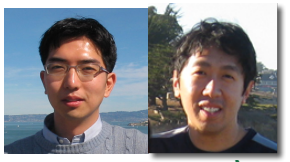
- Humans organize their ideas and concepts hierarchically
- Humans first learn simpler concepts and then compose them to represent more abstract ones
- Engineers break-up solutions into multiple levels of abstraction and processing

It would be good to automatically learn / discover these concepts

(knowledge engineering failed because of superficial introspection?)

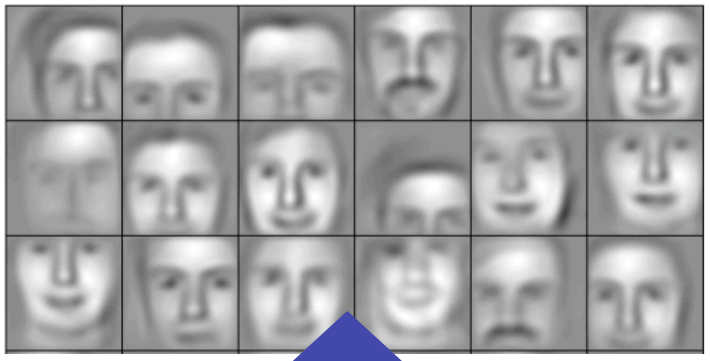


Learning multiple levels of representation



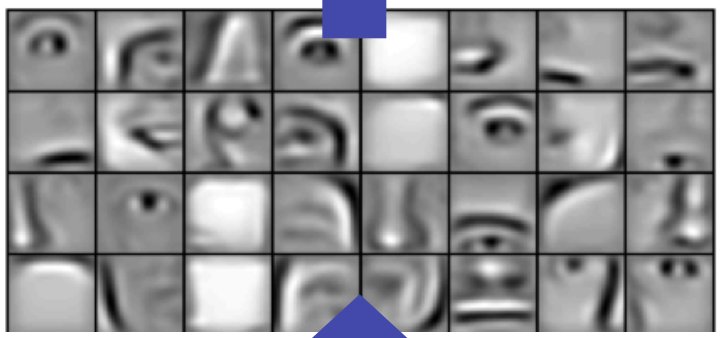
(Lee, Largman, Pham & Ng, NIPS 2009)
(Lee, Grosse, Ranganath & Ng, ICML 2009)

Successive model layers learn deeper intermediate representations



Layer 3

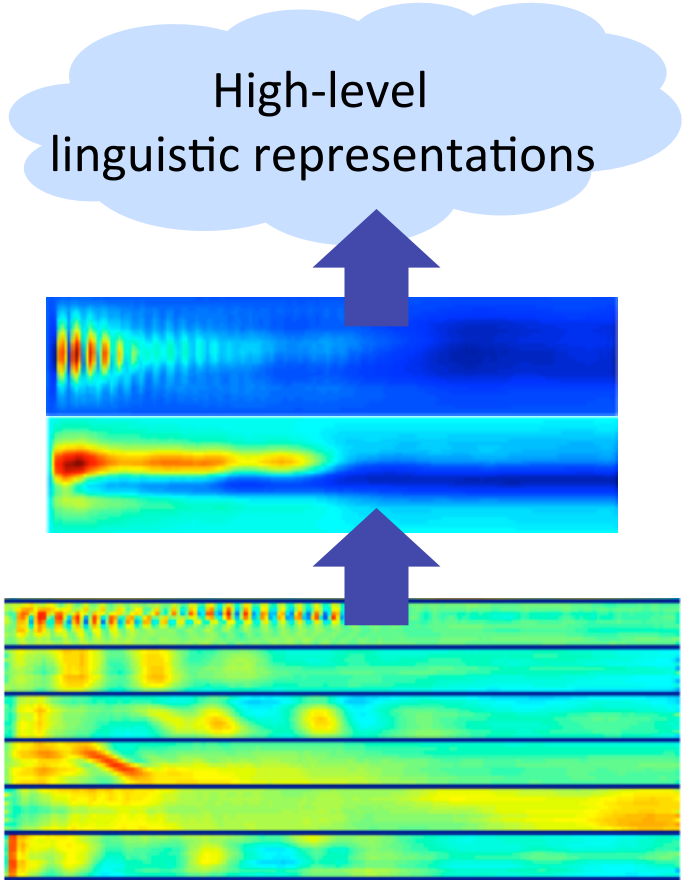
Parts combine to form objects



Layer 2

Layer 1

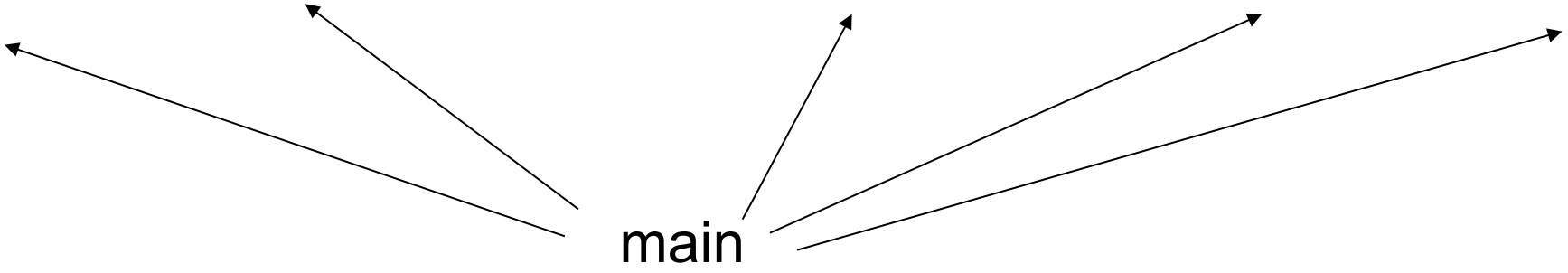
High-level linguistic representations



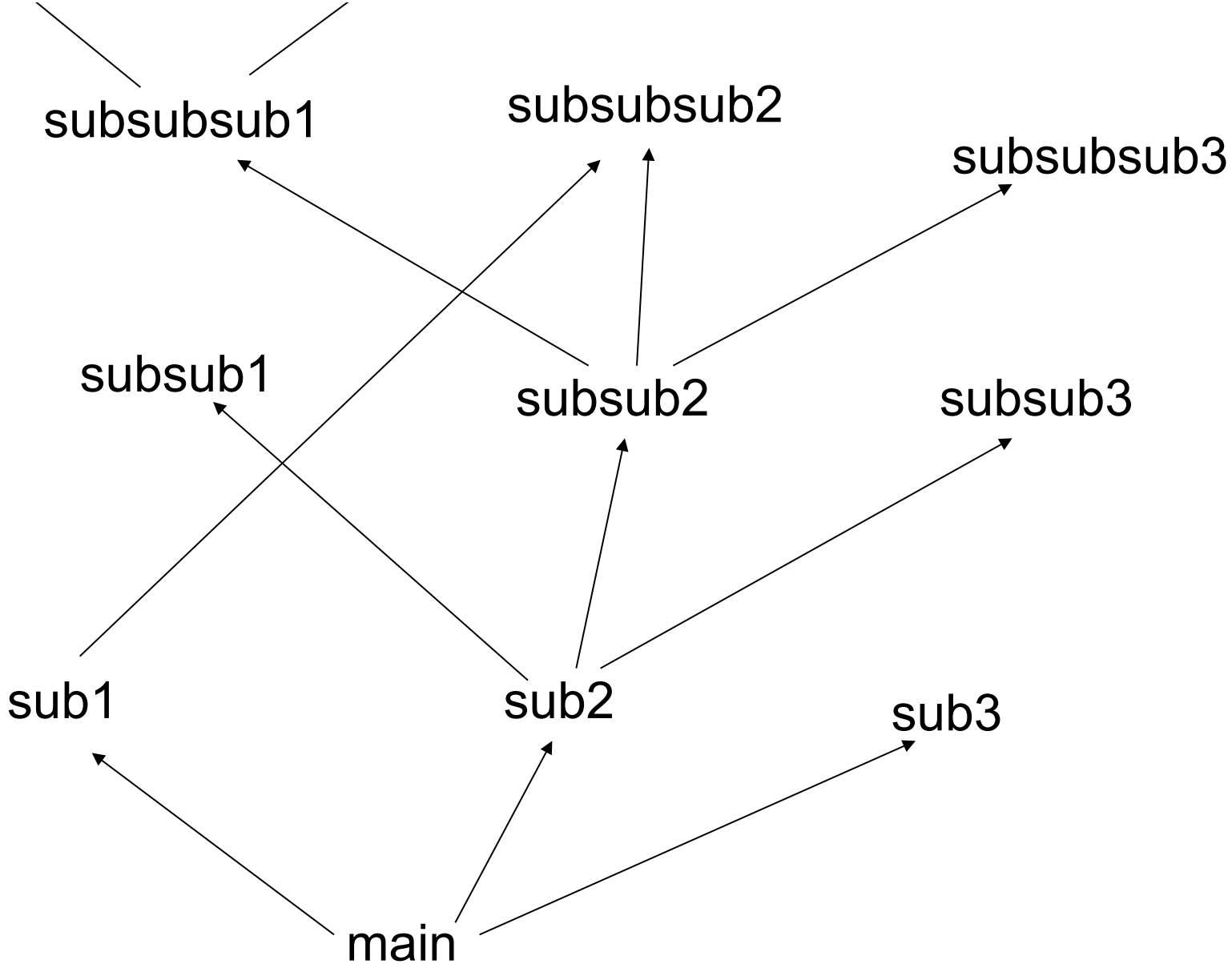
Prior: underlying factors & concepts compactly expressed w/ multiple levels of abstraction

subroutine1 includes
subsub1 code and
subsub2 code and
subsubsub1 code

subroutine2 includes
subsub2 code and
subsub3 code and
subsubsub3 code and …



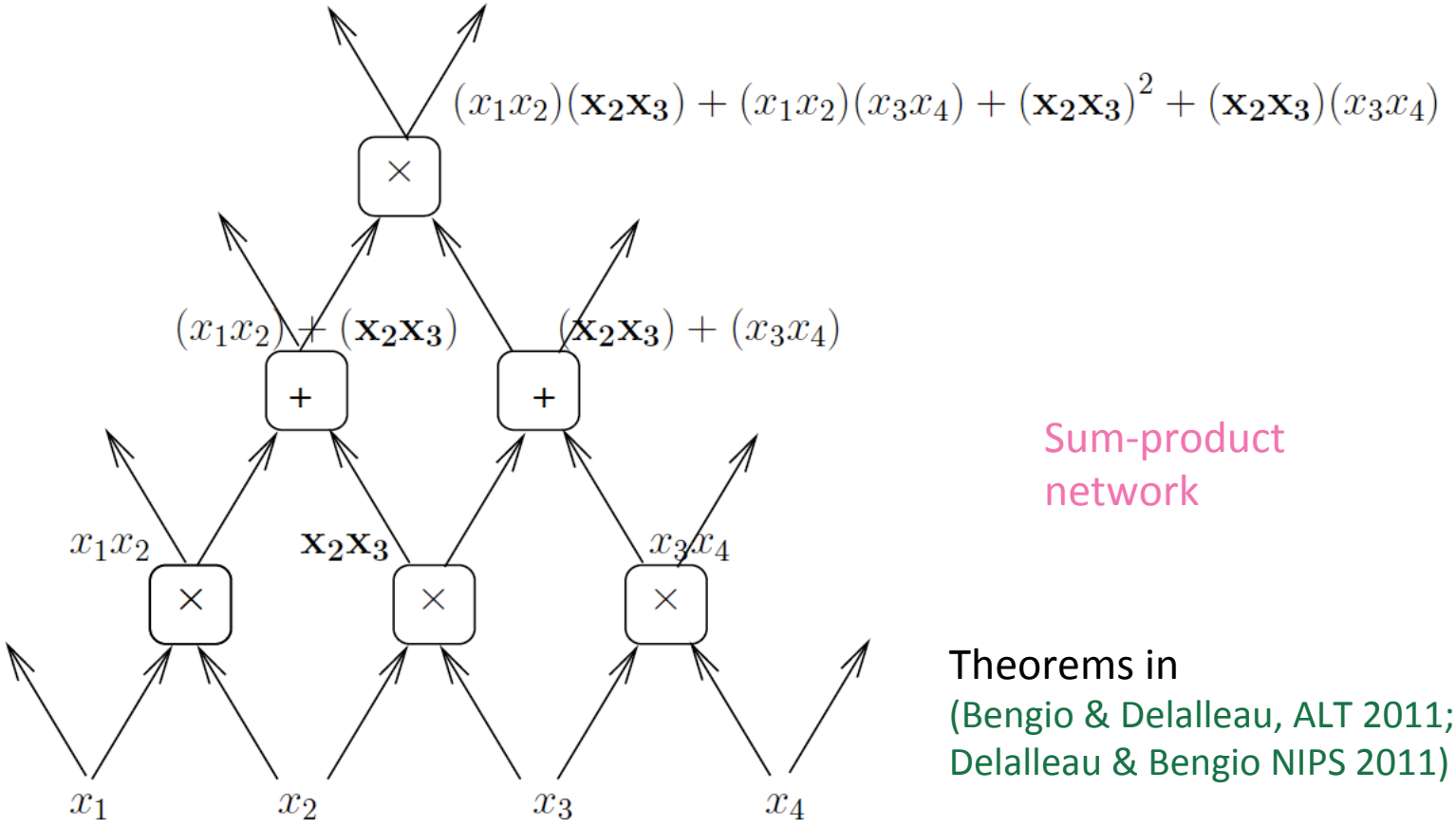
“Shallow” computer program



“Deep” computer program

Sharing Components in a Deep Architecture

Polynomial expressed with shared components: advantage of depth may grow exponentially



Sum-product network

Theorems in
(Bengio & Delalleau, ALT 2011;
Delalleau & Bengio NIPS 2011)

Deep Architectures are More Expressive

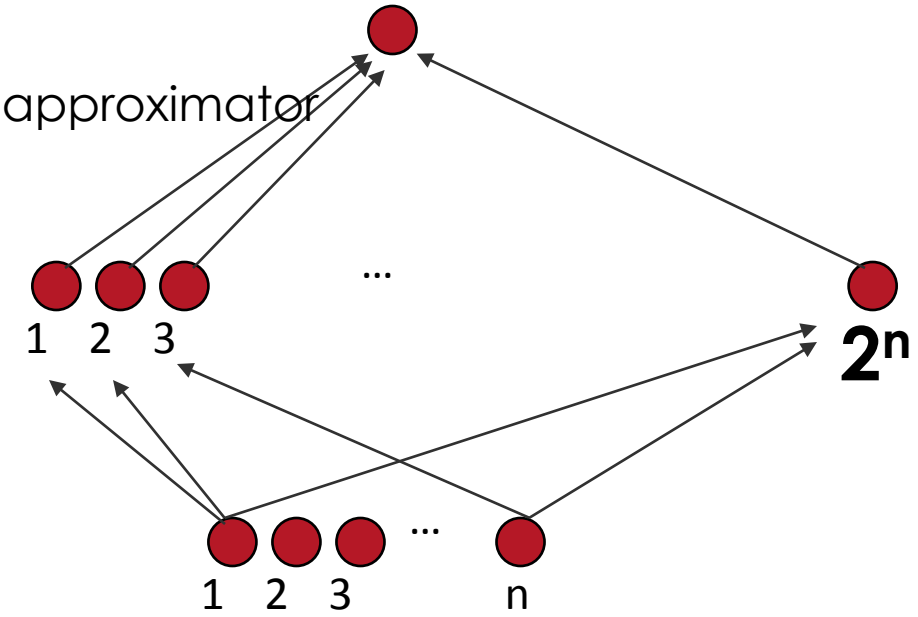
Theoretical arguments:

2 layers of { Logic gates / Formal neurons / RBF units } = universal approximator

RBMs & auto-encoders = universal approximator

Theorems on advantage of depth:
(Hastad et al 86 & 91, Bengio et al 2007, Bengio & Delalleau 2011, Braverman 2011, Pascanu et al 2014, Montufar et al 2014)

Some functions compactly represented with k layers may require exponential size with 2 layers



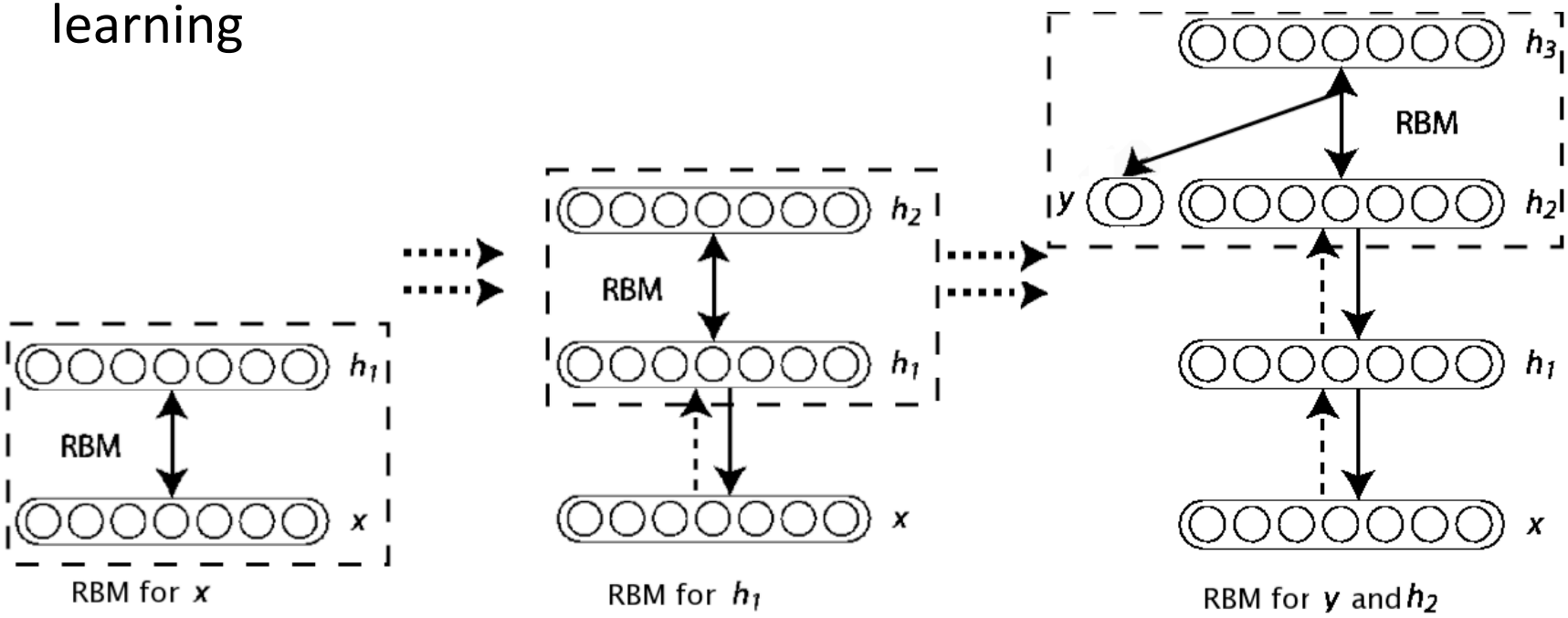
Breakthrough in 2006

- Ability to train deep architectures by using layer-wise unsupervised learning, whereas previous purely supervised attempts had failed

- Unsupervised feature learners:
  - RBMs
  - Auto-encoder variants
  - Sparse coding variants

Stacking Single-Layer Learners

- One of the big ideas from 2006: layer-wise unsupervised feature learning



Stacking Restricted Boltzmann Machines (RBM) → Deep Belief Network (DBN)

Stacking regularized auto-encoders → deep neural nets

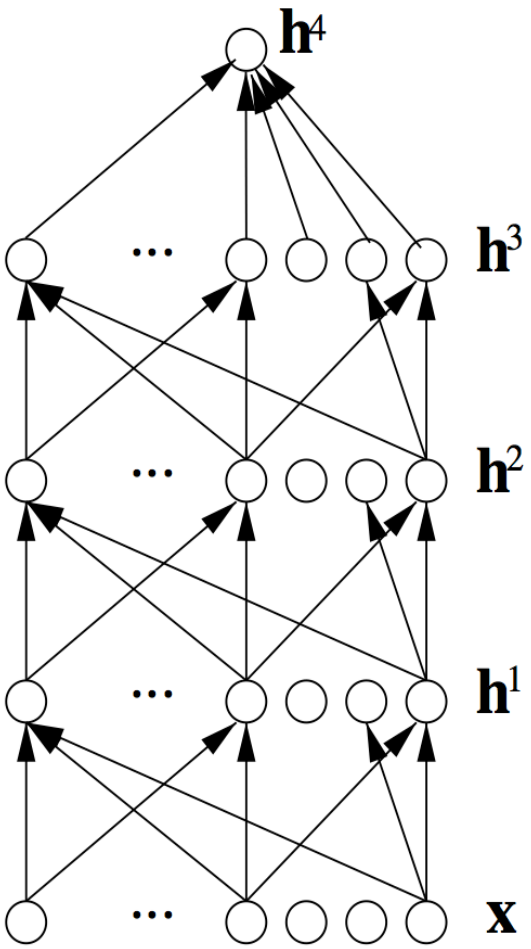
Deep Supervised Neural Nets

- Now can train them even without unsupervised pre-training:

  better initialization and non-linearities (rectifiers, maxout), generalize well with large labeled sets and regularizers (dropout)

- **Unsupervised pre-training:**

  rare classes, transfer, smaller labeled sets, or as extra regularizer.



Deep Learning in the News

WIRED

Researcher Dreams Up Machines That Learn Without Humans
06.27.13

The New York Tim

Monday, June 25, 2012 Last Update: 11:50 PM ET

DIGITAL SUBSCRIPTION: 4 WEEKS

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The New York Times

Scientists See Promise in Deep-Learning Programs

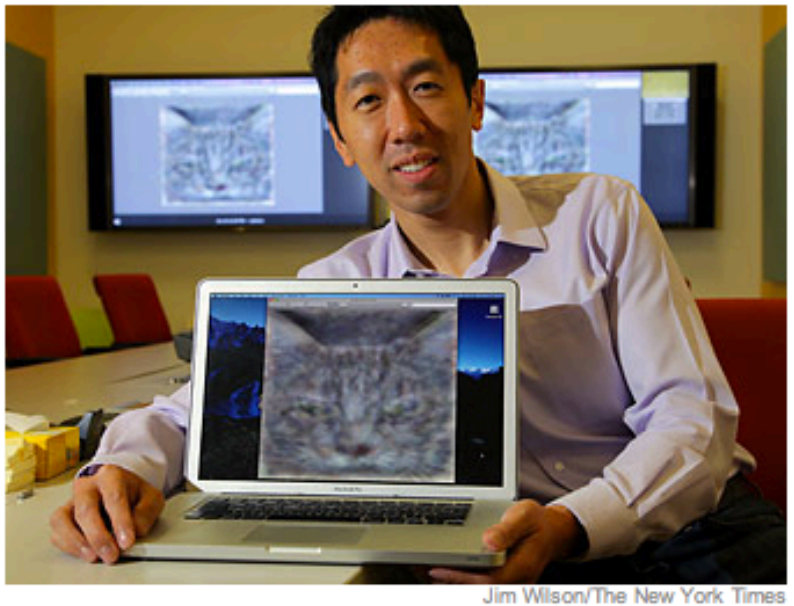
John Markoff

November 23, 2012

WIRED

The Man Behind the Google Brain: Andrew Ng and the Quest for the New AI

BY DANIELA HERNANDEZ 05.07.13 6:30 AM



Jim Wilson/The New York Times

Despite Itself, a Simulated Brain Seeks Cats

By JOHN MARKOFF 12 minutes ago

A Google research team, led by Andrew Y. Ng, above, and Jeff Dean, created a neural network of 16,000 processors that reflected human obsession with Internet felines.

THE GLOBE AND MAIL

CANADA'S NATIONAL NEWSPAPER • FOUNDED 1844

Google taps U of T professor to teach context to computers
03.11.13

MIT Technology Review

10 BREAKTHROUGH TECHNOLOGIES 2013

Intr

Deep Learning

With massive amounts of computational power, machines can now recognize objects and translate speech in real time. Artificial intelligence is finally getting smart. →

Temporary Social Media

Messages that quickly self-destruct could enhance the privacy of online communications and make people freer to be spontaneous. →

Prenatal DNA Sequencing

Reading the DNA of fetuses will be the next frontier of the genomic revolution. But do you really want to know about the genetic problems or musical aptitude of your unborn child? →

Ado Mar

Ske prin wor mar the tech jet p

Memory Implants

A maverick neuroscientist believes he has deciphered the code by which the brain

Smart Watches

Ultra-Efficient Solar Power

Doubling the efficiency of a solar cell would completely

Big Pho

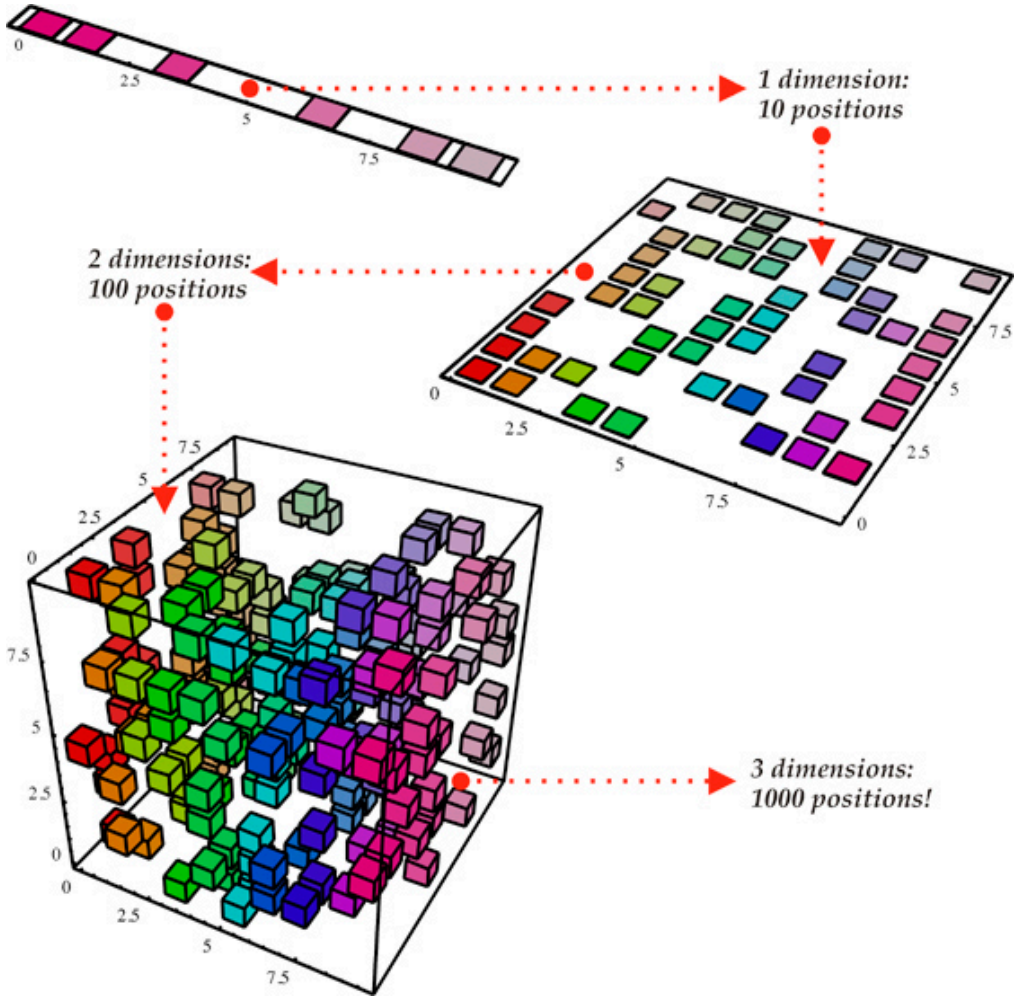
Coll ana from pho

Back to ML Basics

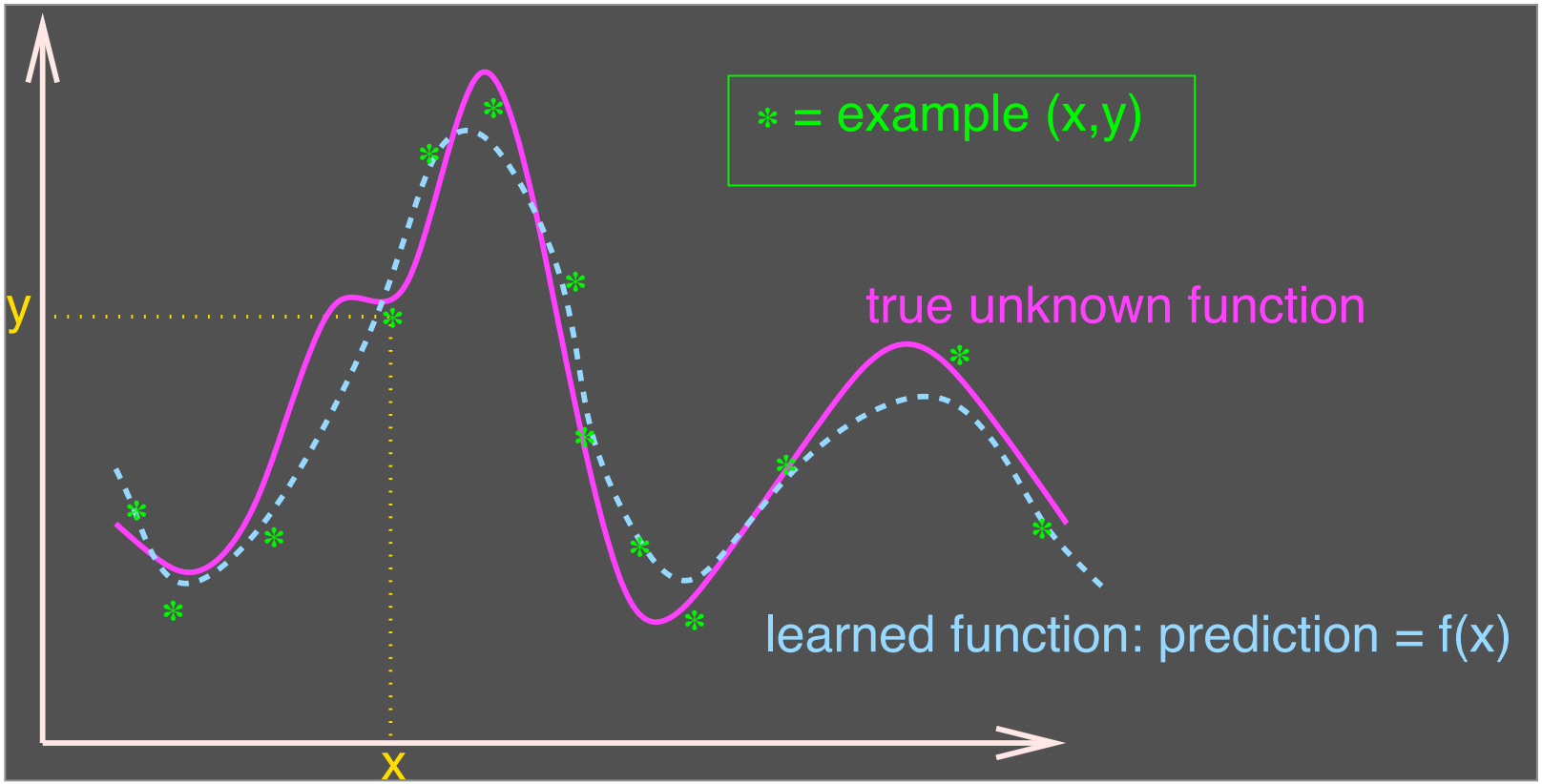
ML 101. What We Are Fighting Against: The Curse of Dimensionality

To generalize locally, need representative examples for all relevant variations!

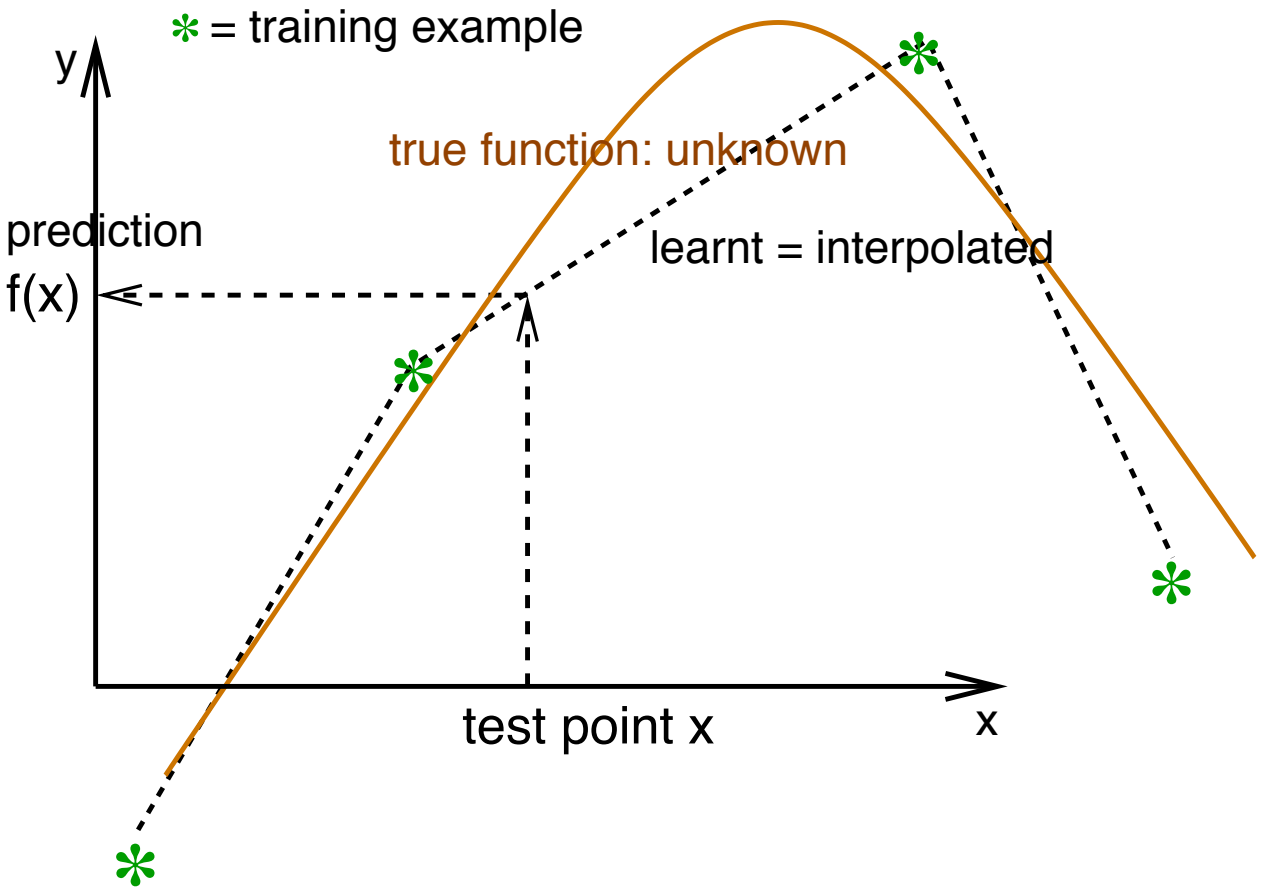
Classical solution: hope for a smooth enough target function, or make it smooth by handcrafting good features / kernel



Easy Learning

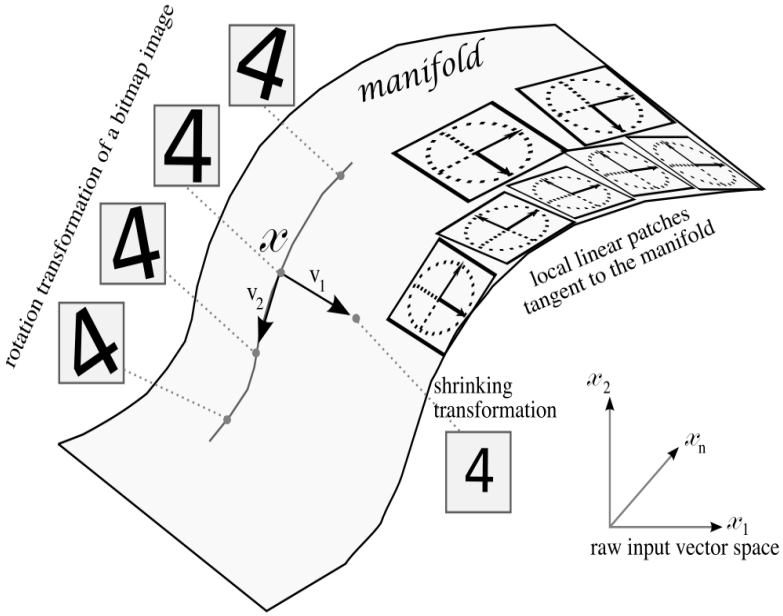


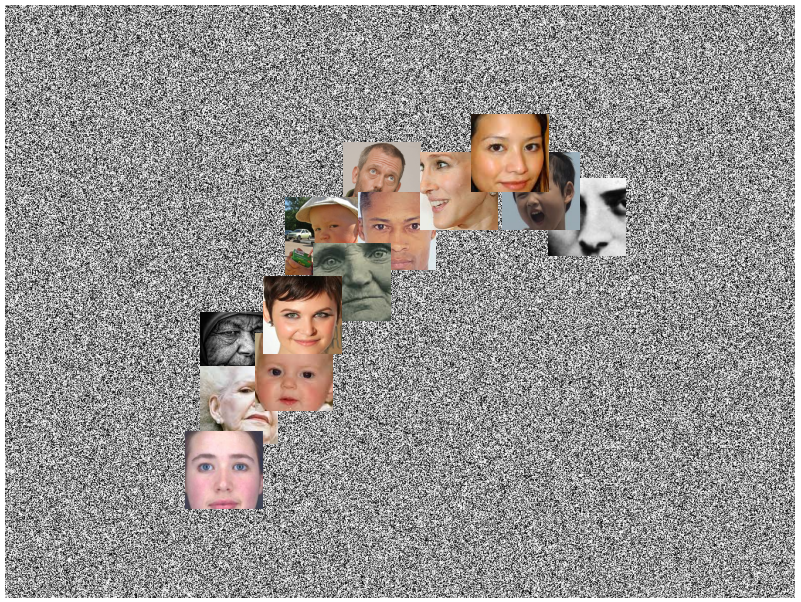
Local Smoothness Prior: Locally Capture the Variations



For AI Tasks: Manifold structure

- examples **concentrate** near a lower dimensional "manifold
- **Evidence: most input configurations are unlikely**

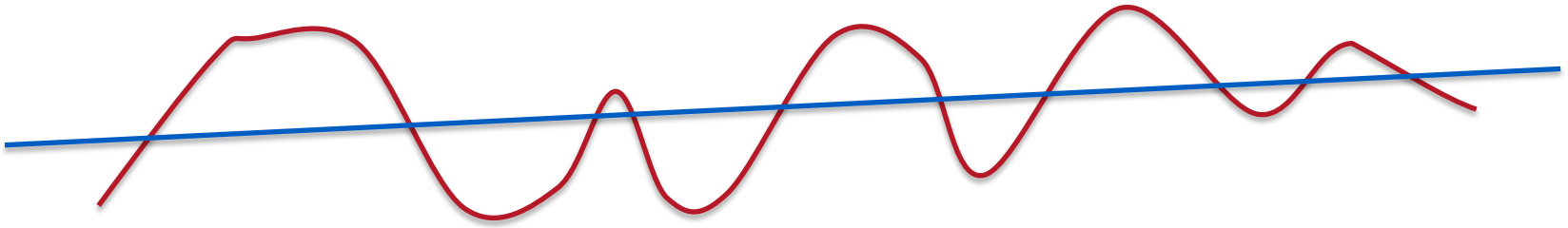




Not Dimensionality so much as Number of Variations

(Bengio, Dellalleau & Le Roux 2007)

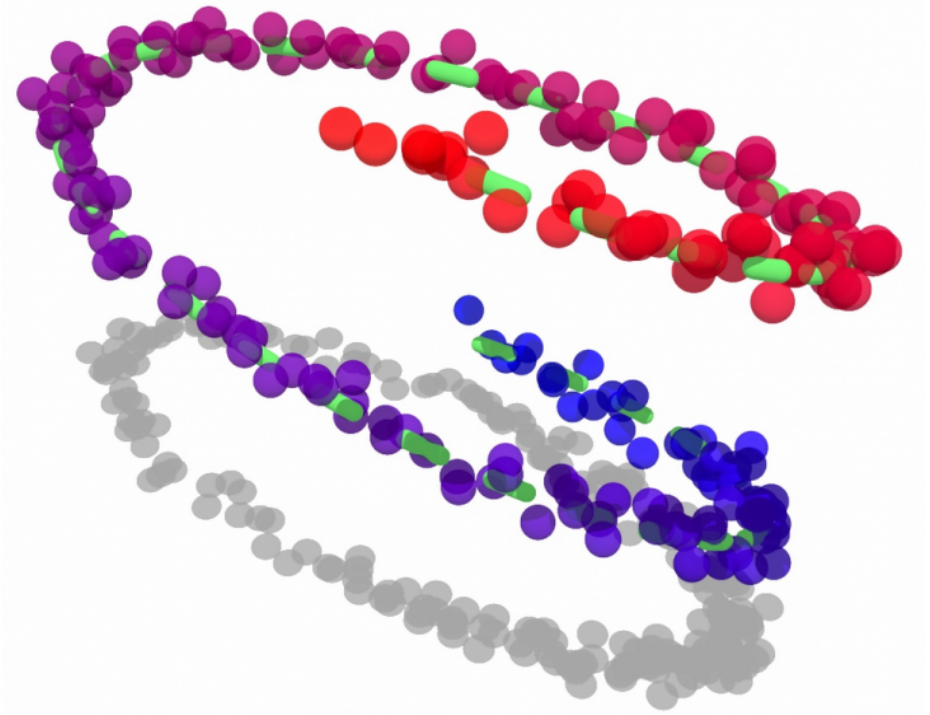
- Theorem: Gaussian kernel machines need at least *k* examples to learn a function that has *2k* zero-crossings along some line



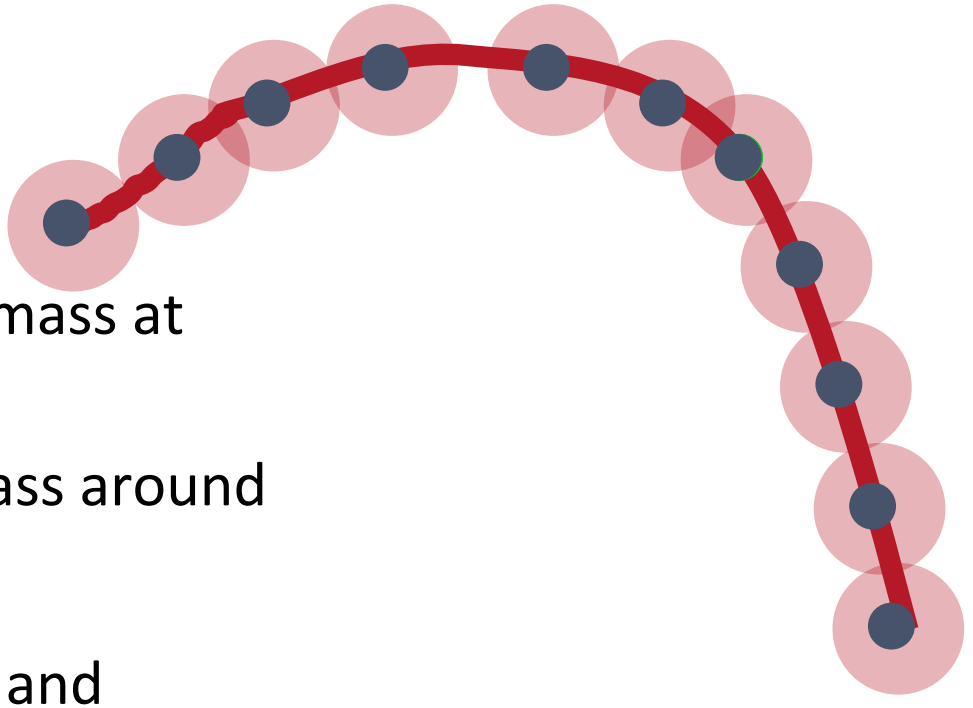
- Theorem: For a Gaussian kernel machine to learn some maximally varying functions over *d* inputs requires $O(2^d)$ examples

Geometrical view on machine learning

- Generalization: guessing **where** *probability* mass concentrates
- Challenge: the curse of dimensionality (exponentially many configurations of the variables to consider)



Putting Probability Mass where Structure is Plausible



- Empirical distribution: mass at training examples
- Smoothness: spread mass around
- Insufficient
- Guess some ‘structure’ and generalize accordingly

Is there any hope to generalize non-locally?

Yes! Need good priors!

Bypassing the curse

We need to build compositionality into our ML models

- Just as human languages exploit compositionality to give representations and meanings to complex ideas

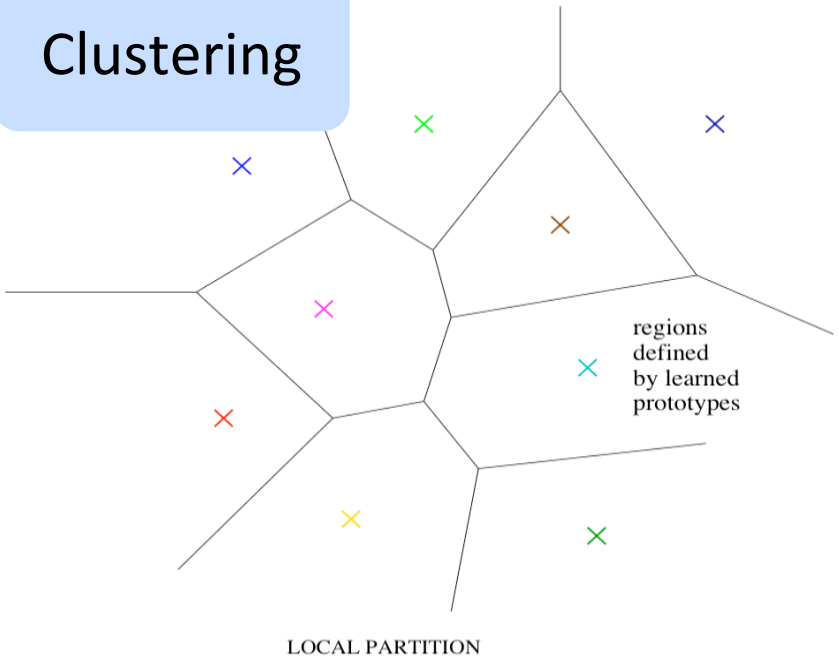
Exploiting compositionality gives an exponential gain in representational power

- Distributed representations / embeddings: feature learning
- Deep architecture: multiple levels of feature learning

Prior: compositionality is useful to describe the world around us efficiently

Non-distributed representations

Clustering



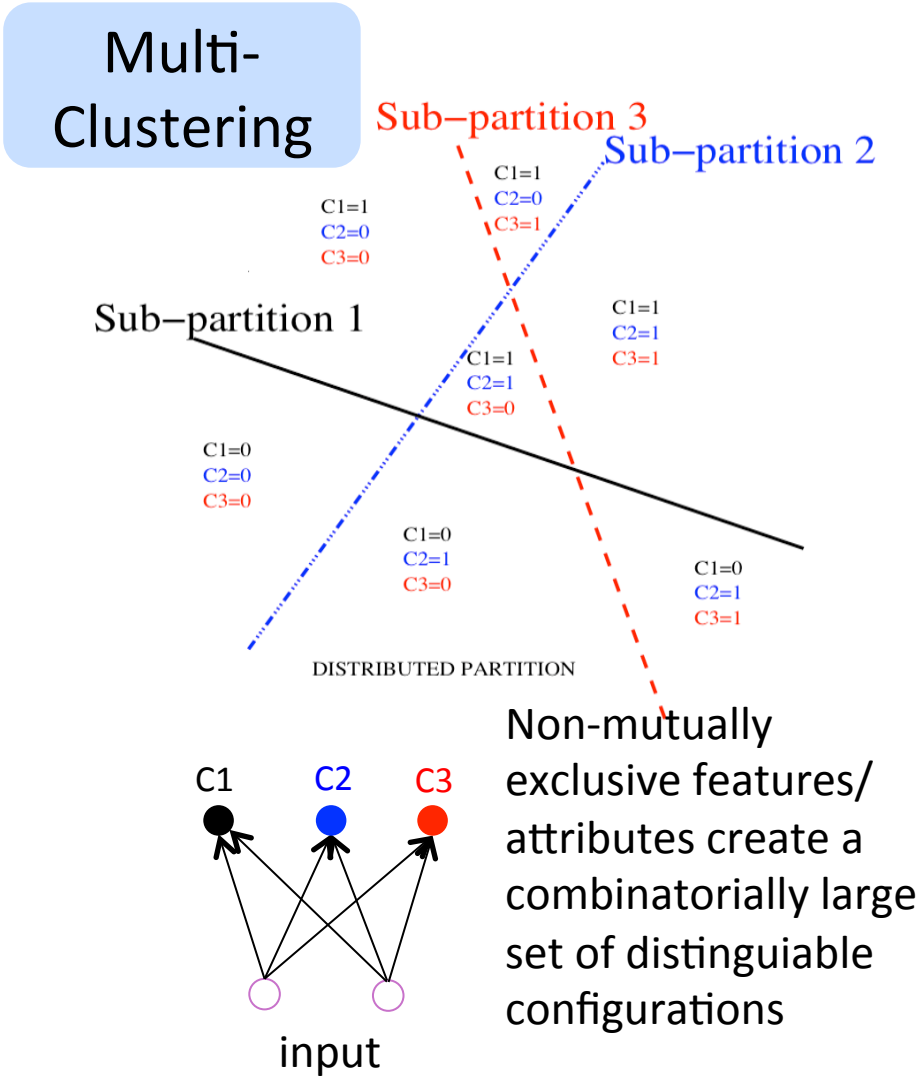
- Clustering, Nearest-Neighbors, RBF SVMs, local non-parametric density estimation & prediction, decision trees, etc.
- Parameters for each distinguishable region
- **# of distinguishable regions is linear in # of parameters**

→ No non-trivial generalization to regions without examples

The need for distributed representations

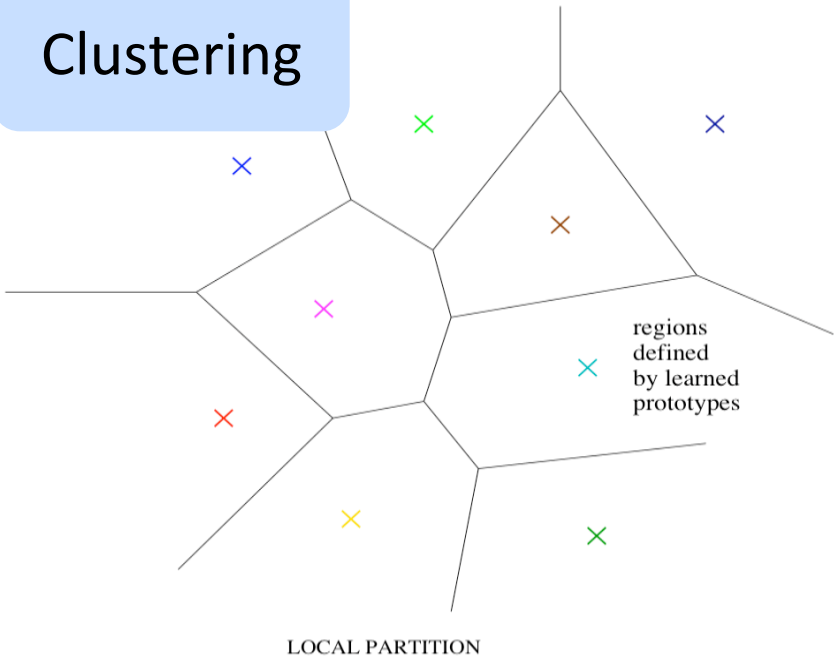
- Factor models, PCA, RBMs, Neural Nets, Sparse Coding, Deep Learning, etc.

- Each parameter influences many regions, not just local neighbors
- **# of distinguishable regions grows almost exponentially with # of parameters**
- **GENERALIZE NON-LOCALLY TO NEVER-SEEN REGIONS**

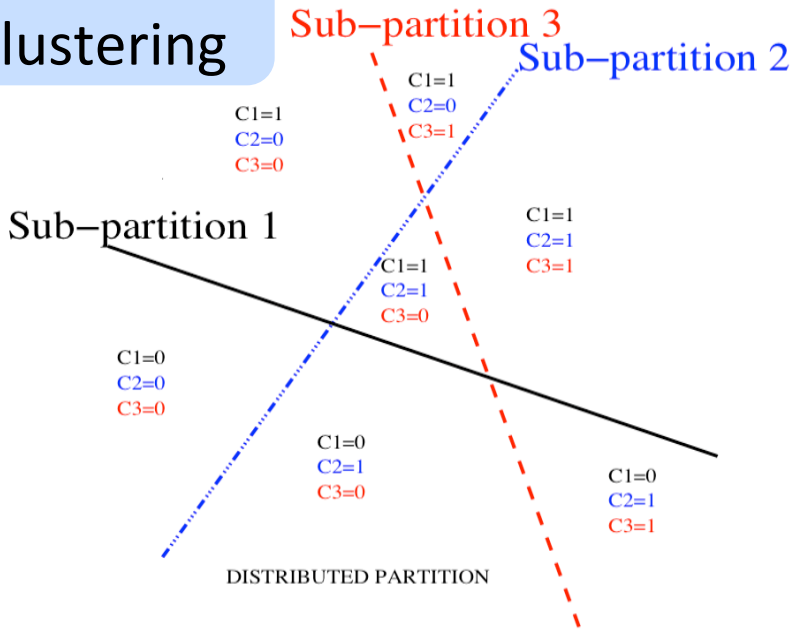


The need for distributed representations

Clustering



Multi-Clustering



Learning a **set of features** that are not mutually exclusive can be exponentially more statistically efficient than having nearest-neighbor-like or clustering-like models

Unsupervised feature learning

Today, most practical ML applications require (lots of) labeled training data

But almost all data is unlabeled, e.g. text, images on the web

Labels cannot possibly provide enough information

Most information acquired in an **unsupervised** fashion

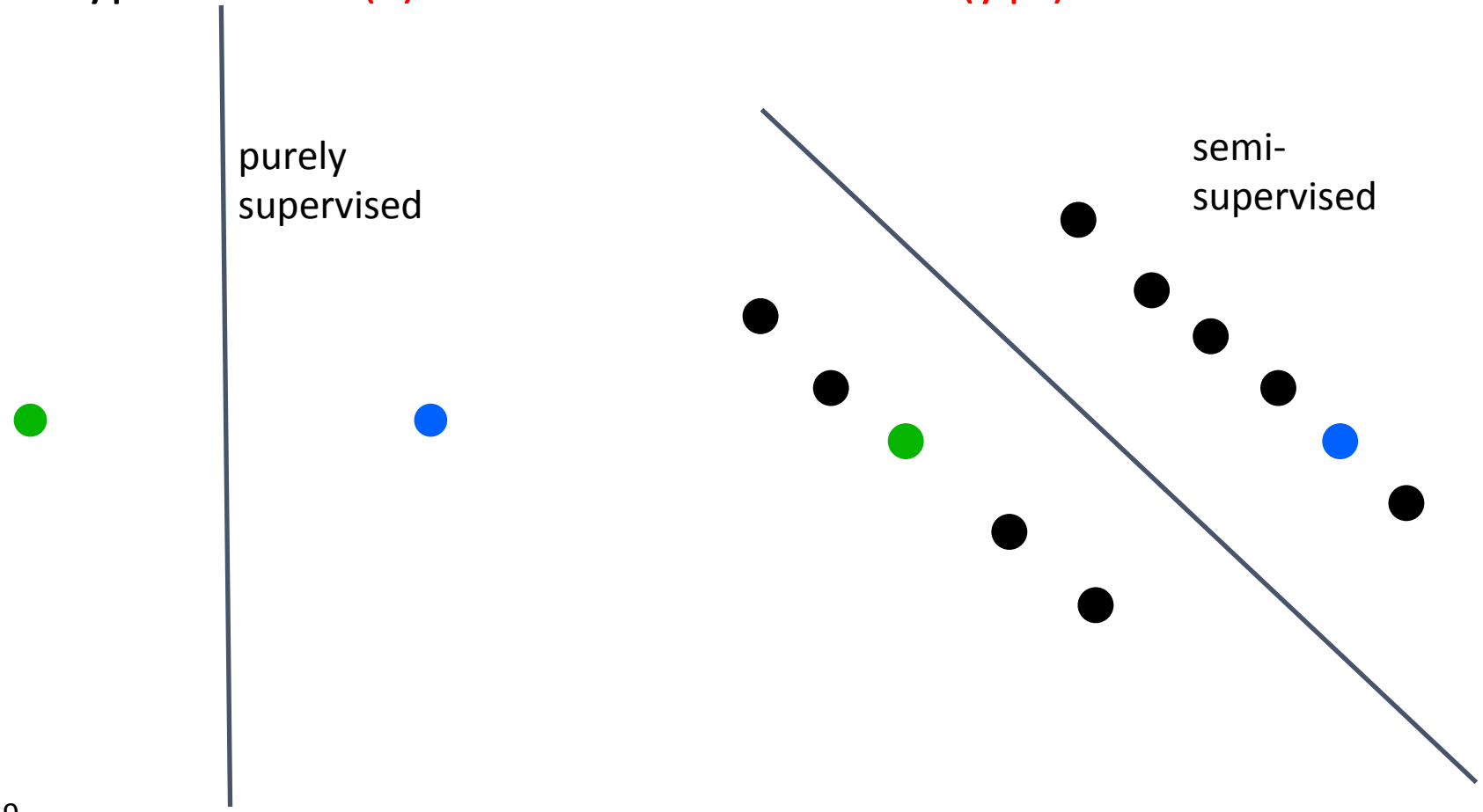
How do humans generalize from very few examples?

- They **transfer** knowledge from previous learning:
  - Representations
  - Explanatory factors
- Previous learning from: unlabeled data

  \+ labels for other tasks
- **Prior: shared underlying explanatory factors, in particular between P(x) and P(Y|x)**

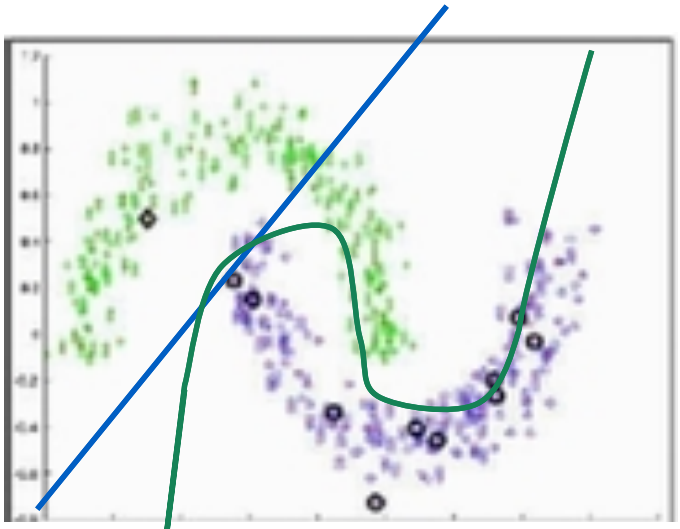
Sharing Statistical Strength by Semi-Supervised Learning

- Hypothesis: P(x) shares structure with P(y|x)



Why Semi-Supervised Learning Works

- The labeled examples (circles) help to identify the class of each cluster of unlabeled examples.
- The unlabeled examples (colored dots) help to identify the shape of each cluster.



few labeled examples

"happiness"

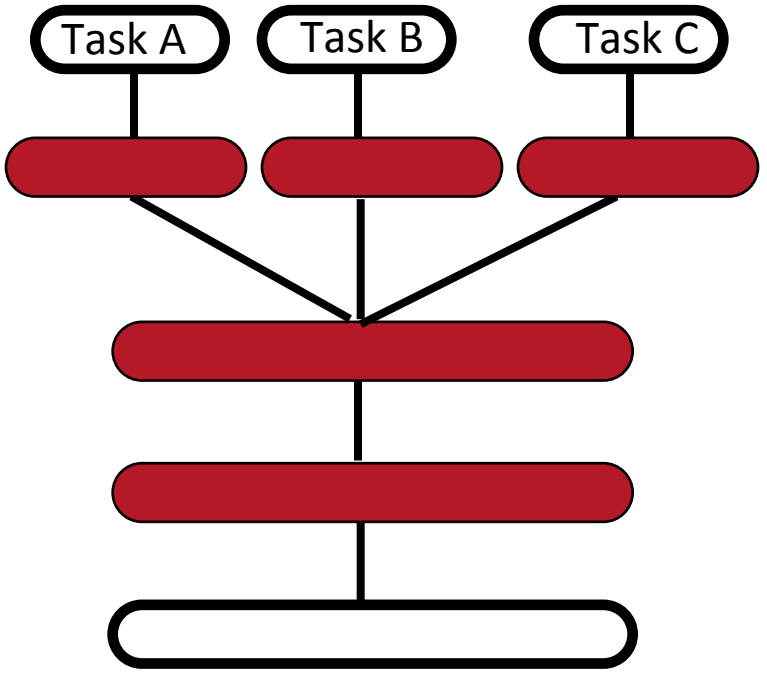
+

many unlabeled examples

Multi-Task Learning

- Generalizing better to new tasks (tens of thousands!) is crucial to approach AI
- Deep architectures learn good intermediate representations that can be shared across tasks

  (Collobert & Weston ICML 2008, Bengio et al AISTATS 2011)
- Good representations that disentangle underlying factors of variation make sense for many tasks because **each task concerns a subset of the factors**



E.g. dictionary, with intermediate concepts re-used across many definitions

Prior: shared underlying explanatory factors between tasks

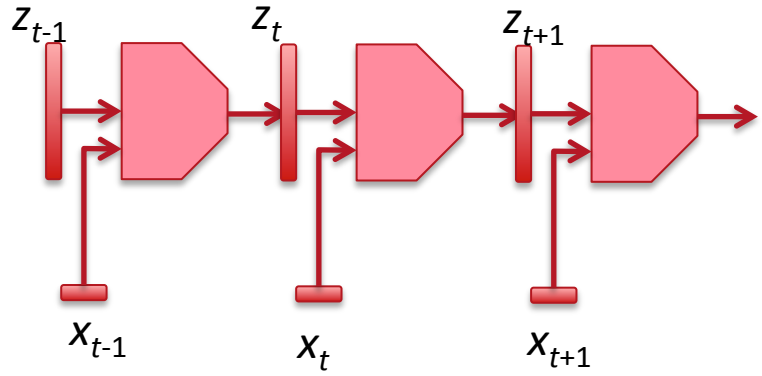
Better Representations → Better Transfer → Better Domain Adaptation

- What is a good representation?

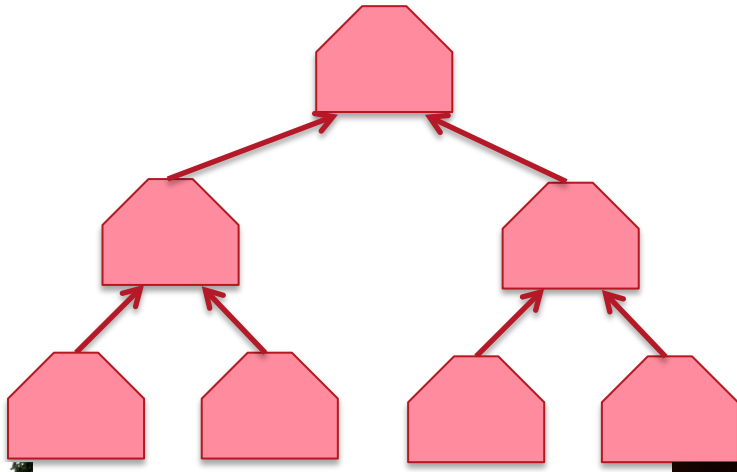
- Separate the « noise » from the « signal »
- Disentangle the underlying causal factors from each other

Handling the compositionality of human language and thought

- Human languages, ideas, and artifacts are composed from simpler components



- **Recursion**: the same operator (same parameters) is applied repeatedly on different states/components of the computation

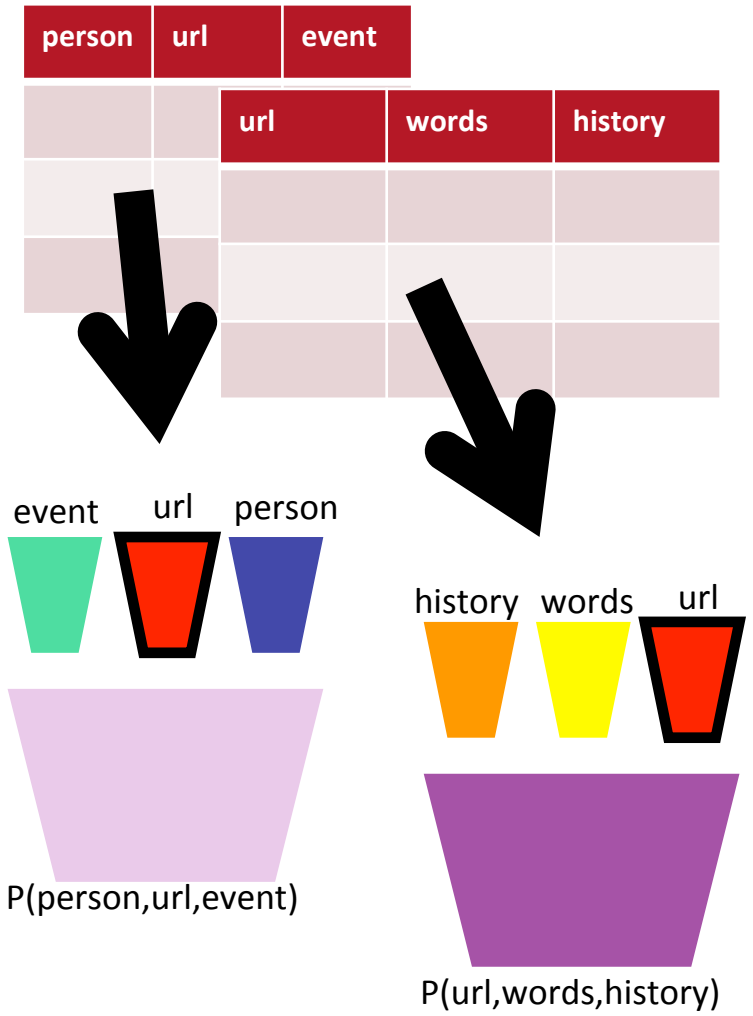


- Result after unfolding = deep computation / representation

(Bottou 2011, Socher et al 2011)

Combining Multiple Sources of Evidence with Shared Representations

- Traditional ML: data = matrix
- Relational learning: multiple sources, different tuples of variables
- Share representations of same types across data sources
- Shared learned representations help propagate information among data sources: e.g., WordNet, XWN, Wikipedia, **FreeBase**, ImageNet… (Bordes et al AISTATS 2012, ML J. 2013)
- **FACTS = DATA**
- **Deduction = Generalization**



Invariance and Disentangling

- Invariant features

- Which invariances?
- Alternative: learning to disentangle factors
- Good disentangling →

  avoid the curse of dimensionality

Emergence of Disentangling

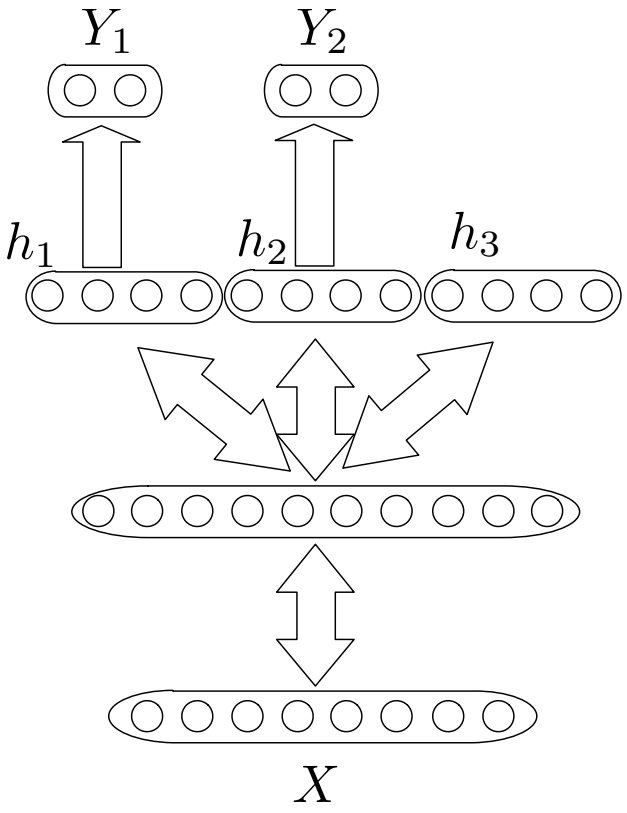
- (Goodfellow et al. 2009): sparse auto-encoders trained on images
  - some higher-level features more invariant to geometric factors of variation

- (Glorot et al. 2011): sparse rectified denoising auto-encoders trained on bags of words for sentiment analysis
  - different features specialize on different aspects (domain, sentiment)

WHY?

Hints to Help Disentangling

- (Rifai et al, ECCV 2012, *Disentangling factors of variation for facial expression recognition*)
- (Kingma & Welling, NIPS 2014, *Semi-Supervised Learning with Deep Generative Models*)
- Some hidden units predict some of the factors, others are free to be used to reconstruct the input. Different groups of hidden units assigned to different factors. Orthogonality or penalty or independence prior between hidden units of different groups

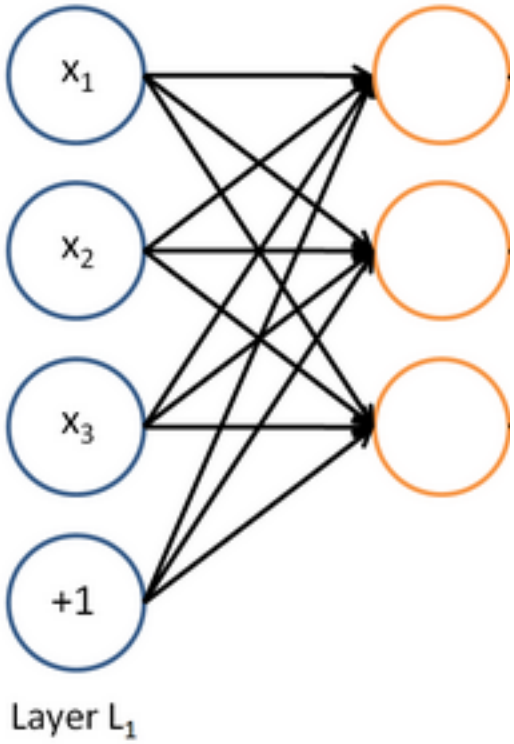


Part 2

Representation Learning Algorithms

A neural network = running several logistic regressions at the same time

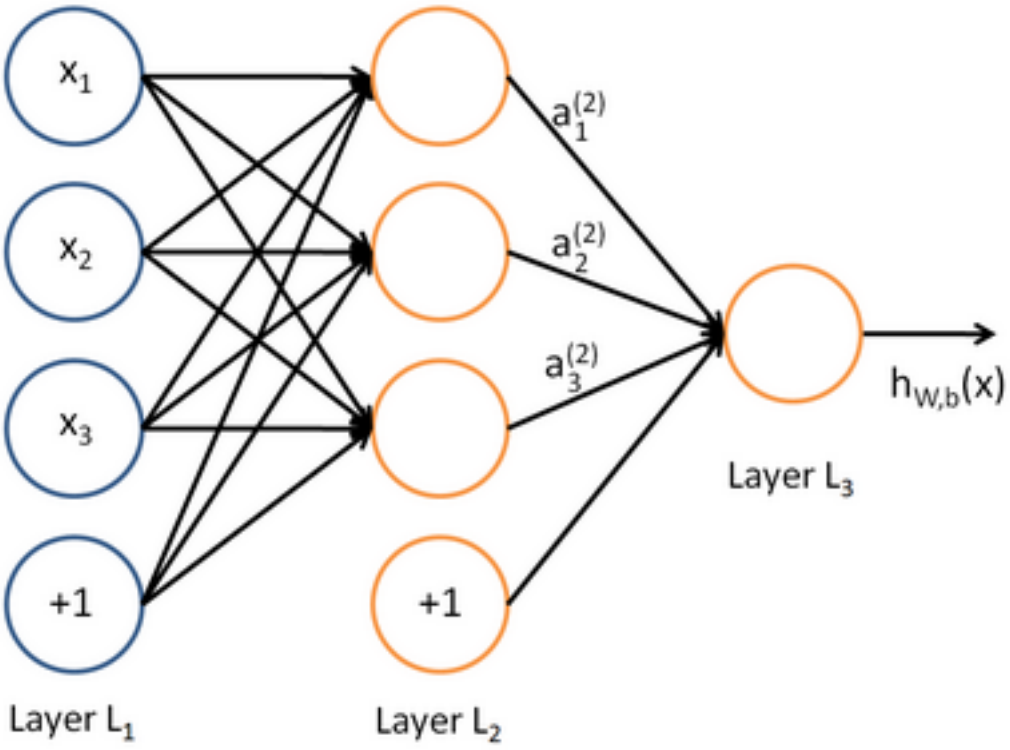
If we feed a vector of inputs through a bunch of logistic regression functions, then we get a vector of outputs



But we don't have to decide ahead of time what variables these logistic regressions are trying to predict!

A neural network = running several logistic regressions at the same time

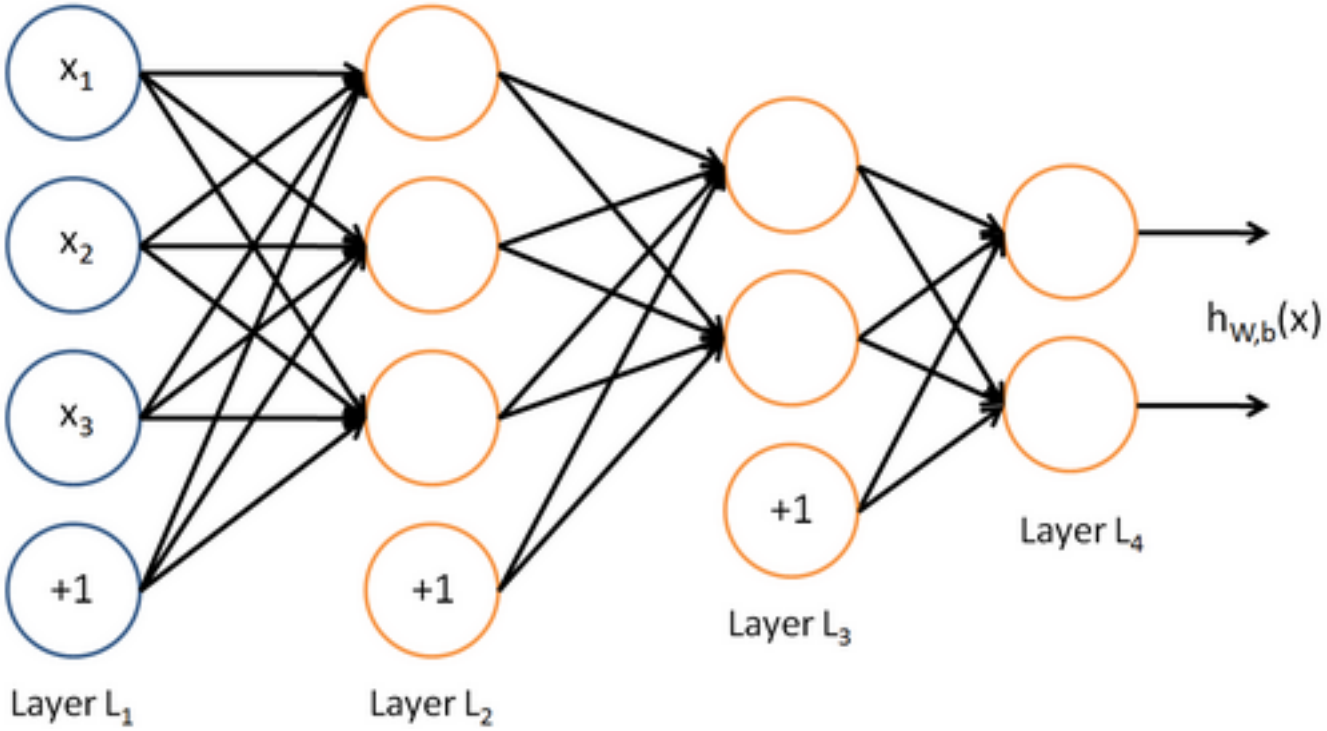
… which we can feed into another logistic regression function



and it is the training criterion that will decide what those intermediate binary target variables should be, so as to make a good job of predicting the targets for the next layer, etc.

A neural network = running several logistic regressions at the same time

- Before we know it, we have a multilayer neural network….



Back-Prop

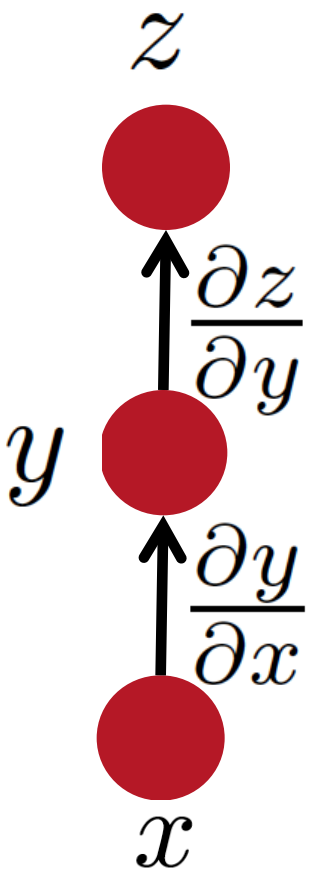
- Compute gradient of example-wise loss wrt parameters

- Simply applying the derivative chain rule wisely

$$z = f(y) \quad y = g(x) \quad \frac{\partial z}{\partial x} = \frac{\partial z}{\partial y}\frac{\partial y}{\partial x}$$

- *If computing the loss(example, parameters) is O(n) computation, then so is computing the gradient*

Simple Chain Rule



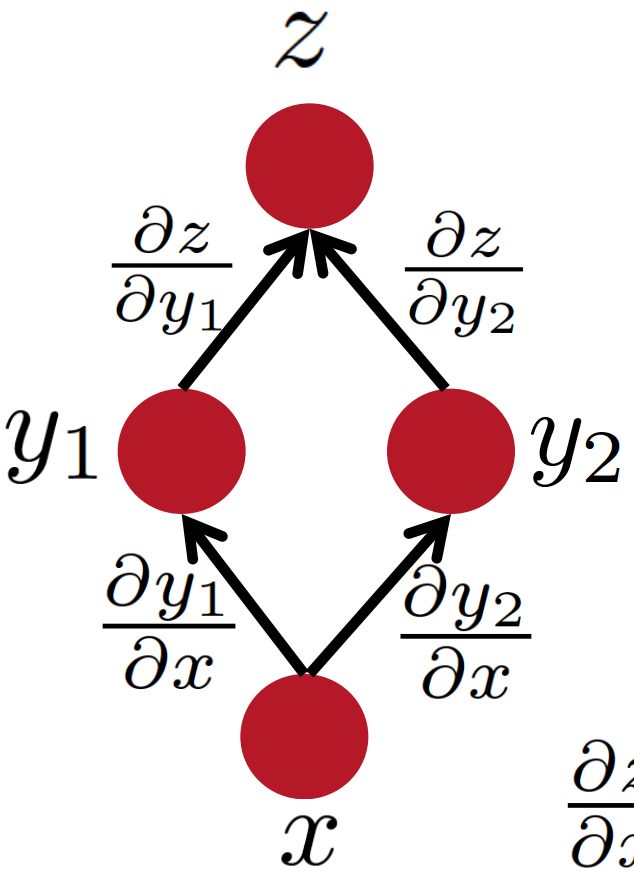
$$\Delta z = \frac{\partial z}{\partial y}\Delta y$$

$$\Delta y = \frac{\partial y}{\partial x}\Delta x$$

$$\Delta z = \frac{\partial z}{\partial y}\frac{\partial y}{\partial x}\Delta x$$

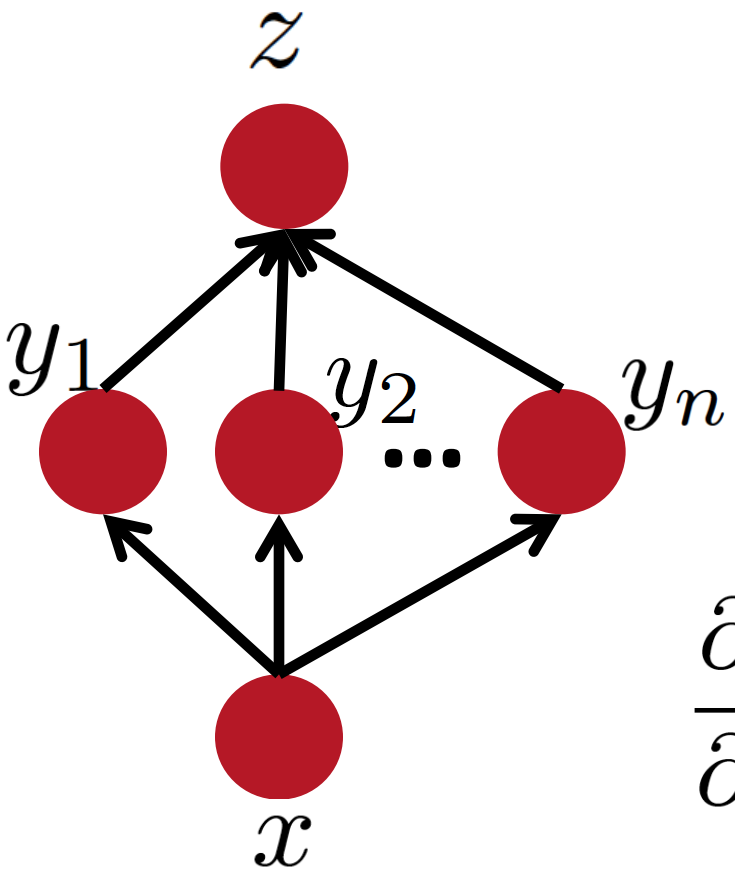
$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y}\frac{\partial y}{\partial x}$$

Multiple Paths Chain Rule



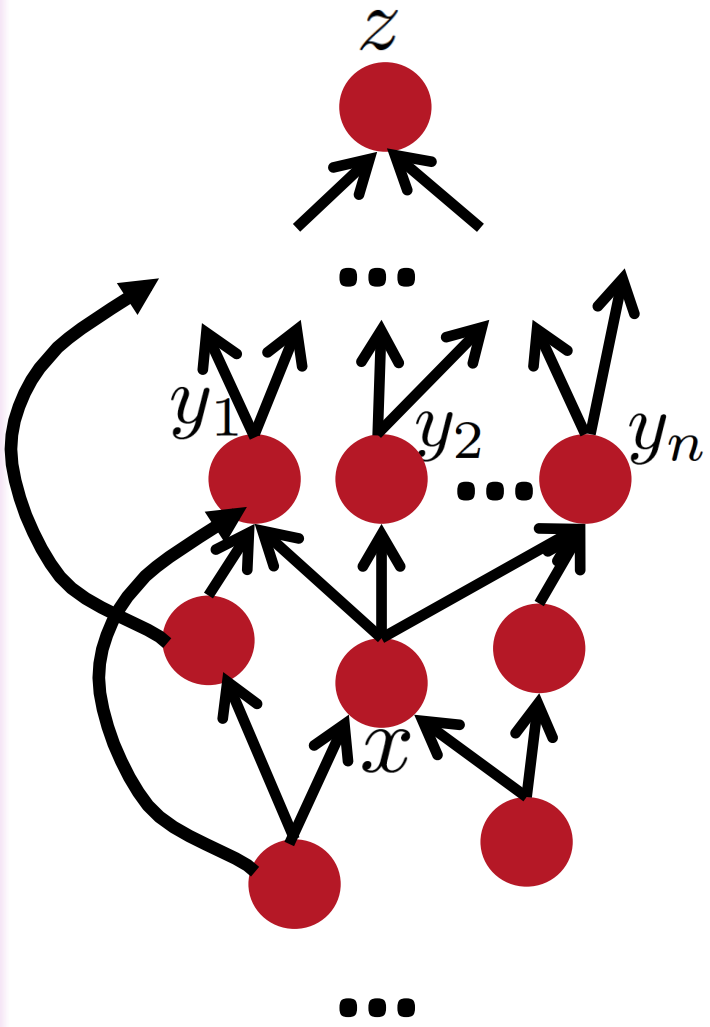
$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y_1}\frac{\partial y_1}{\partial x} + \frac{\partial z}{\partial y_2}\frac{\partial y_2}{\partial x}$$

Multiple Paths Chain Rule - General



$$\frac{\partial z}{\partial x} = \sum_{i=1}^{n} \frac{\partial z}{\partial y_i} \frac{\partial y_i}{\partial x}$$

Chain Rule in Flow Graph

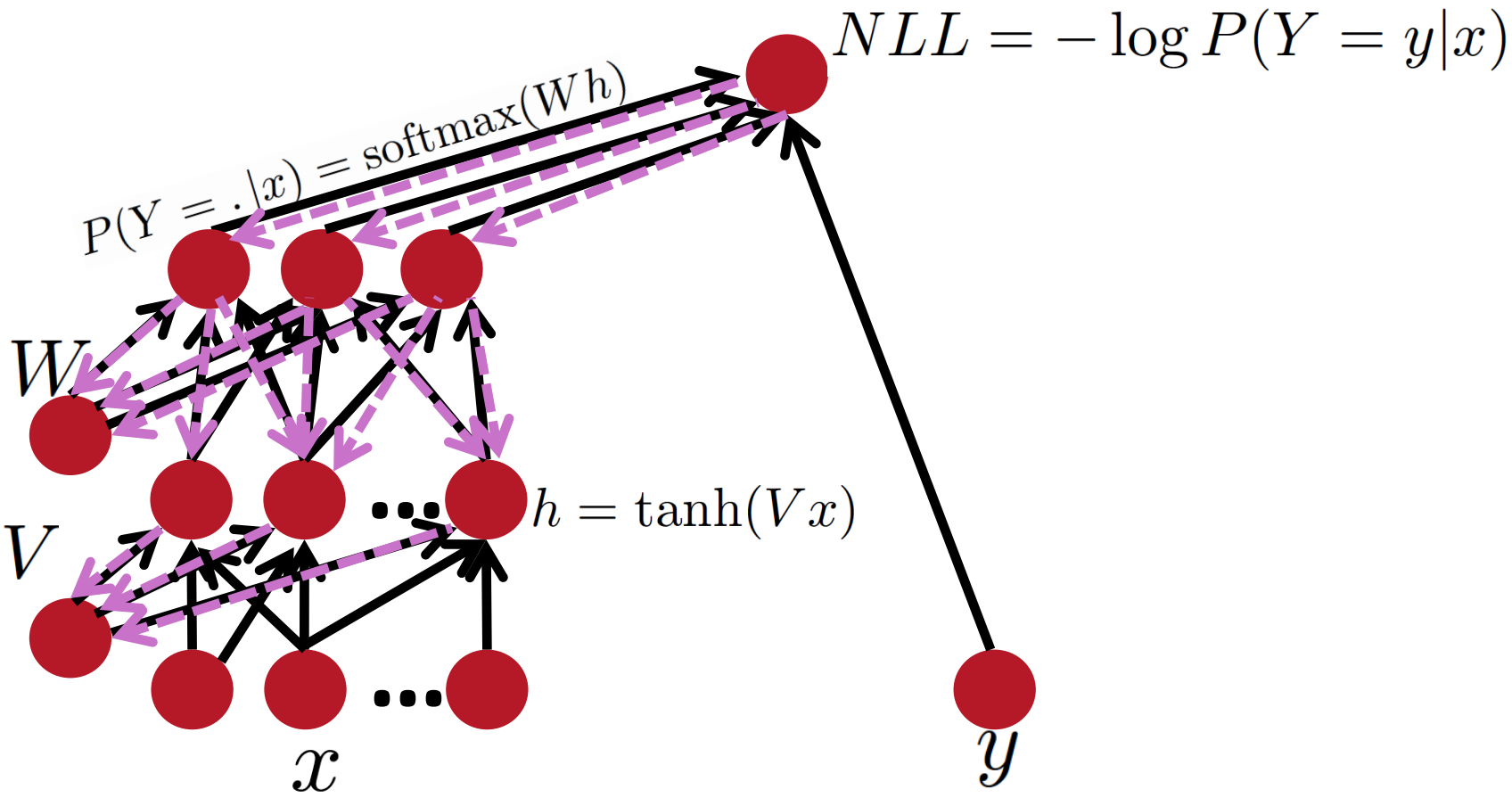


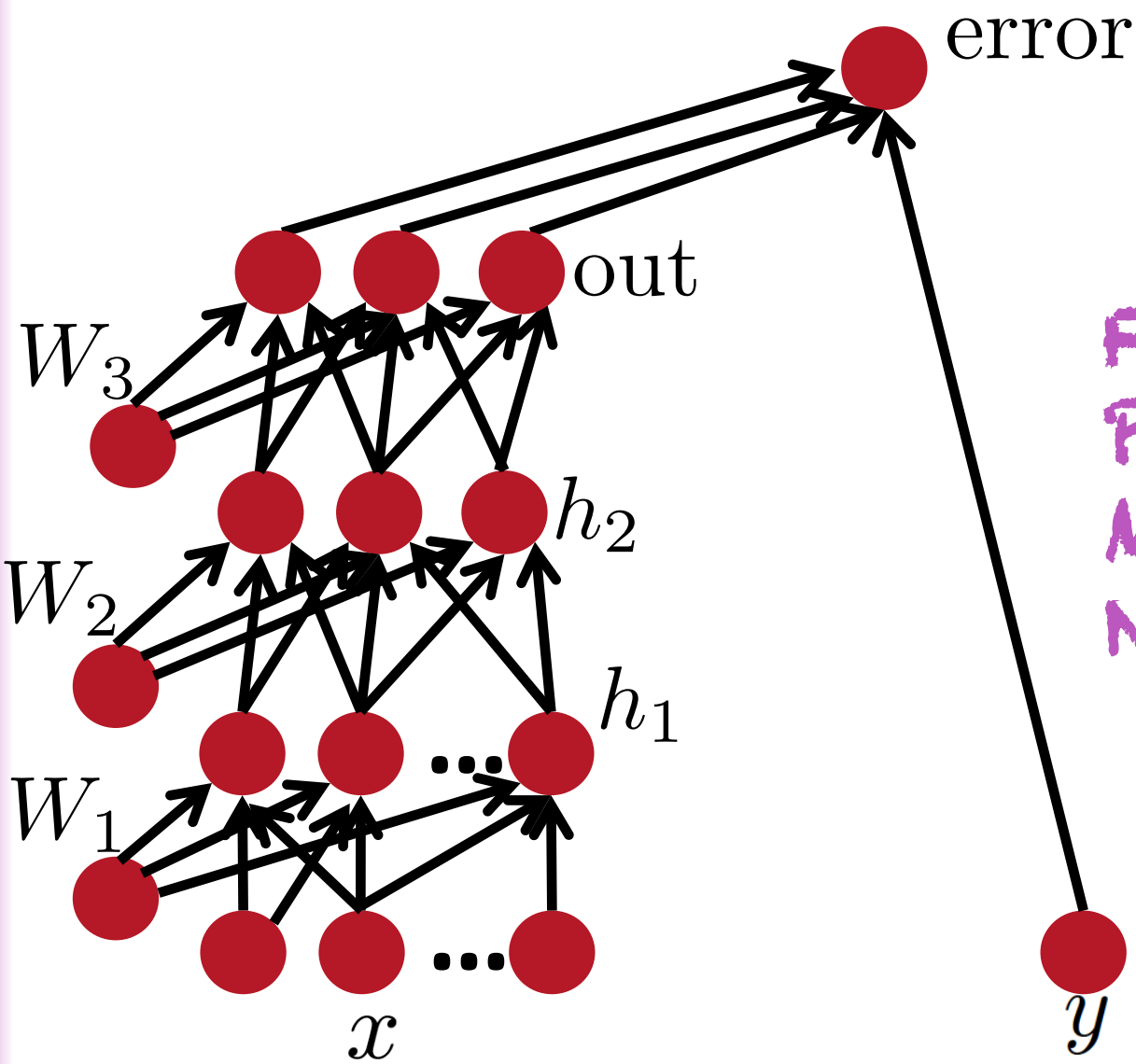
Flow graph: any directed acyclic graph
node = computation result
arc = computation dependency

$\{y_1, y_2, \ldots y_n\}$ = successors of x

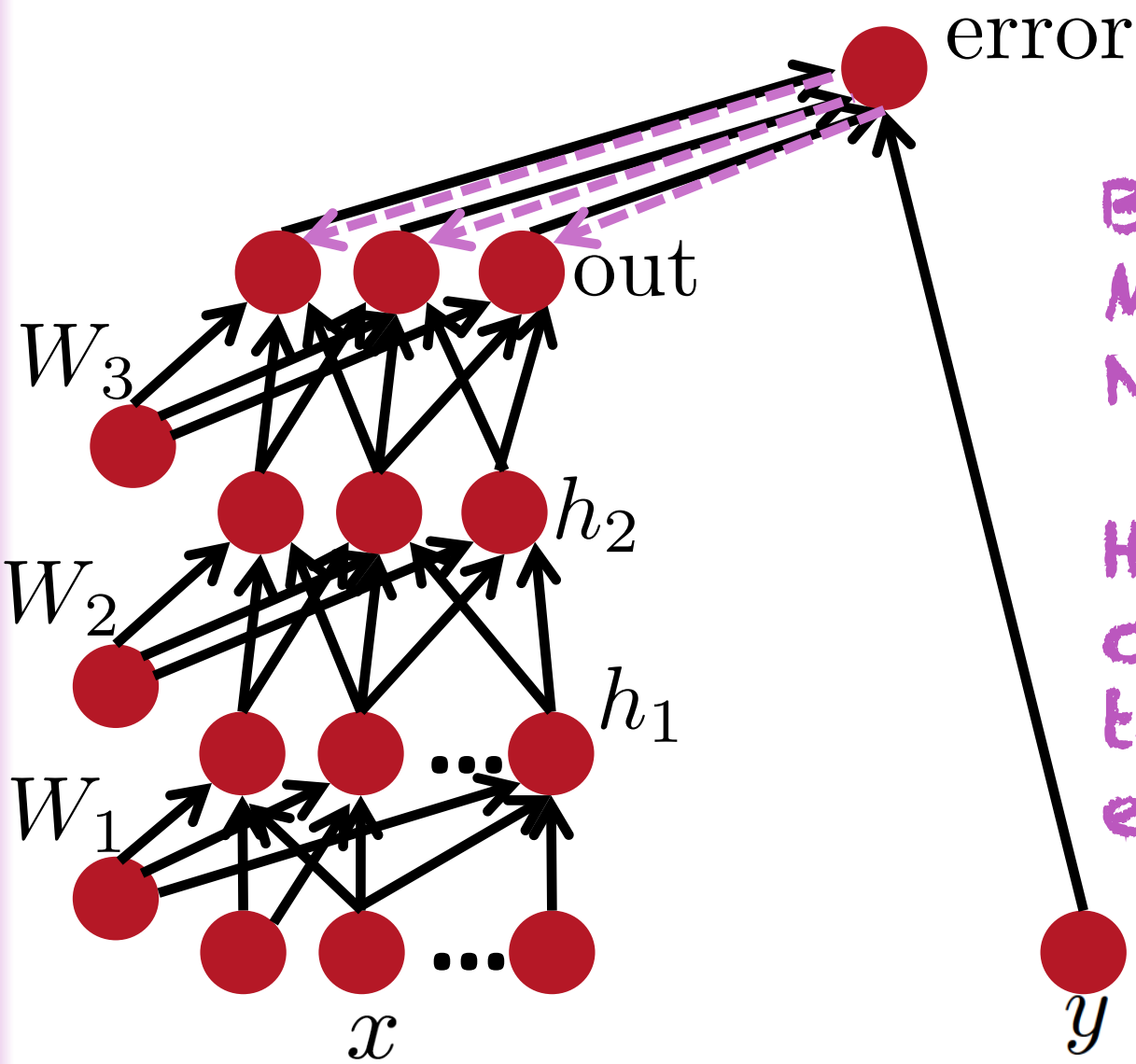
$$\frac{\partial z}{\partial x} = \sum_{i=1}^{n} \frac{\partial z}{\partial y_i} \frac{\partial y_i}{\partial x}$$

Back-Prop in Multi-Layer Net



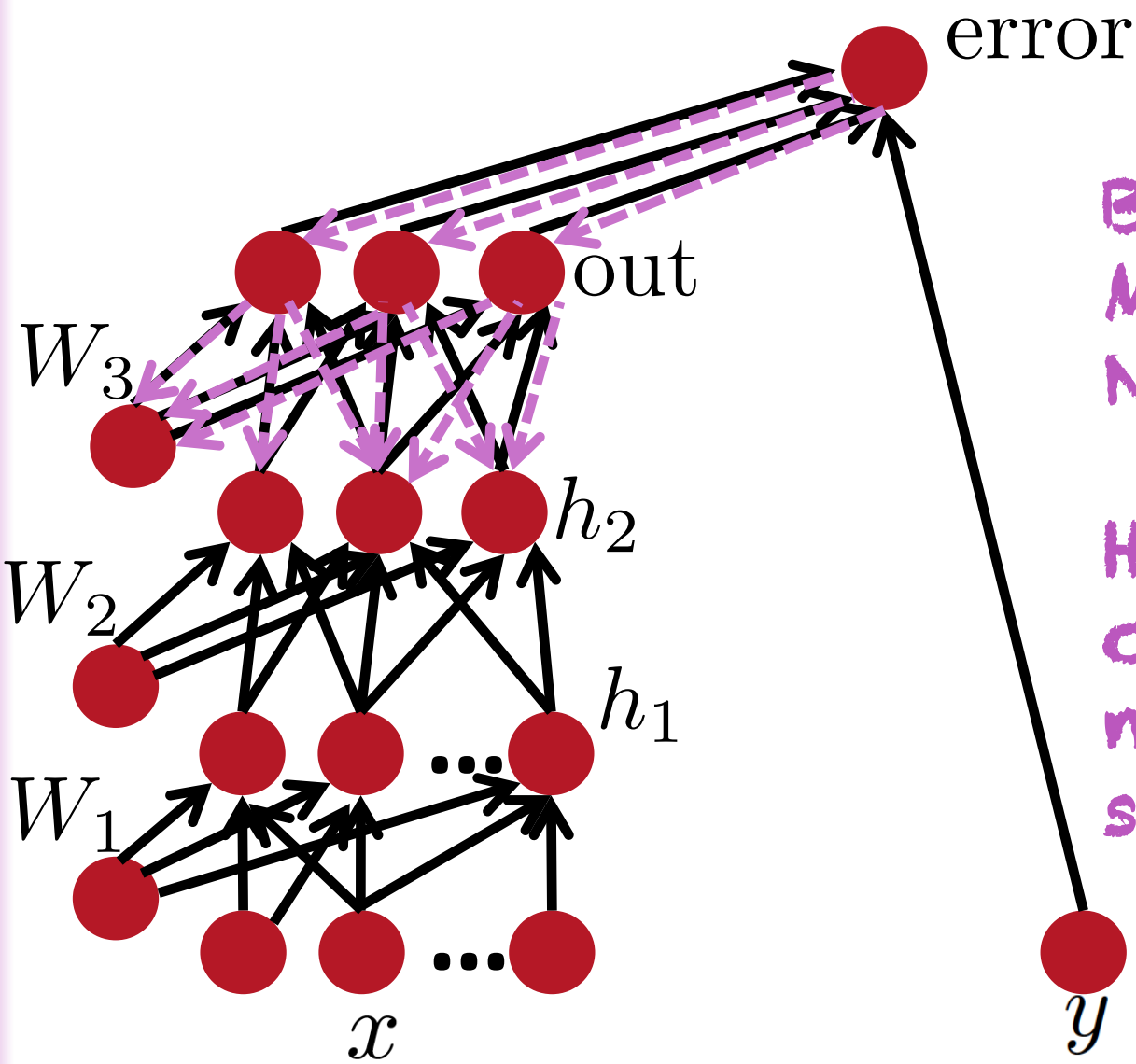


Forward-Prop in Multi-Layer Net



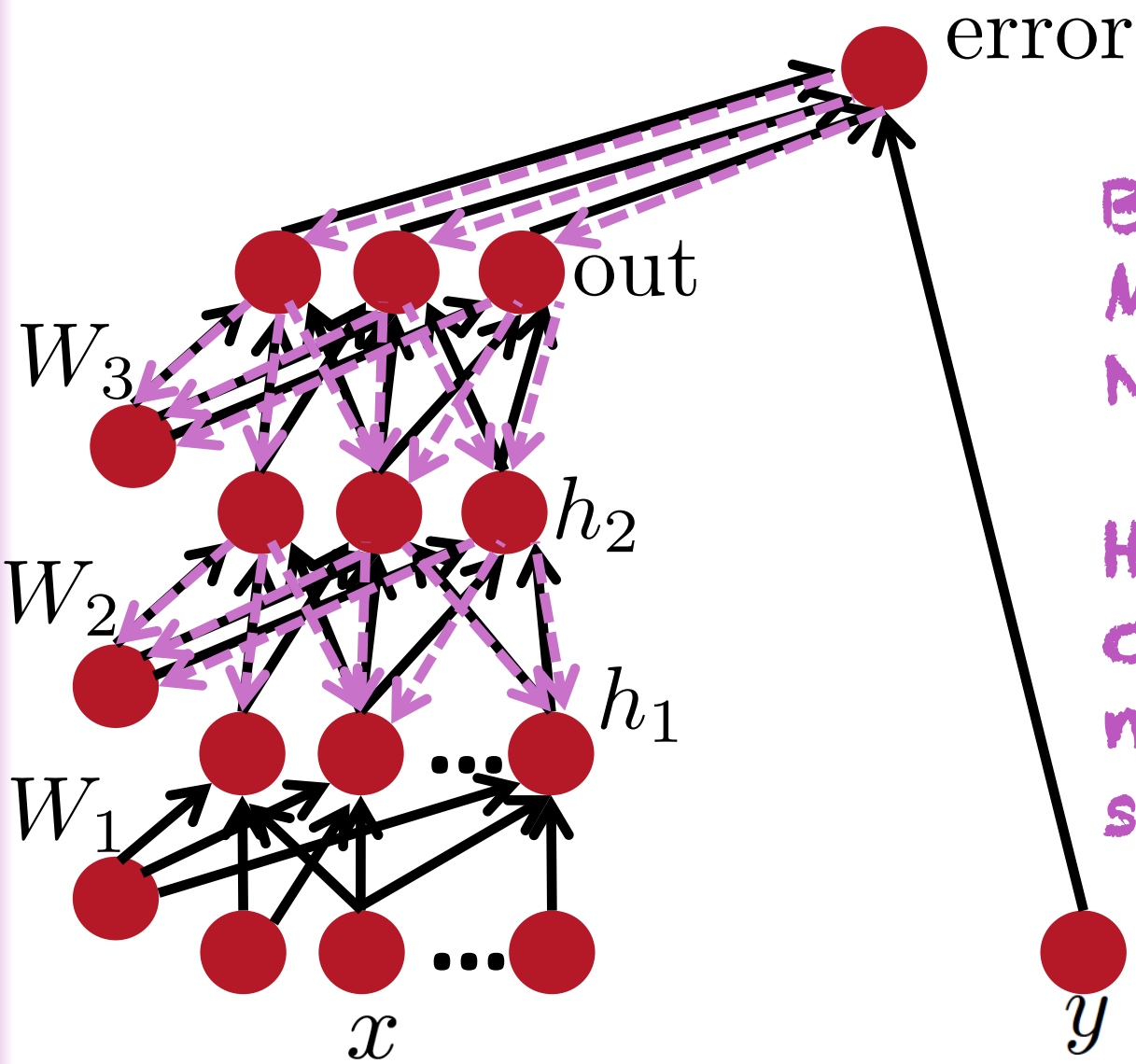
Backprop in Multi-Layer Net:

How outputs could change to make error smaller



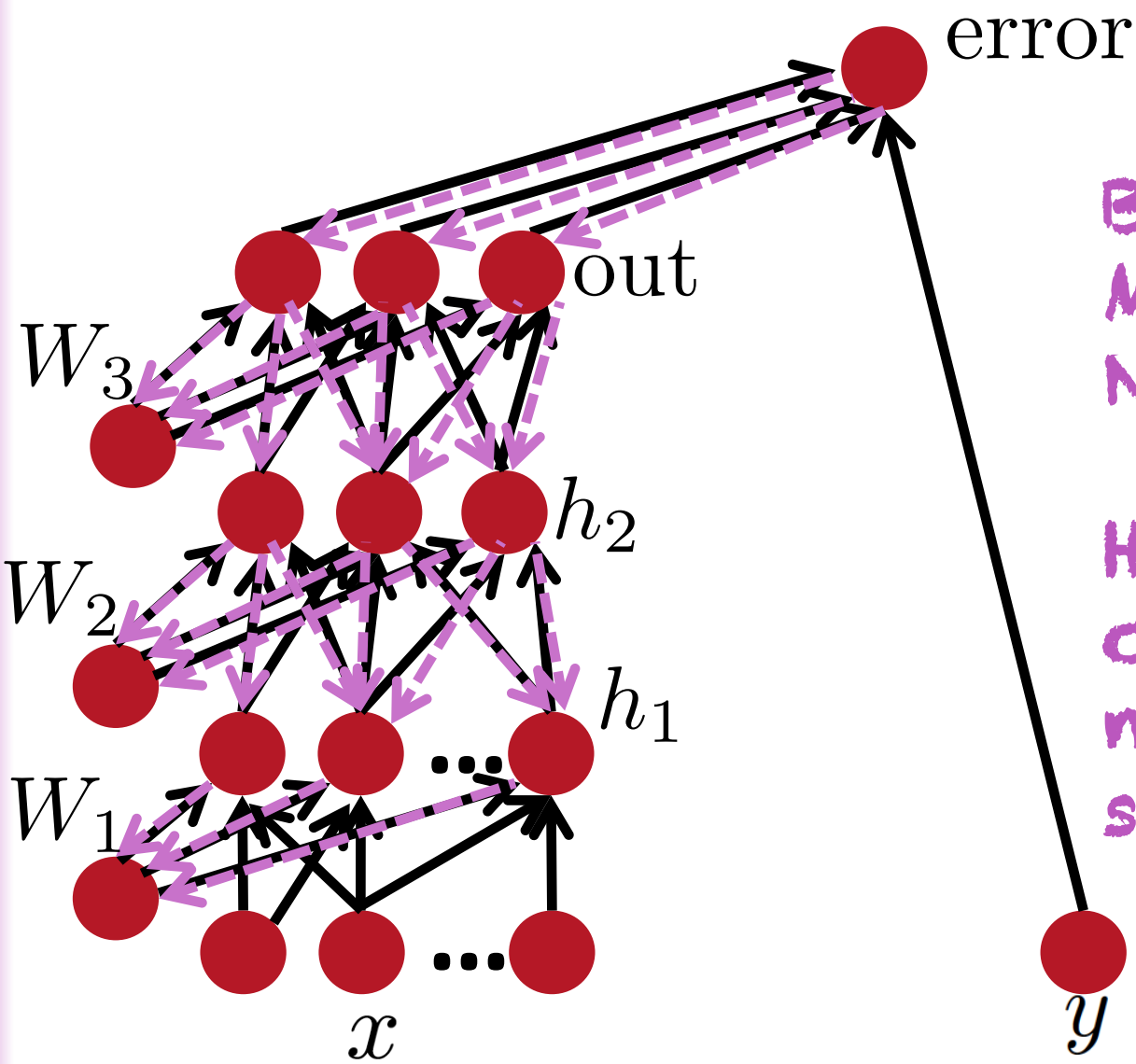
Backprop in Multi-Layer Net:

How h_2 could change to make error smaller



Backprop in Multi-Layer Net:

How h_1 could change to make error smaller

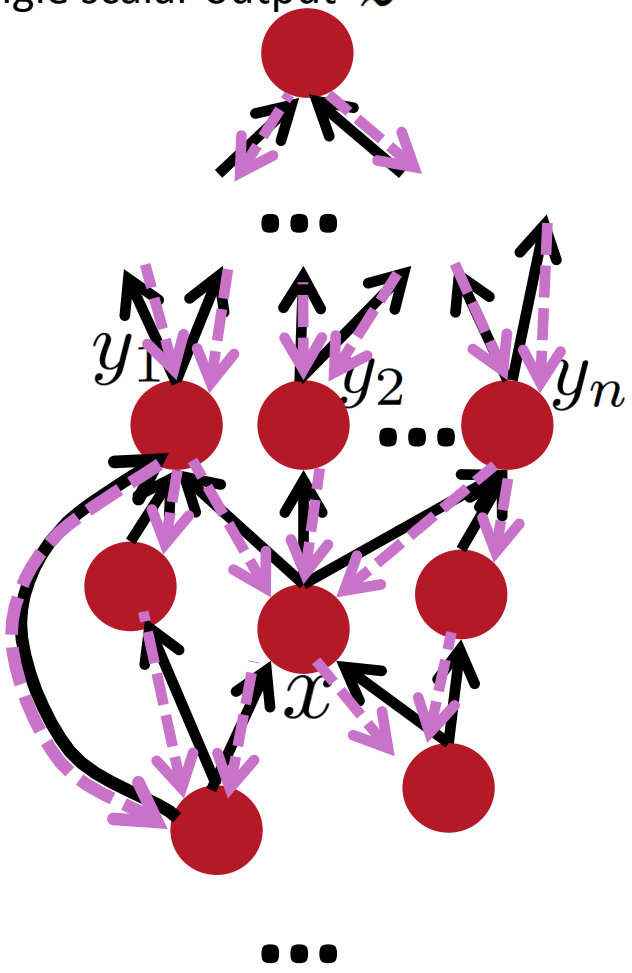


Backprop in Multi-Layer Net:

How W_1 could change to make error smaller

Back-Prop in General Flow Graph

Single scalar output z



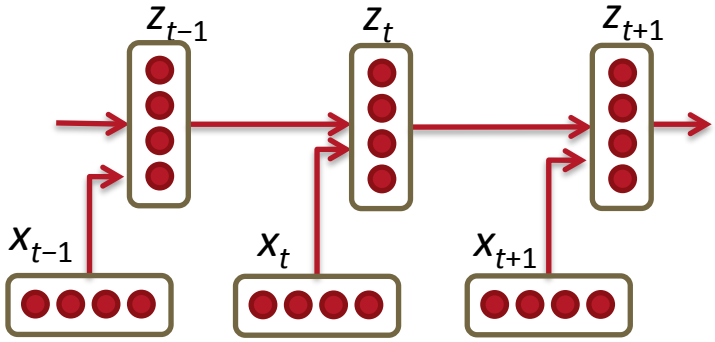
1. Fprop: visit nodes in topo-sort order
   - Compute value of node given predecessors
2. Bprop:
   - initialize output gradient = 1
   - visit nodes in reverse order:
     Compute gradient wrt each node using gradient wrt successors

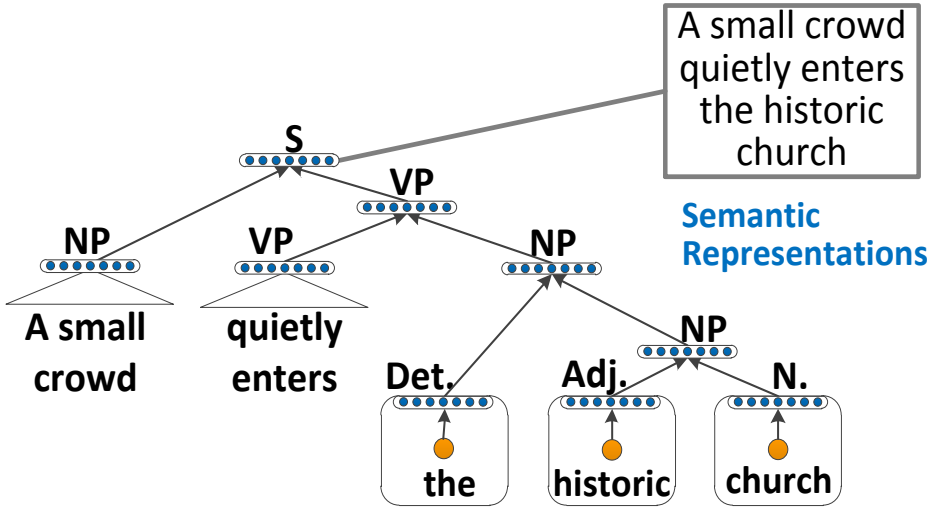
$\{y_1, y_2, \ldots y_n\}$ = successors of x

$$\frac{\partial z}{\partial x} = \sum_{i=1}^{n} \frac{\partial z}{\partial y_i} \frac{\partial y_i}{\partial x}$$

Back-Prop in Recurrent & Recursive Nets

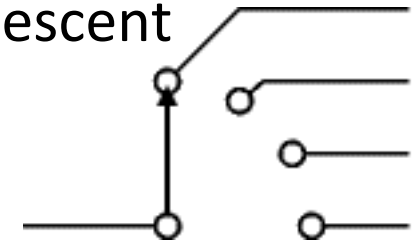
- Replicate a parameterized function over different time steps or nodes of a DAG
- Output state at one time-step / node is used as input for another time-step / node



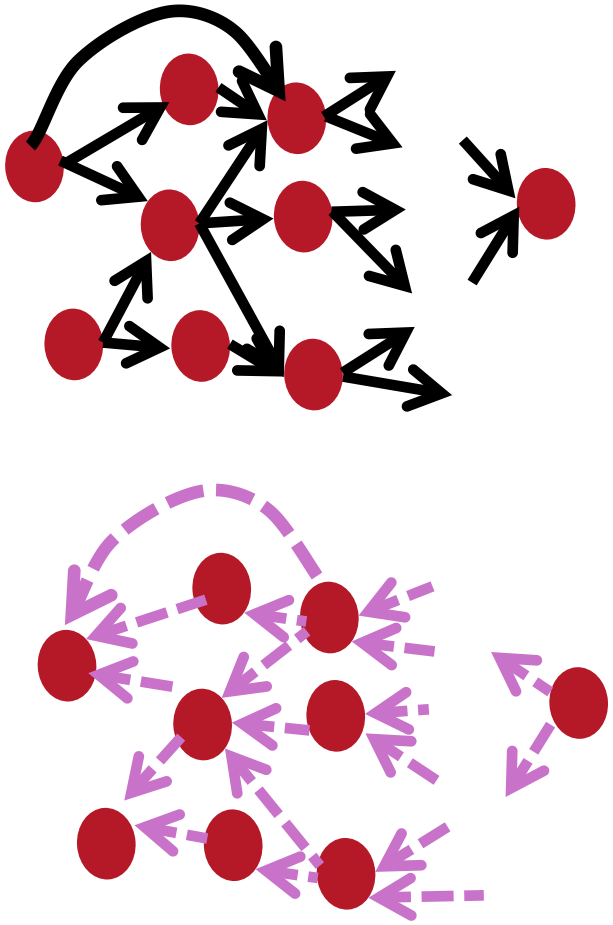


Backpropagation Through Structure

- Inference → discrete choices
  - (e.g., shortest path in HMM, best output configuration in CRF)
- E.g. Max over configurations or sum weighted by posterior
- The loss to be optimized depends on these choices
- The inference operations are flow graph nodes
- If continuous, can perform stochastic gradient descent
  - Max(a,b) is continuous.



Automatic Differentiation



- The gradient computation can be automatically inferred from the symbolic expression of the fprop.
- Each node type needs to know how to compute its output and how to compute the gradient wrt its inputs given the gradient wrt its output.
- Easy and fast prototyping

theano

Machine Learning 101

- Family of functions f_θ
- Tunable parameters θ
- Examples *Z* ~ unknown data generating distribution *P(Z)*
- Loss *L* maps *Z* and f_θ to a scalar
- Regularizer *R* (typically on depends on θ but possibly also on *Z*)
- Training criterion:
$$C(\theta) = \text{average}_{Z \sim \text{dataset}} L(f_\theta, Z) + R(\theta, Z)$$
- Approximate minimization algorithm to search for good θ
- Supervised learning:
  - *Z=(X,Y)* and $L = L(f_\theta(X), Y)$

Log-Likelihood for Neural Nets

- Estimating a conditional probability $P(Y|X)$
- Parametrize it by $P(Y|X) = P(Y|\omega = f_\theta(X))$
- Loss = $-\log P(Y|X)$
- E.g. Gaussian *Y*, $\omega = (\mu, \sigma)$

  typically only μ is the network output, depends on *X*

  Equivalent to MSE criterion:

  Loss = $-\log P(Y|X) = \log \sigma + ||f_\theta(X) - Y||^2/\sigma^2$
- E.g. Multinoulli *Y* for classification,

  $\omega_i = P(Y = i|x) = f_{\theta,i}(X) = \mathrm{softmax}_i(a(X))$

  Loss = $-\log \omega_Y = -\log f_{\theta,Y}(X)$

Multiple Output Variables

- If they are conditionally independent (given X), the individual prediction losses add up:

$$-\log P(Y|X) = -\log P(Y_1, \ldots Y_k|X) = -\log \prod_i P(Y_i|X) = -\sum_i \log P(Y_i|X)$$

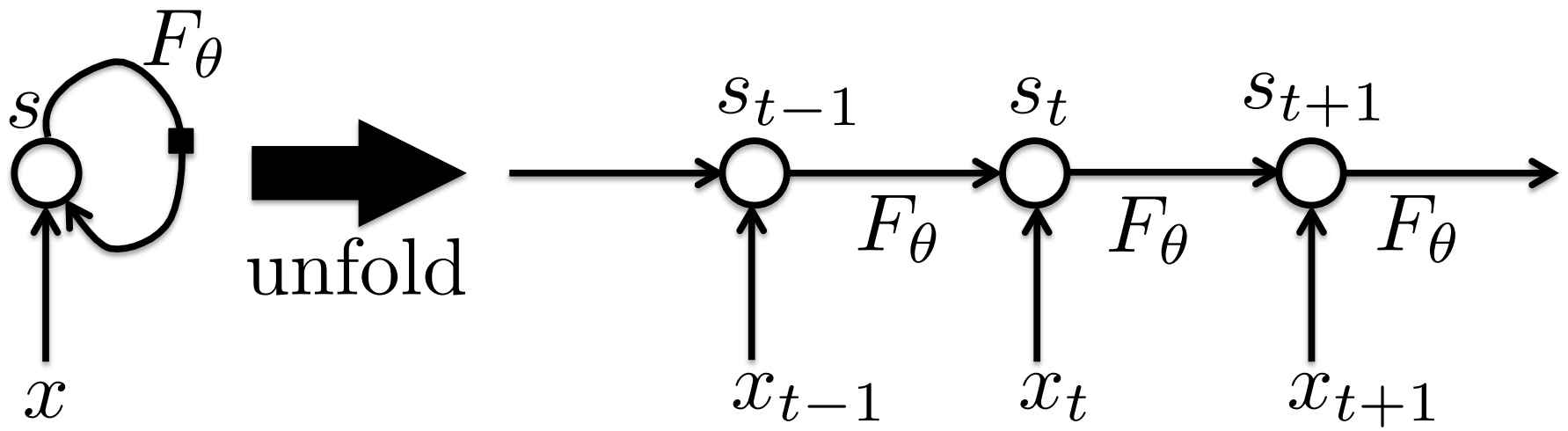
- Likelihood if some Y_i's are missing: just ignore those losses

- If not conditionally independent, need to capture the conditional joint distribution
  - Example: output = image, sentence, tree, etc.
  - $P(Y_1, \ldots Y_k|X)$
  - Similar to unsupervised learning problem of capturing joint
  - Exact likelihood may similarly be intractable, depending on model

Recurrent Neural Networks

- Selectively summarize an input sequence in a fixed-size state vector via a recursive update

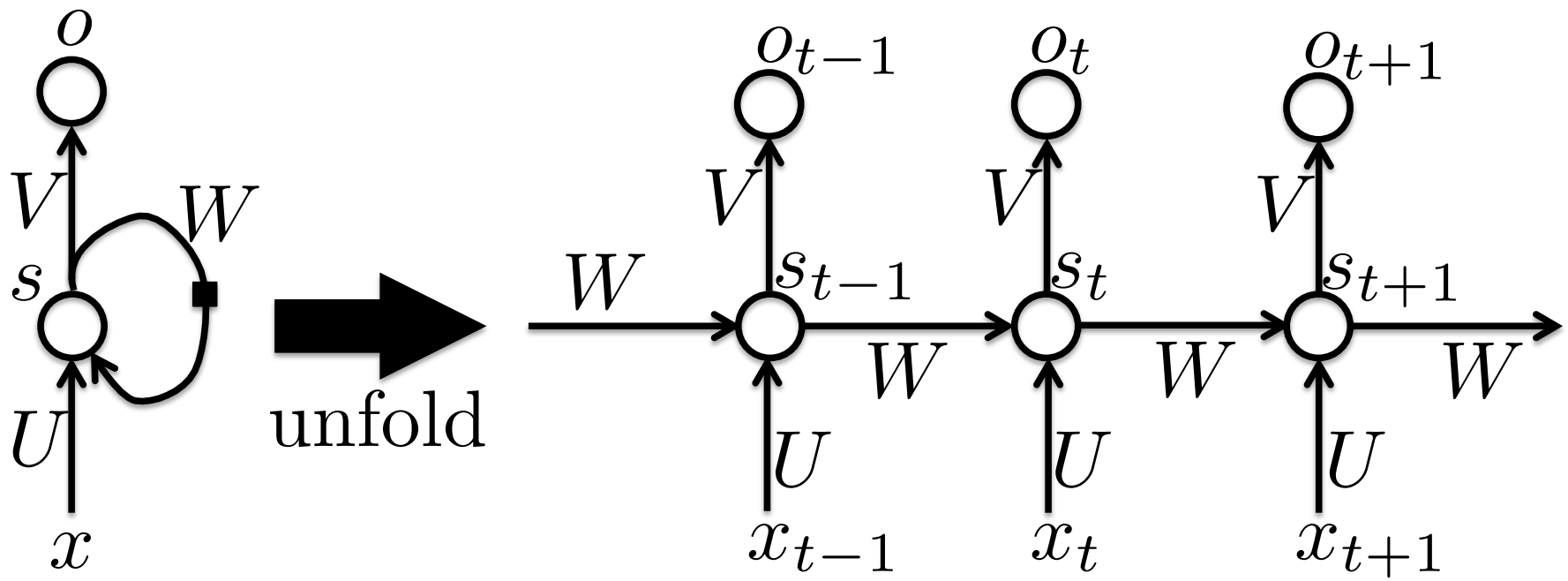
$$s_t = F_\theta(s_{t-1}, x_t)$$



$$s_t = G_t(x_t, x_{t-1}, x_{t-2}, \ldots, x_2, x_1)$$

Recurrent Neural Networks

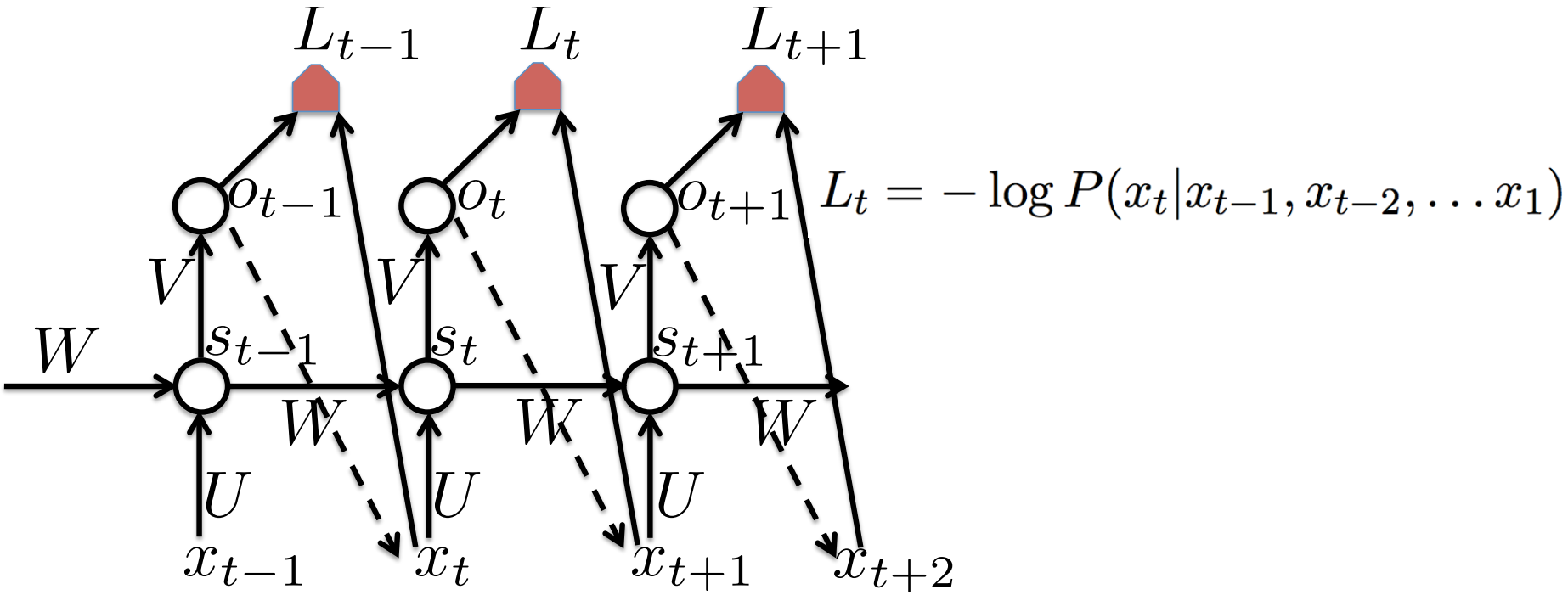
- Can produce an output at each time step: unfolding the graph tells us how to back-prop through time.



Generative RNNs

- An RNN can represent a fully-connected directed generative model: every variable predicted from all previous ones.

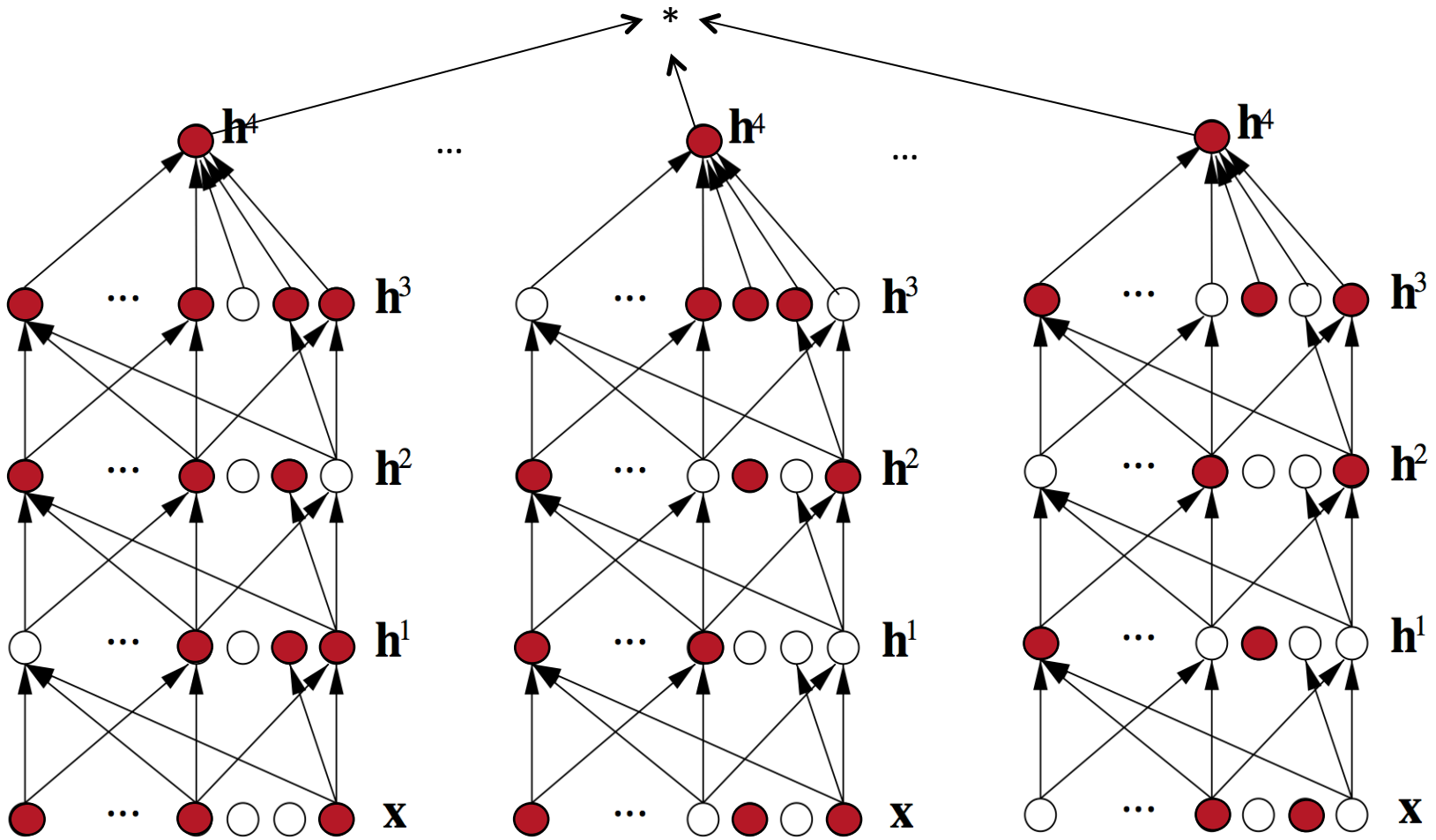
$$P(\mathbf{x}) = P(x_1, \ldots x_T) = \prod_{t=1}^{T} P(x_t | x_{t-1}, x_{t-2}, \ldots x_1)$$



Stochastic Neurons as Regularizer:
Improving neural networks by preventing co-adaptation of feature detectors (Hinton et al 2012, arXiv)

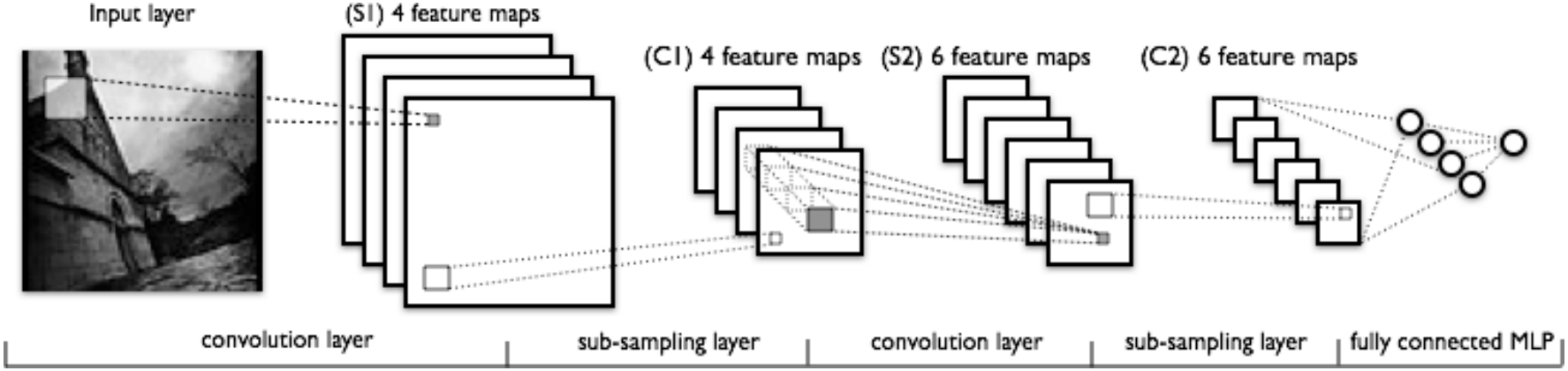
- **Dropouts** trick: during training multiply neuron output by random bit (p=0.5), during test by 0.5
- Used in deep supervised networks
- Similar to denoising auto-encoder, but corrupting every layer
- Works better with some non-linearities (rectifiers, maxout) (Goodfellow et al. ICML 2013)
- Equivalent to averaging over exponentially many architectures
  - Used by Krizhevsky et al to break through ImageNet SOTA
  - Also improves SOTA on CIFAR-10 (18→16% err)
  - Knowledge-free MNIST with DBMs (.95→.79% err)
  - TIMIT phoneme classification (22.7→19.7% err)

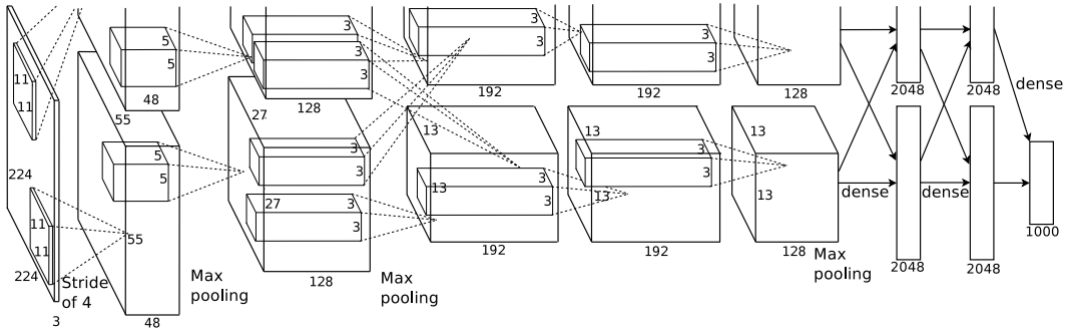
Dropout Regularizer: Super-Efficient Bagging

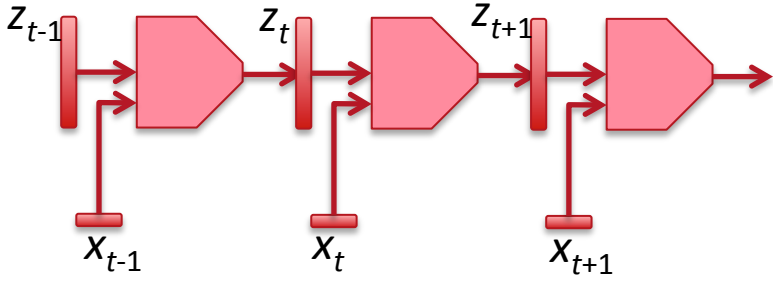


Temporal & Spatial Inputs: Convolutional & Recurrent Nets

- Local connectivity across time/space
- Sharing weights across time/space (translation equivariance)
- Pooling (translation invariance, cross-channel pooling for learned invariances)





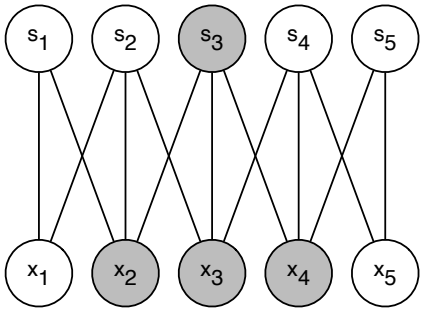


Recurrent nets (RNNs) can summarize information from the past

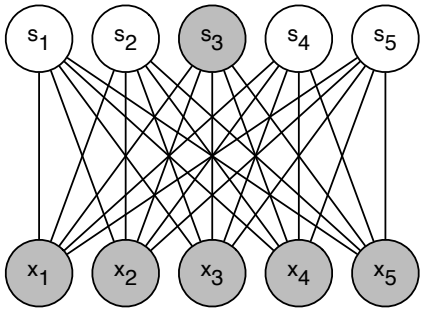
Bidirectional RNNs also summarize information from the future

Convolution = sparse connectivity + parameter sharing

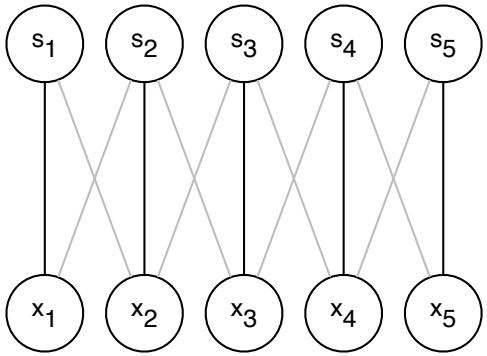
$$s[t] = (x * w)(t) = \sum_{a=-\infty}^{\infty} x[a]w[t-a]$$



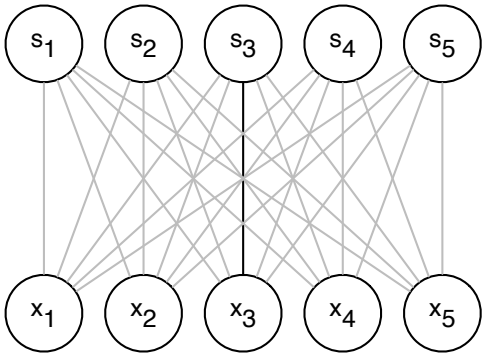
sparse



dense



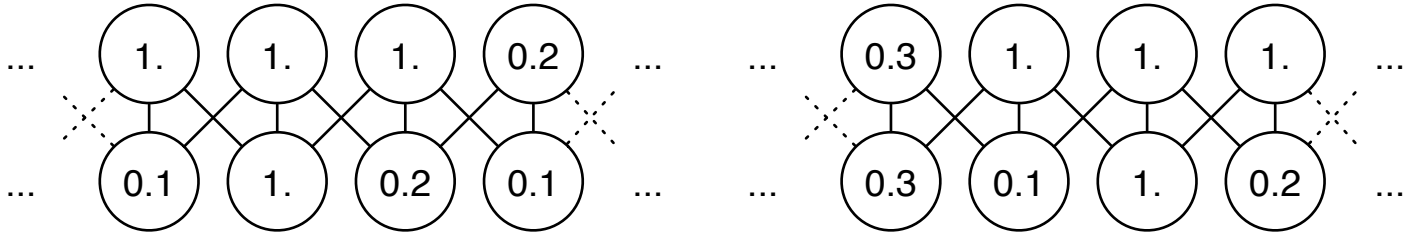
shared



not shared

Pooling Layers

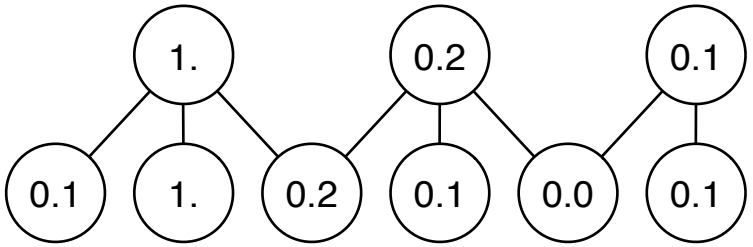
- Aggregate to achieve local invariance



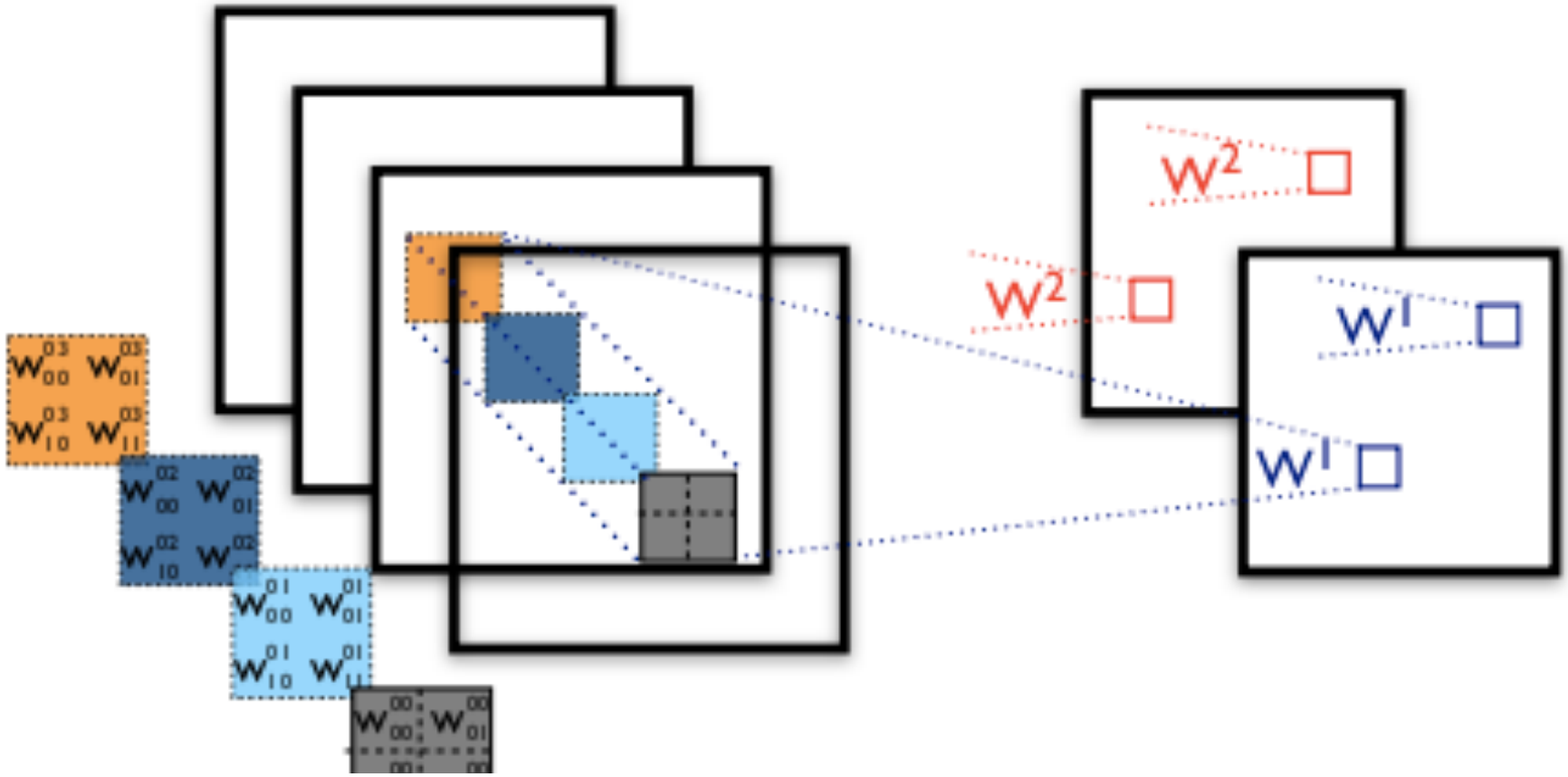
Max-pooling

Effect of translation

- Subsampling to reduce temporal/spatial scale and computation

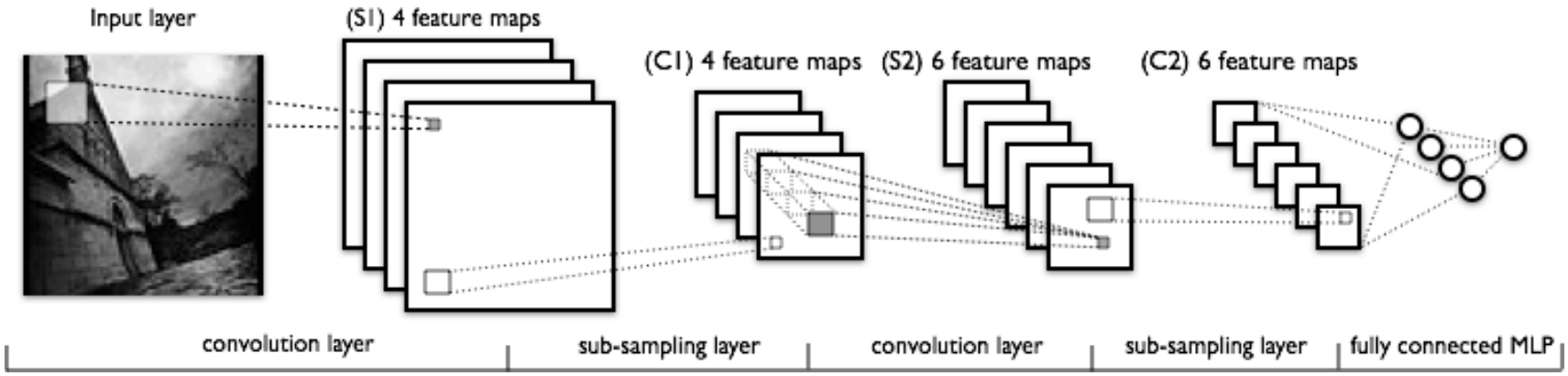


Multiple Convolutions: Feature Maps



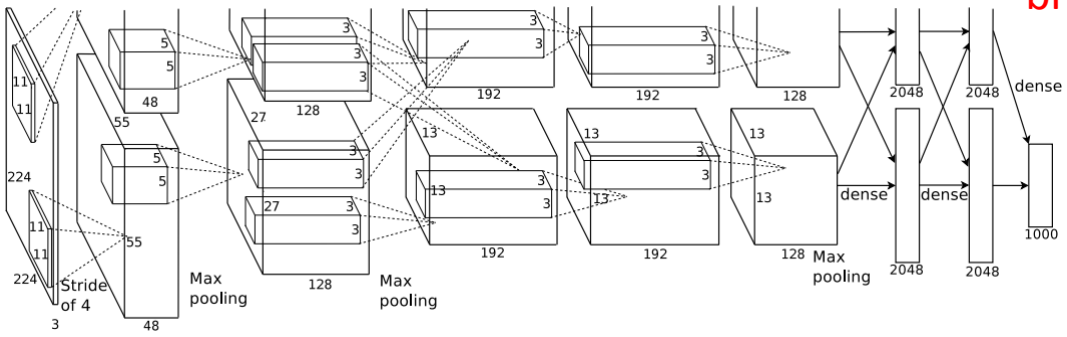
Alternating convolutions & pooling

- Inspired by visual cortex, idea from Fukushima's Neocognitron, combined with back-prop and developped by **LeCun** since 1989



- Increasing number of features, decreasing spatial resolution
- Top layers are fully connected

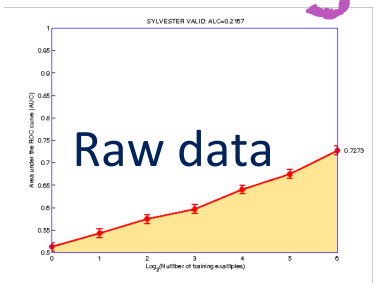
Krizhevsky, Sutskever & Hinton 2012
breakthrough in object recognition

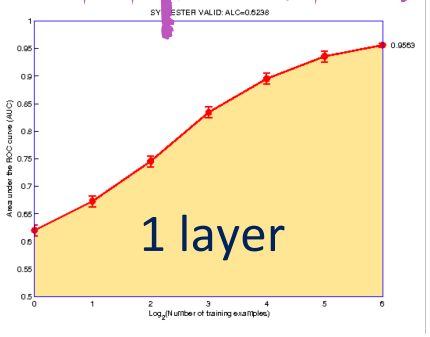


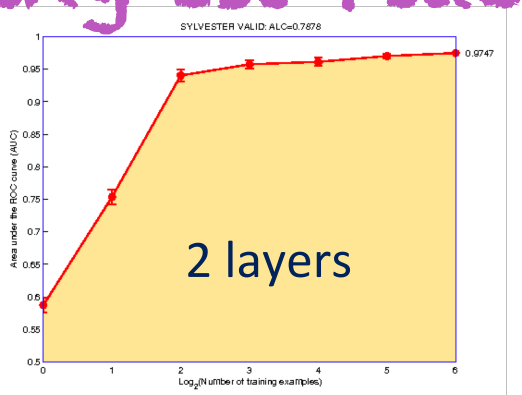
Distributed Representations & Neural Nets:

How to do unsupervised training?

Unsupervised and Transfer Learning Challenge + Transfer Learning Challenge: Deep Learning 1st Place

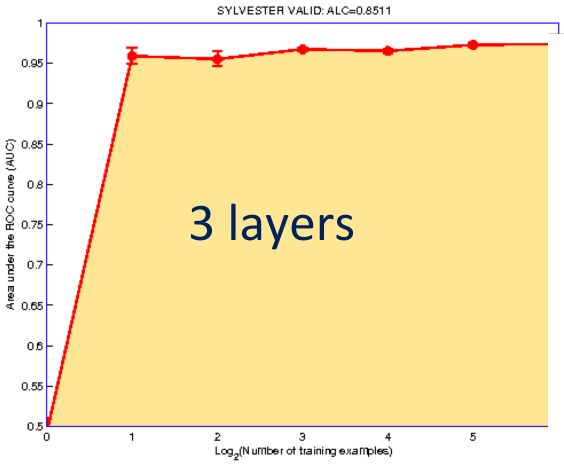


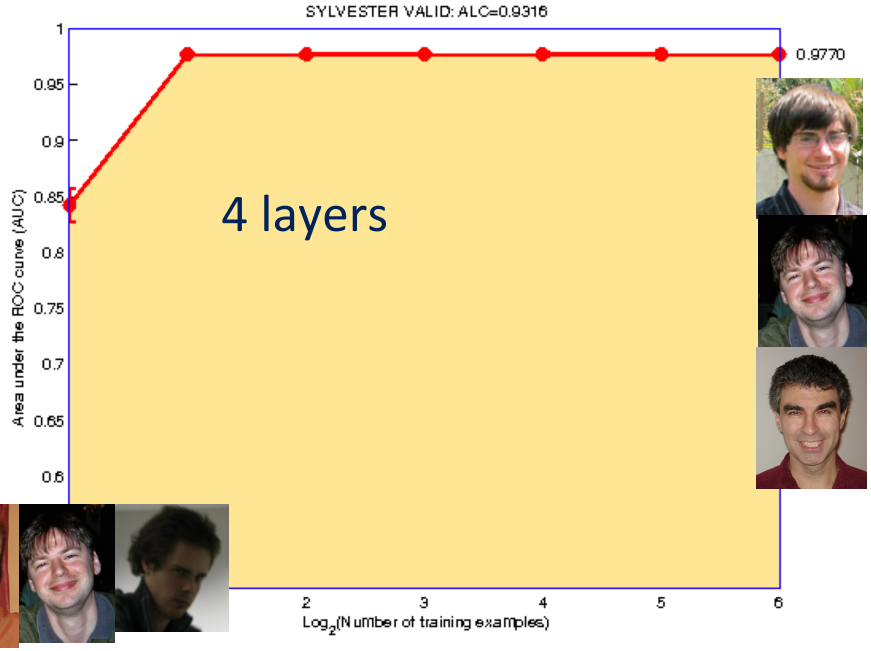




NIPS'2011 Transfer Learning Challenge Paper: ICML'2012

ICML'2011 workshop on Unsup. & Transfer Learning





Why Unsupervised Learning?

- Recent progress mostly in supervised DL
- ∃ real challenges for unsupervised DL
- Potential benefits:
  - Exploit tons of unlabeled data
  - Answer new questions about the variables observed
  - Regularizer – transfer learning – domain adaptation
  - Easier optimization (local training signal)
  - Structured outputs
  - Simulate future for RL and planning

Why Unsupervised Representation Learning? Because of Causality.

- If Ys of interest are among the causal factors of X, then

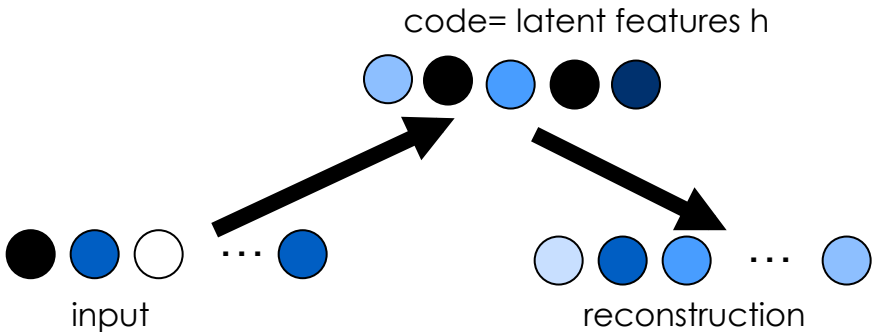
$$P(Y|X) = \frac{P(X|Y)P(Y)}{P(X)}$$

is tied to P(X) and P(X|Y), and P(X) is defined in terms of P(X|Y), i.e.

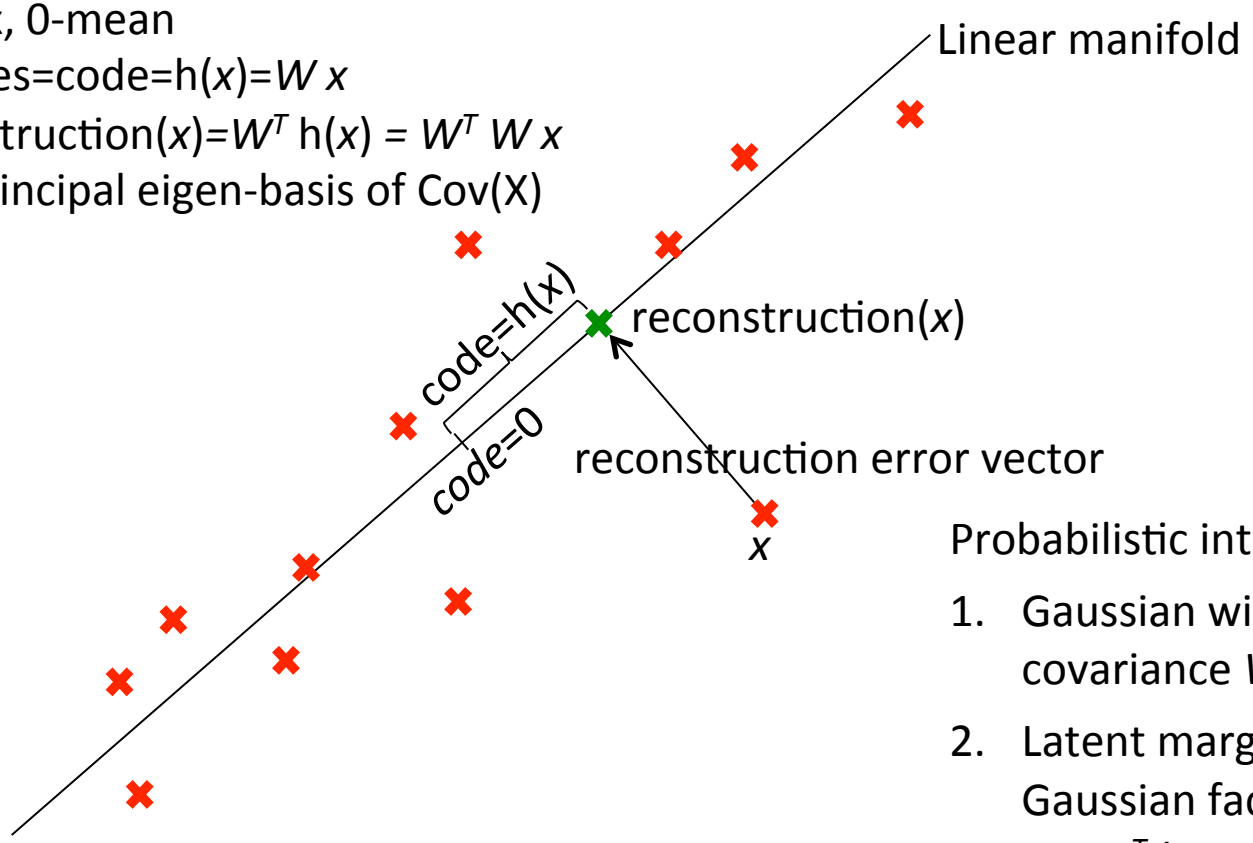
- The best possible model of X (unsupervised learning) MUST involve Y as a latent factor, implicitly or explicitly.
- Representation learning SEEKS the latent variables H that explain the variations of X, making it likely to also uncover Y.
- We need 3 pieces:
  - latent variable model P(H),
  - generative decoder P(X|H), and
  - approximate inference encoder Q(H|X).

PCA

= Linear Manifold
= Linear Auto-Encoder
= Linear Gaussian Factors



input x, 0-mean
features=code=h(x)=$W\,x$
reconstruction(x)=W^T h(x) = $W^T\,W\,x$
W = principal eigen-basis of Cov(X)



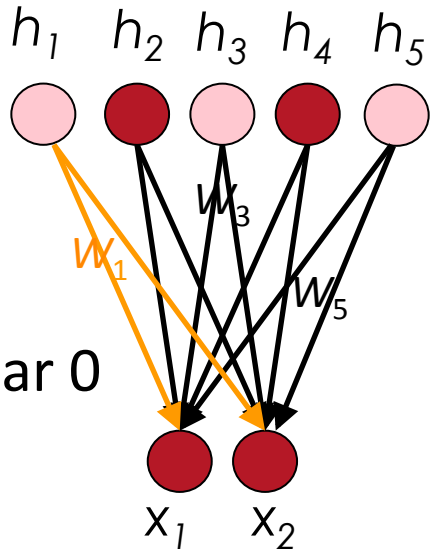
Probabilistic interpretations:

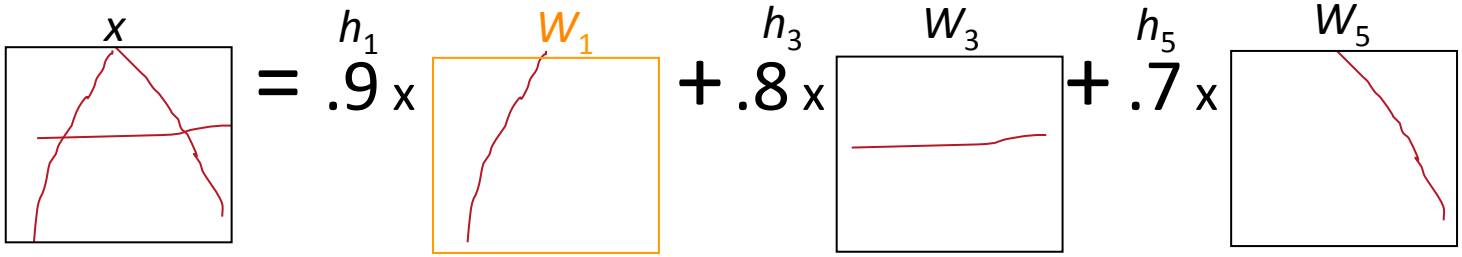
1. Gaussian with full covariance $W^T\,W+\lambda I$
2. Latent marginally iid Gaussian factors h with x = $W^T\,h$ + *noise*

Directed Factor Models: $P(x,h)=P(h)P(x|h)$

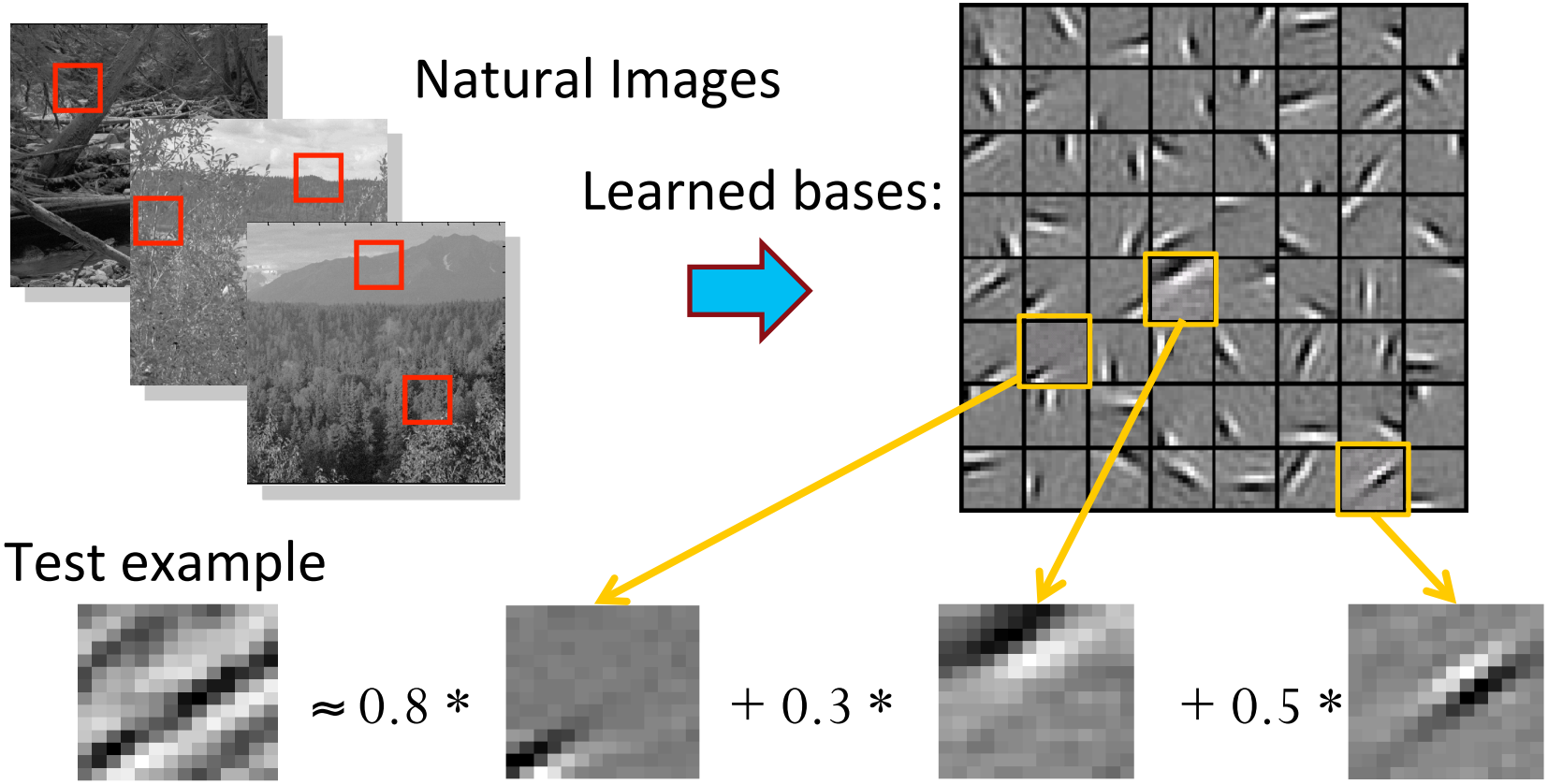
factors prior likelihood

- P(h) factorizes into P(h_1) P(h_2)…
- Different priors:
  - PCA: P(h_i) is Gaussian
  - ICA: P(h_i) is non-parametric
  - **Sparse coding**: P(h_i) is concentrated near 0
- Likelihood is typically Gaussian x | h with mean given by $W^T h$
- Inference procedures (predicting h, given x) differ
- Sparse h: x is explained by the weighted addition of selected filters h_i





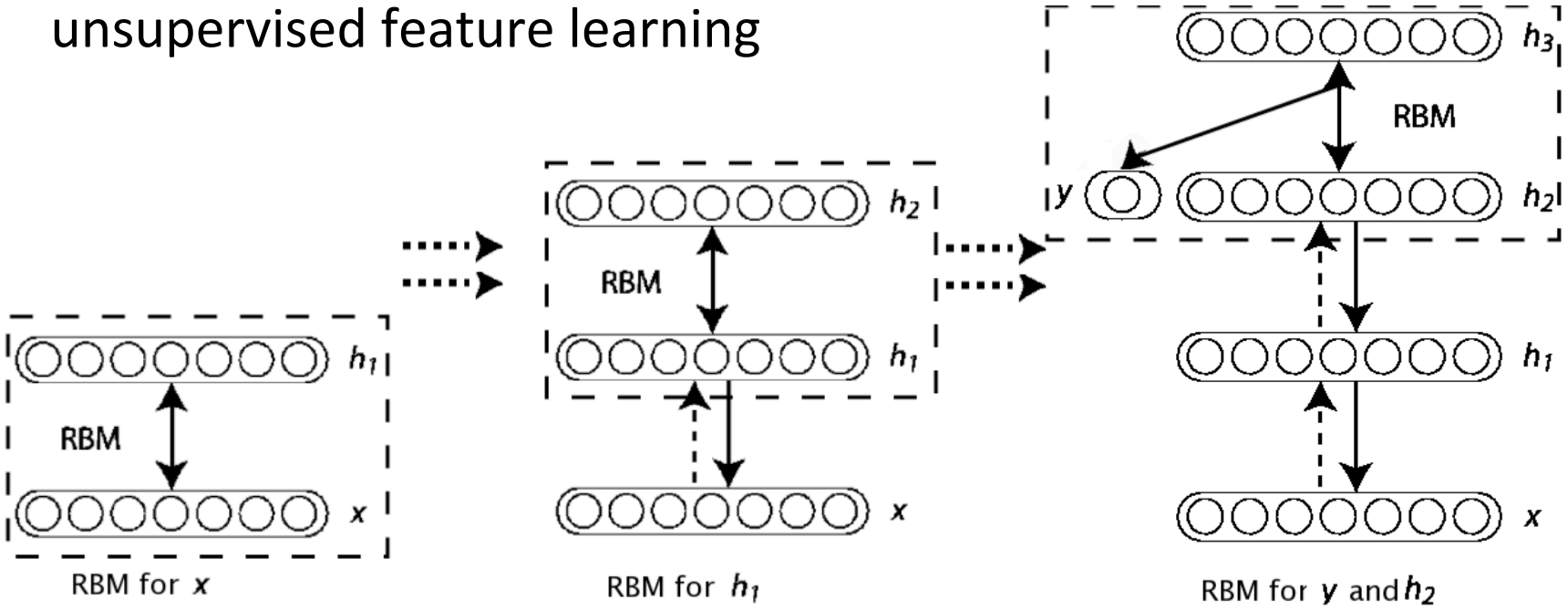
Sparse autoencoder illustration for images



$[h_1, \ldots, h_{64}] = [0, 0, \ldots, 0, \mathbf{0.8}, 0, \ldots, 0, \mathbf{0.3}, 0, \ldots, 0, \mathbf{0.5}, 0]$
(feature representation)

Stacking Single-Layer Learners

- PCA is great but can't be stacked into deeper more abstract representations (linear x linear = linear)
- One of the big ideas from Hinton et al. 2006: layer-wise unsupervised feature learning



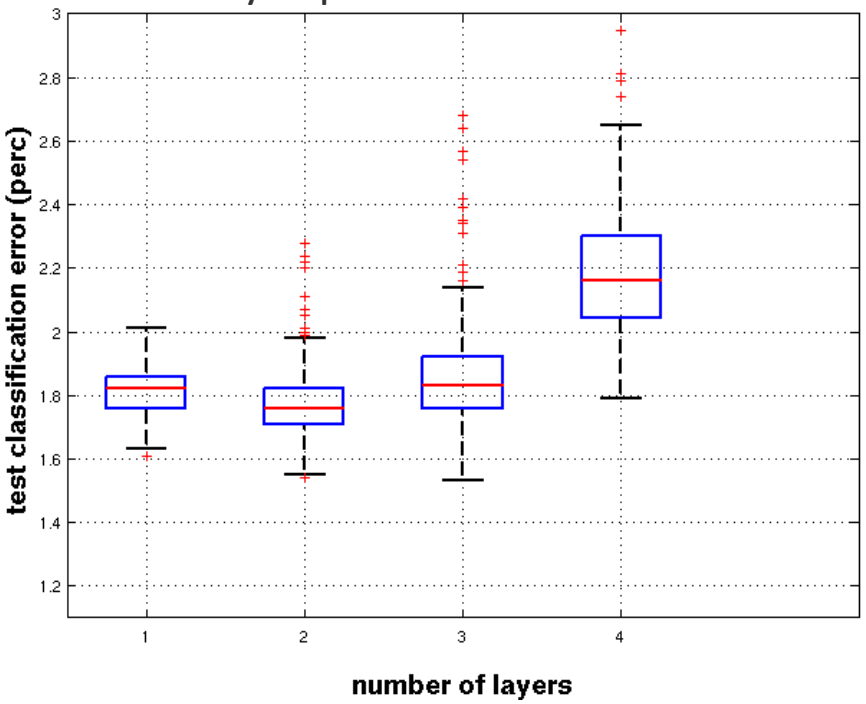
Stacking Restricted Boltzmann Machines (RBM) → Deep Belief Network (DBN)

Effective deep learning first became possible with unsupervised pre-training

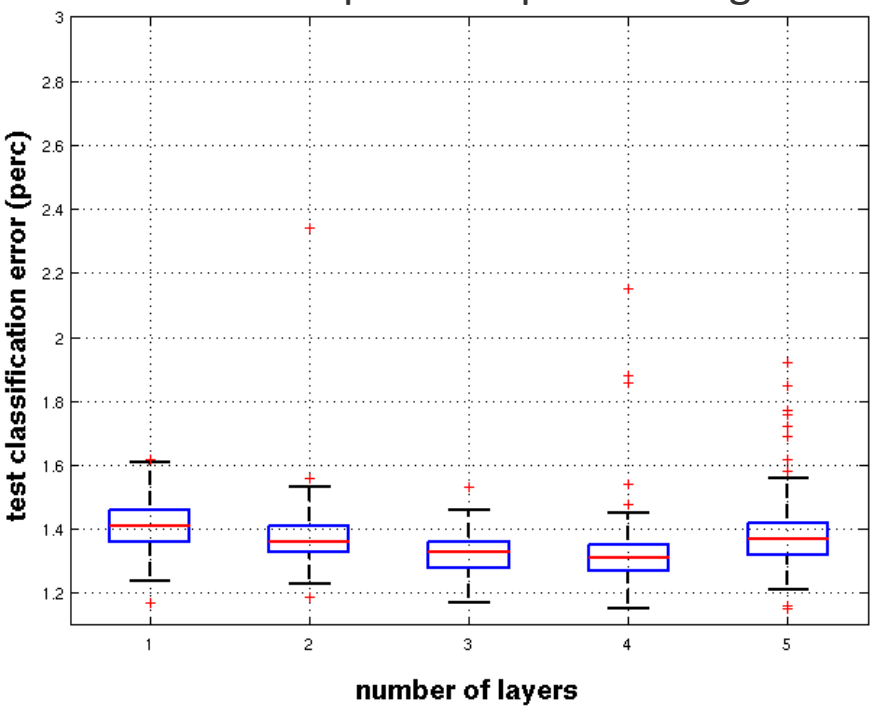
[Erhan et al., JMLR 2010]

(with RBMs and Denoising Auto-Encoders)

Purely supervised neural net



With unsupervised pre-training



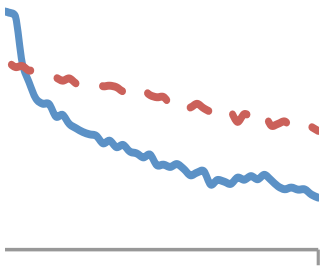
Optimizing Deep Non-Linear Composition of Functions Seems Hard

- Failure of training deep supervised nets before 2006
- Regularization effect + optimization effect of unsupervised pre-training
- Is optimization difficulty due to
  - ill-conditioning?
  - local minima?
  - something else?
- The jury is still out, but we now have many successes training deep supervised nets without unsupervised pre-training

Order & Selection of Examples Matters

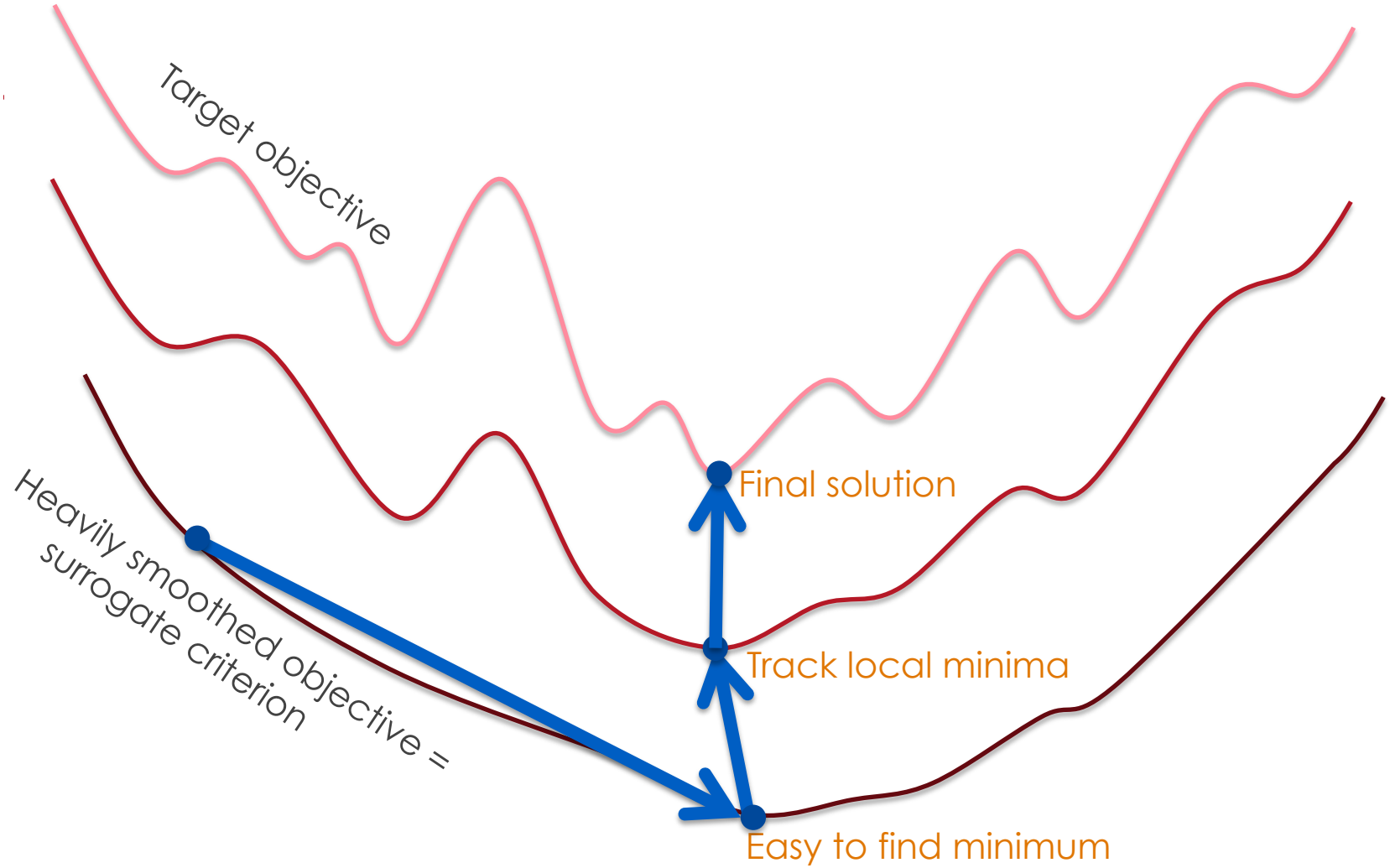
(Bengio, Louradour, Collobert & Weston, ICML'2009)

- Curriculum learning
- (Bengio et al 2009, Krueger & Dayan 2009)
- **Start with easier examples**



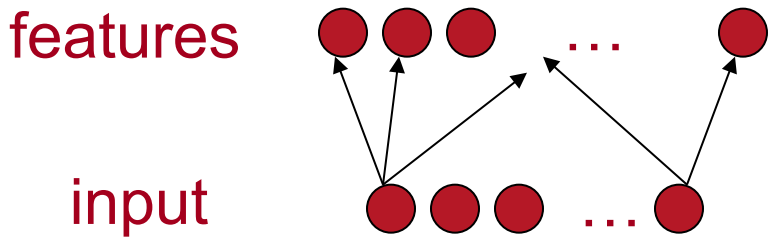
- Faster convergence to a better local minimum in deep architectures

Continuation Methods

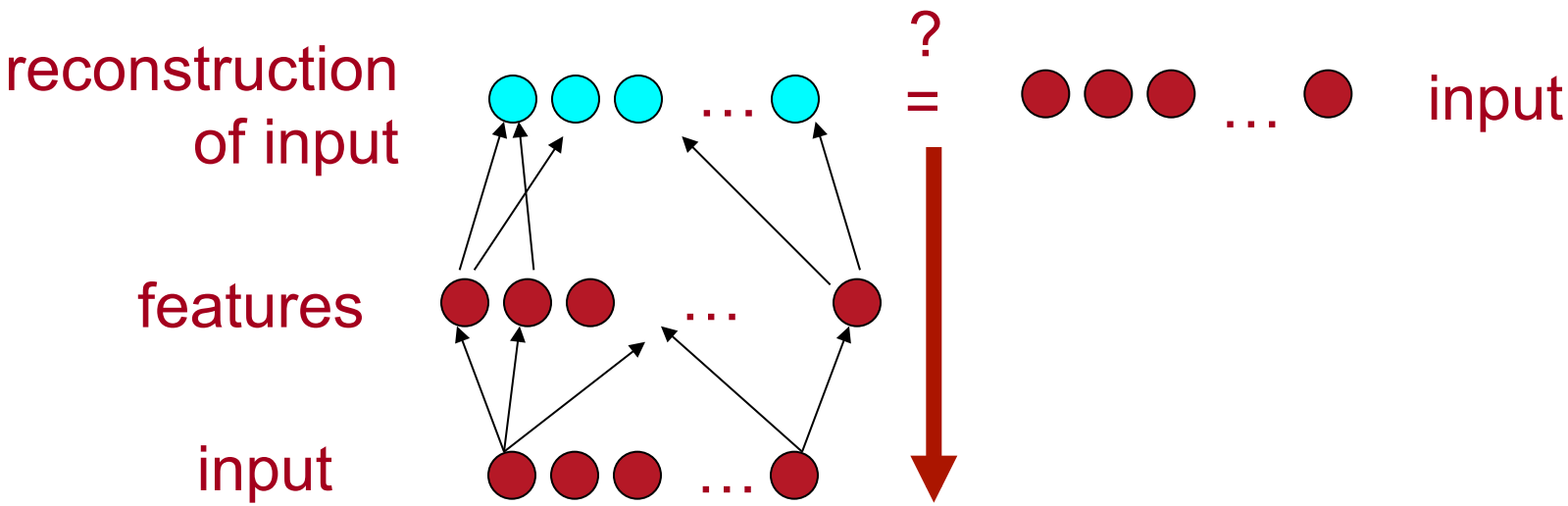


Layer-wise Unsupervised Learning

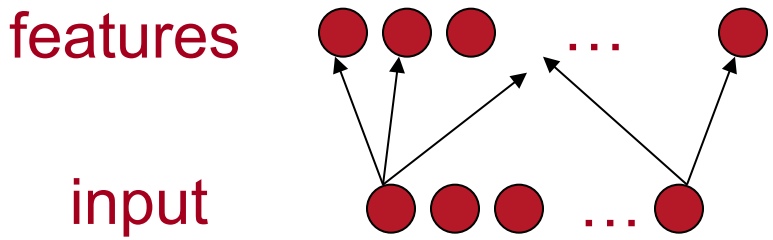
Layer-Wise Unsupervised Pre-training



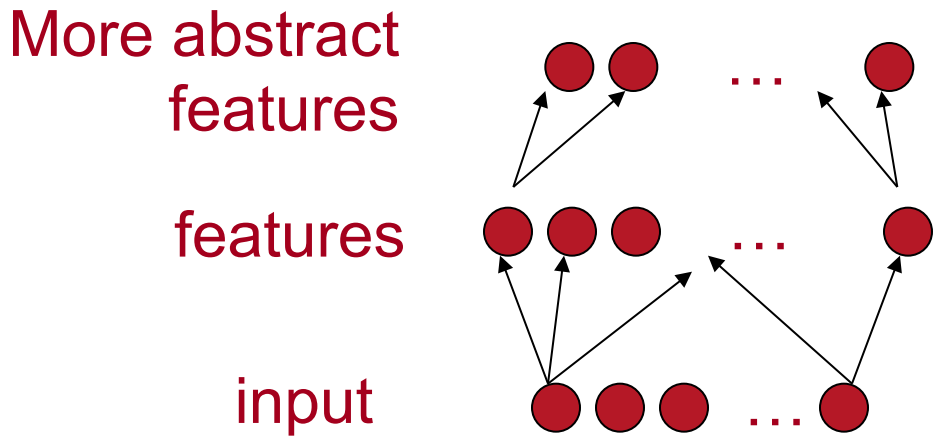
Layer-Wise Unsupervised Pre-training



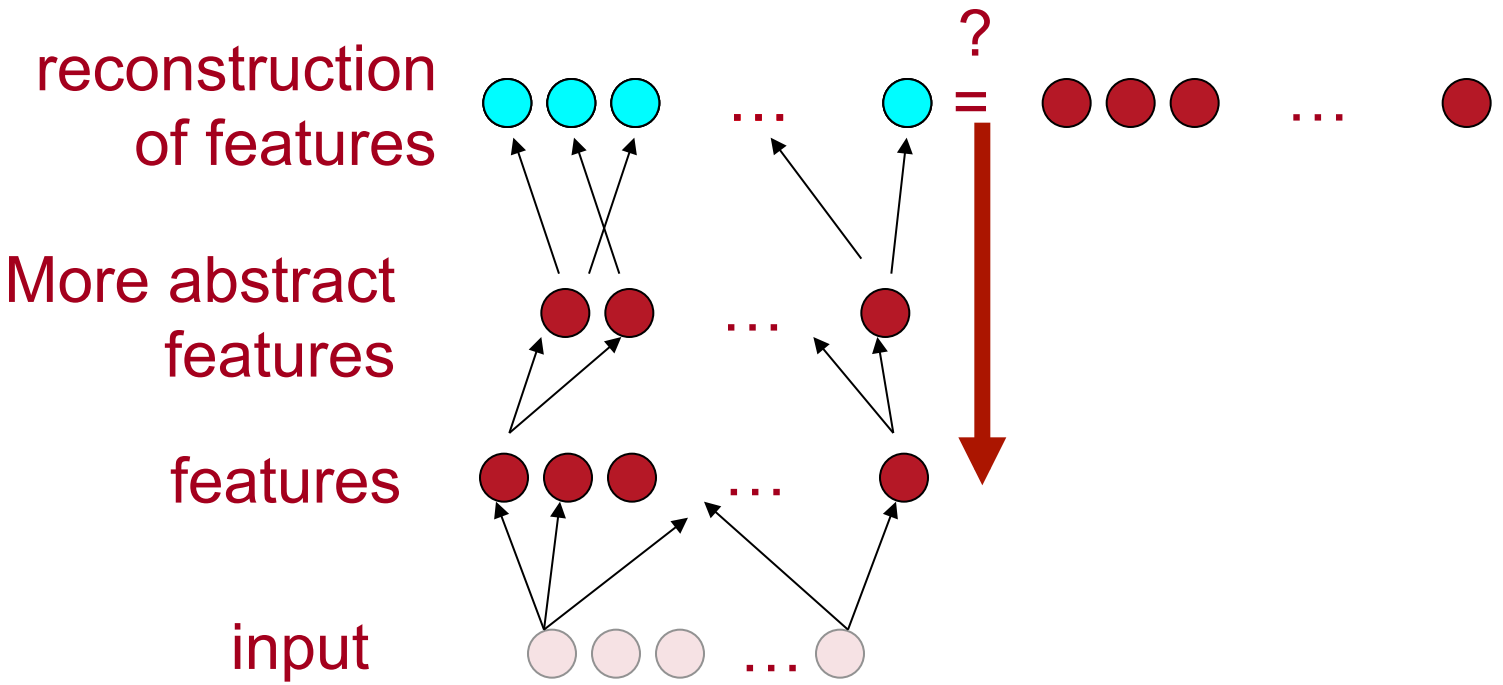
Layer-Wise Unsupervised Pre-training



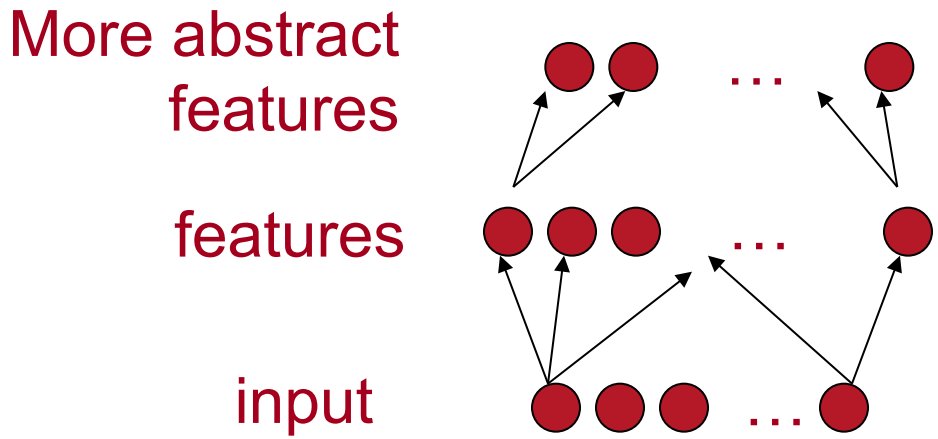
Layer-Wise Unsupervised Pre-training



Layer-wise Unsupervised Learning



Layer-Wise Unsupervised Pre-training



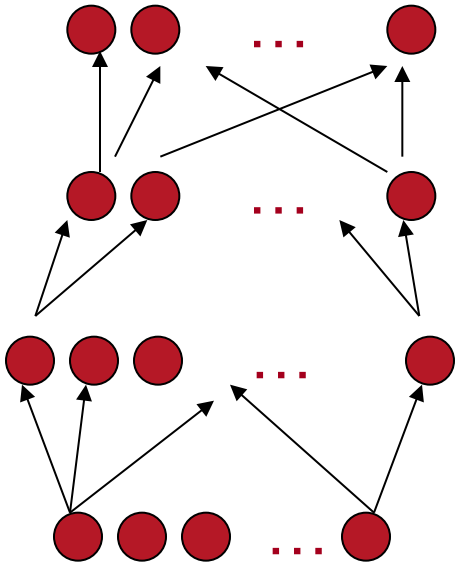
Layer-wise Unsupervised Learning

Even more abstract features

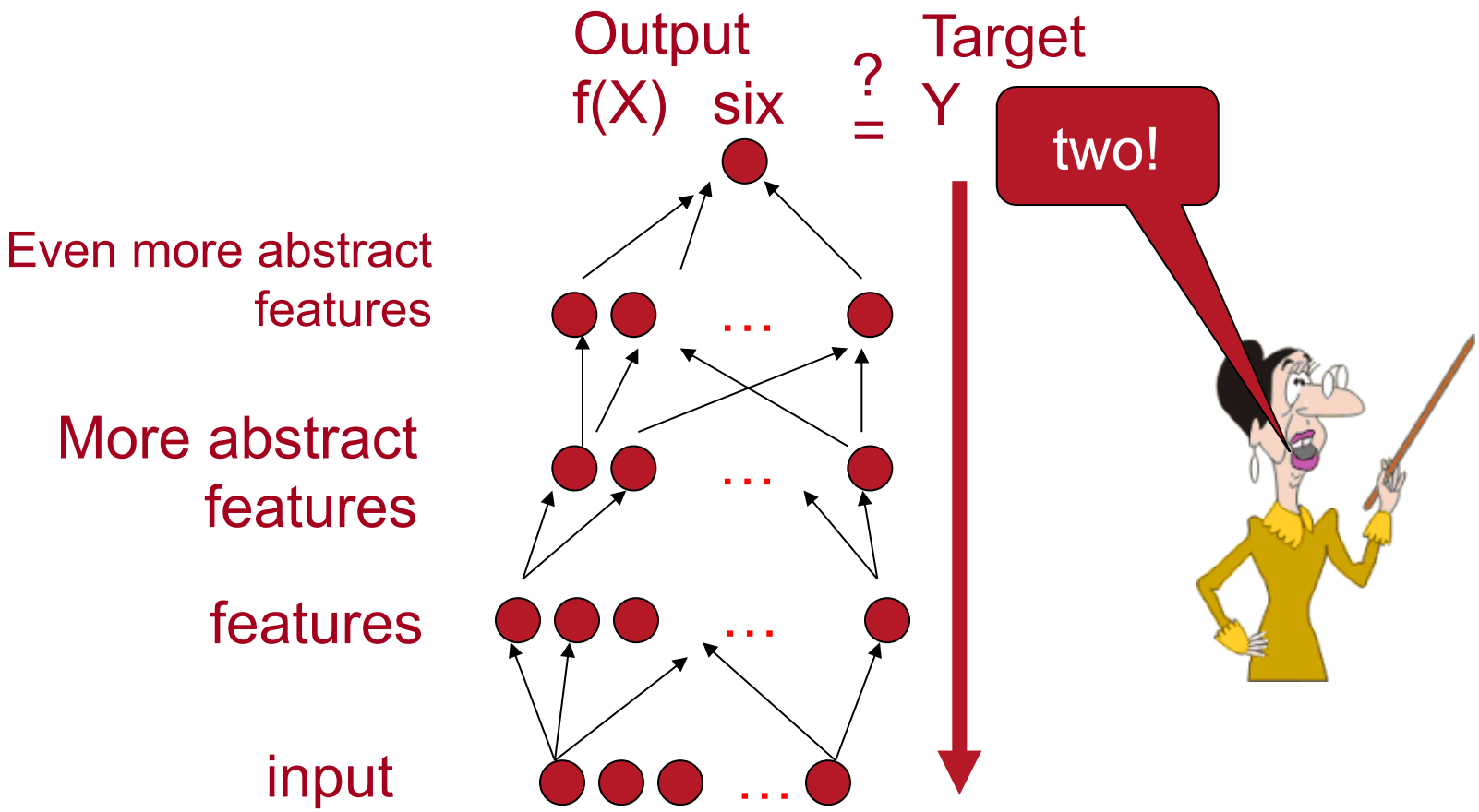
More abstract features

features

input

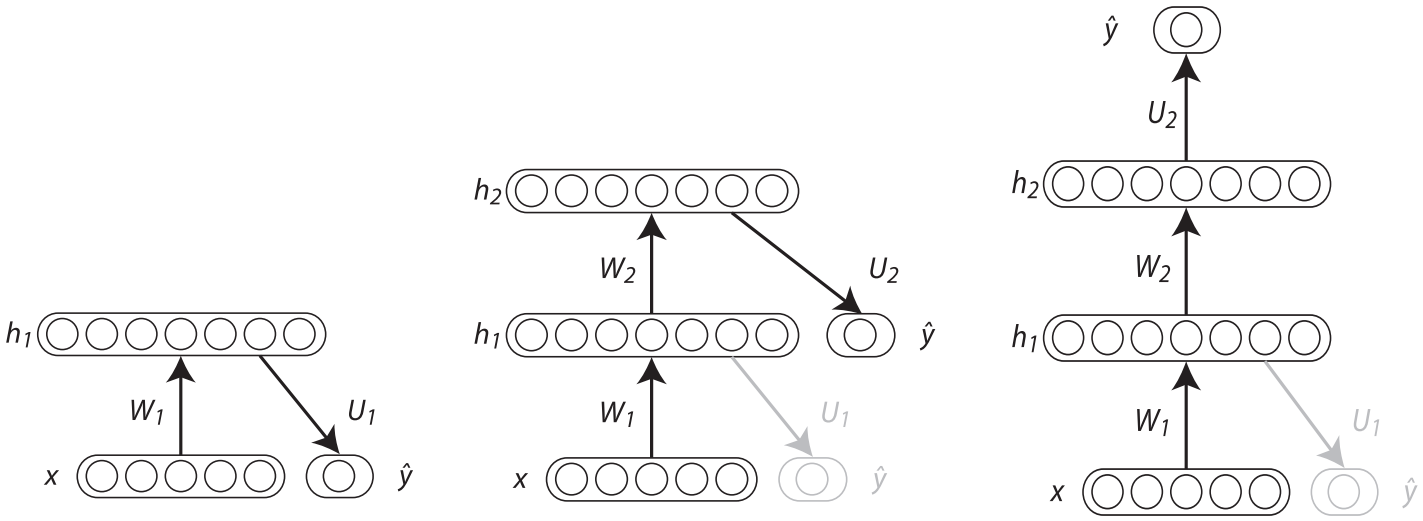


Supervised Fine-Tuning



- Additional hypothesis: features good for P(x) good for P(y|x)

Greedy Layerwise Supervised Training



Generally worse than unsupervised pre-training but better than ordinary training of a deep neural network (Bengio et al. NIPS'2006). Has been used successfully on large labeled datasets, where unsupervised pre-training did not make as much of an impact.

Understanding the difficulty of training deep feedforward supervised neural networks

(Glorot & Bengio, AISTATS 2010)


Study the activations and gradients

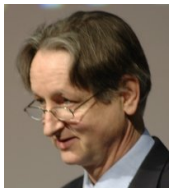
- wrt depth
- as training progresses
- for different initializations → big difference
- for different non-linearities → big difference

First demonstration that deep supervised nets can be successfully trained almost as well as with unsupervised pre-training, by setting up the optimization problem appropriately…

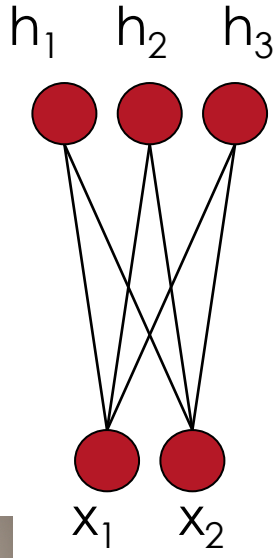
Restricted Boltzmann Machines

Undirected Models: the Restricted Boltzmann Machine

[Hinton et al 2006]



- Probabilistic model of the joint distribution of the observed variables (inputs alone or inputs and targets) x
- Latent (hidden) variables h model high-order dependencies
- Inference is easy, $P(h|x)$ factorizes into product of $P(h_i \mid x)$



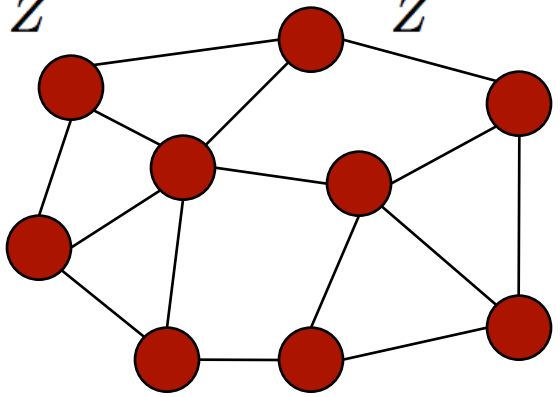
- See Bengio (2009) detailed monograph/review: *"Learning Deep Architectures for AI"*.
- See Hinton (2010) *"A practical guide to training Restricted Boltzmann Machines"*

Boltzmann Machines & MRFs

- Boltzmann machines:

(Hinton 84) $$P(x) = \frac{1}{Z} e^{-\text{Energy}(x)} = \frac{1}{Z} e^{c^T x + x^T W x} = \frac{1}{Z} e^{\sum_i c_i x_i + \sum_{i,j} x_i W_{ij} x_j}$$

- Markov Random Fields:



Undirected graphical models

$$P(x) = \frac{1}{Z} e^{\sum_i w_i f_i(x)}$$

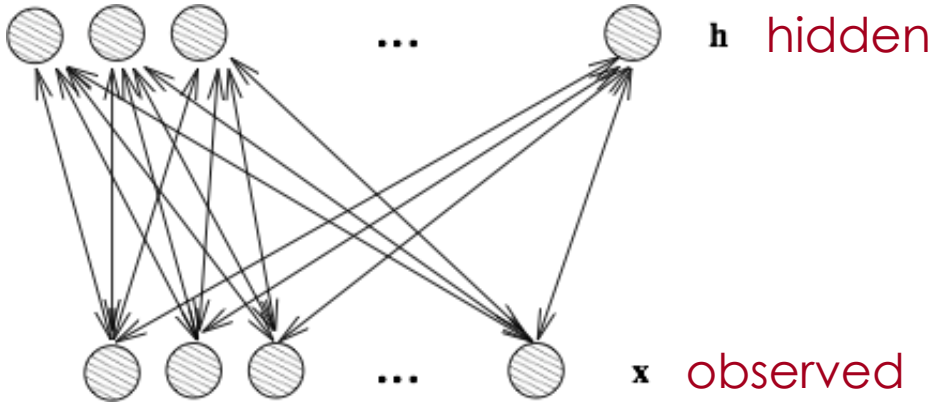
Soft constraint / probabilistic statement

- More interesting with latent variables!

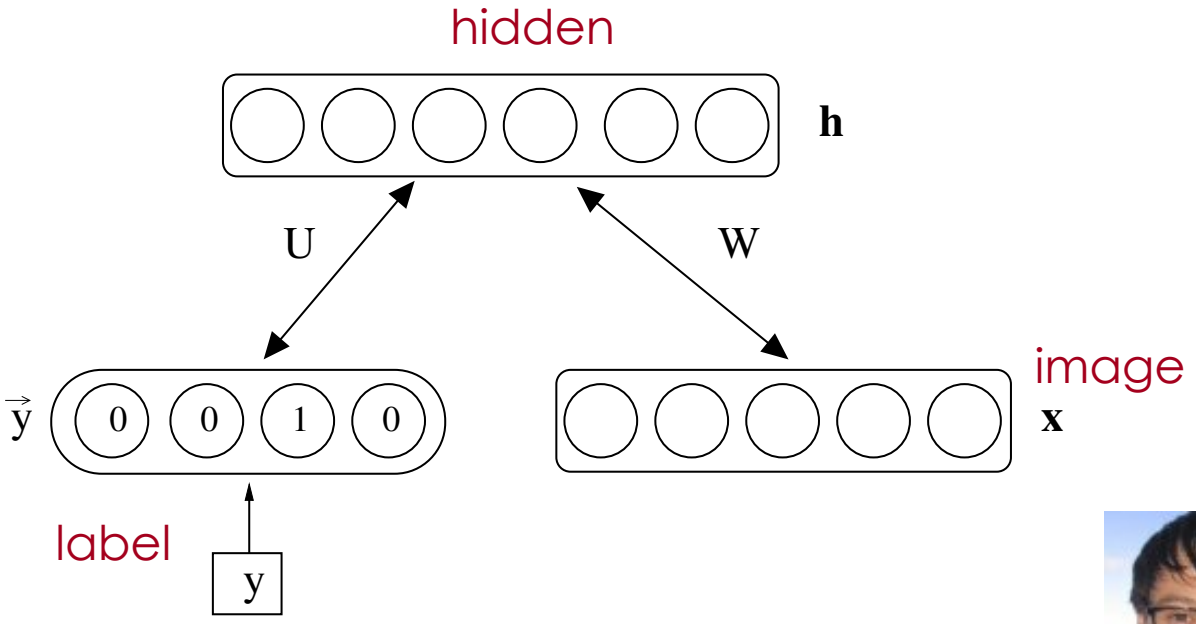
Restricted Boltzmann Machine (RBM)

$$P(x,h) = \frac{1}{Z} e^{b^T h + c^T x + h^T W x} = \frac{1}{Z} e^{\sum_i b_i h_i + \sum_j c_j x_j + \sum_{i,j} h_i W_{ij} x_j}$$

- A popular building block for deep architectures
- **Bipartite** undirected graphical model



RBM with (image, label) visible units



(Larochelle & Bengio 2008)

RBMs are Universal Approximators

(Le Roux & Bengio 2008)


- Adding one hidden unit (with proper choice of parameters) guarantees increasing likelihood
- With enough hidden units, can perfectly model any discrete distribution
- RBMs with variable # of hidden units = non-parametric

Boltzmann Machine Gradient

$$P(x) = \frac{1}{Z}\sum_h e^{-\text{Energy}(x,h)} = \frac{1}{Z}e^{-\text{FreeEnergy}(x)}$$

- Gradient has two components:

"positive phase" "negative phase"

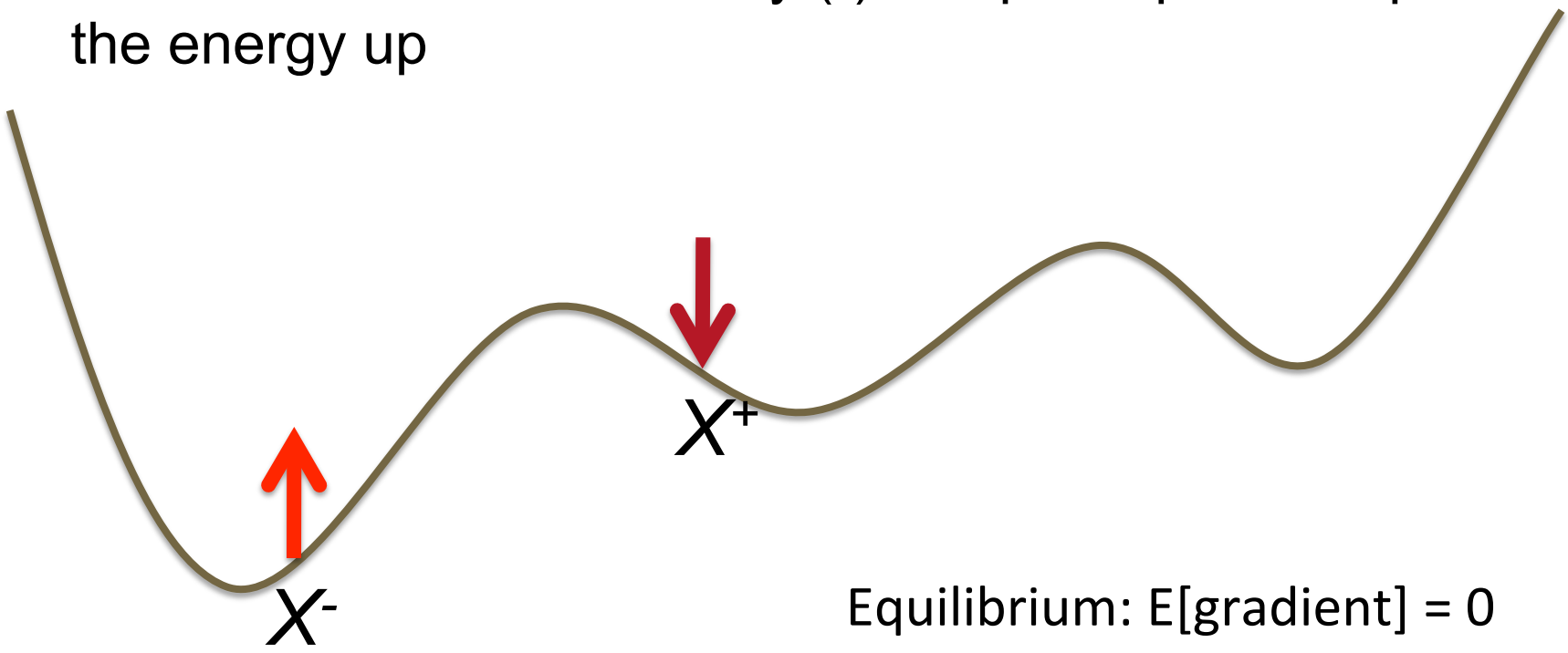
$$\frac{\partial \log P(x)}{\partial \theta} = -\frac{\partial \text{FreeEnergy}(x)}{\partial \theta} + \sum_{\tilde{x}} P(\tilde{x}) \frac{\partial \text{FreeEnergy}(\tilde{x})}{\partial \theta}$$

$$= -\sum_h P(h|x) \frac{\partial \text{Energy}(x,h)}{\partial \theta} + \sum_{\tilde{x},\tilde{h}} P(\tilde{x},\tilde{h}) \frac{\partial \text{Energy}(\tilde{x},\tilde{h})}{\partial \theta}$$

- In RBMs, easy to sample or sum over $h|x$
- Difficult part: sampling from $P(x)$, typically with a Markov chain

Positive & Negative Samples

- Observed (+) examples push the energy down
- Generated / dream / fantasy (-) samples / particles push the energy up



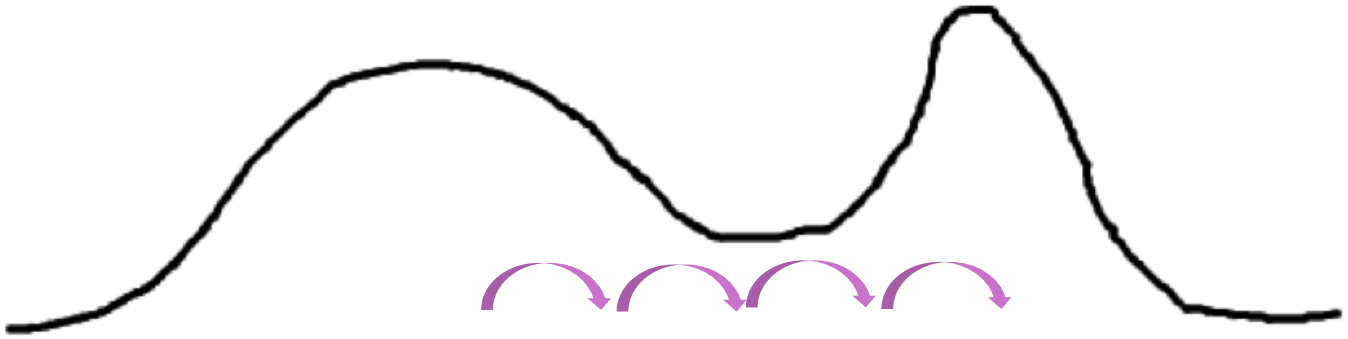
Equilibrium: E[gradient] = 0

Training RBMs

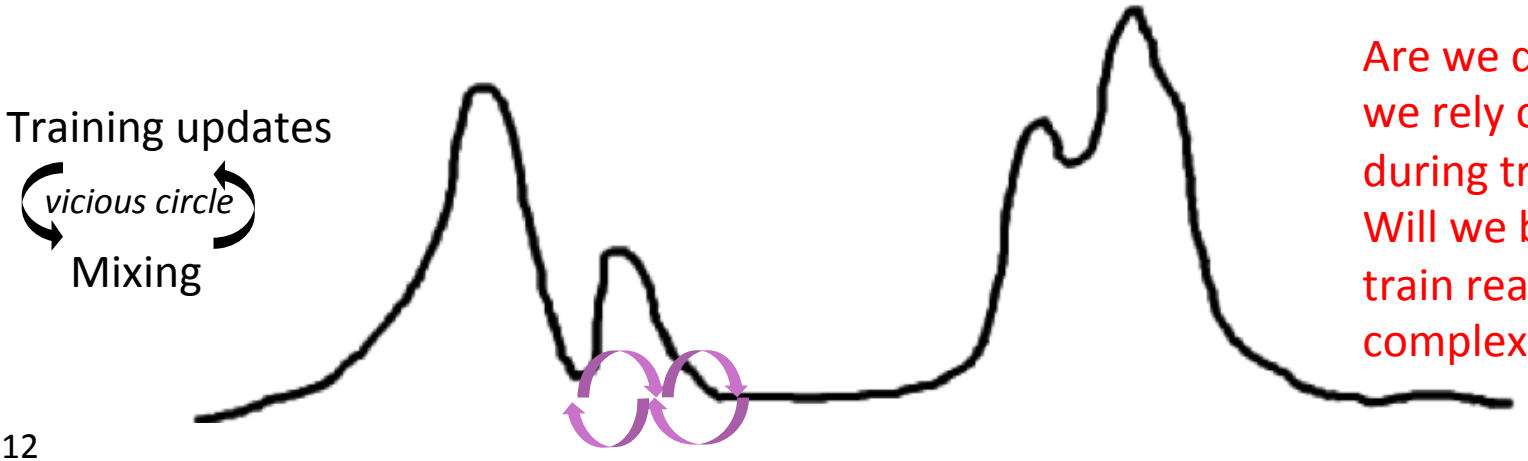
Contrastive Divergence: (CD-k)	start negative Gibbs chain at observed x, run k Gibbs steps
SML/Persistent CD: (PCD)	run negative Gibbs chain in background while weights slowly change
Fast PCD:	two sets of weights, one with a large learning rate only used for negative phase, quickly exploring modes
Herding:	Deterministic near-chaos dynamical system defines both learning and sampling
Tempered MCMC:	use higher temperature to escape modes

Obstacle: Vicious Circle Between Learning and MCMC Sampling

- Early during training, density smeared out, mode bumps overlap



- Later on, hard to cross empty voids between modes

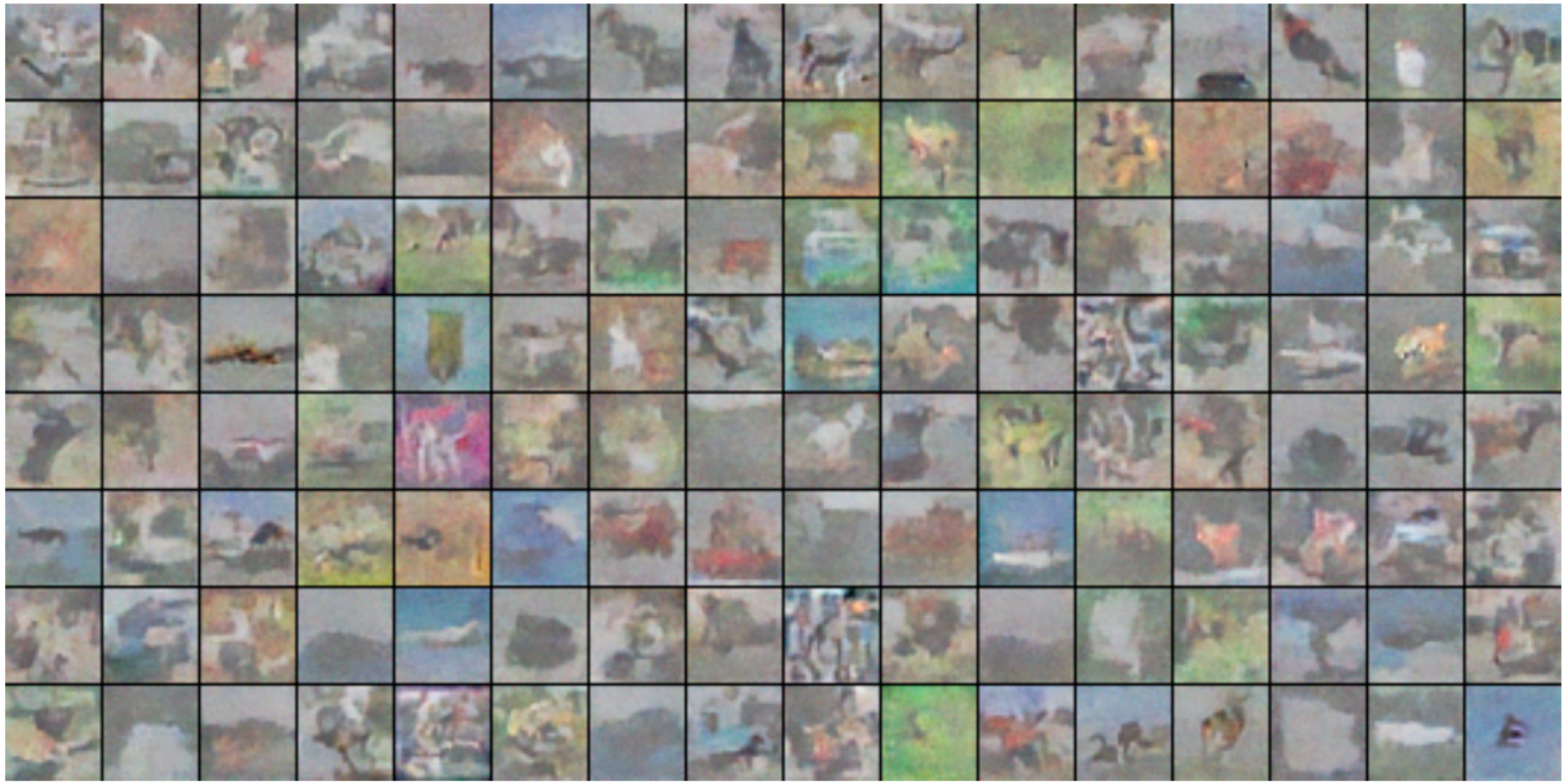


Are we doomed if we rely on MCMC during training? Will we be able to train really large & complex models?

Some RBM Variants

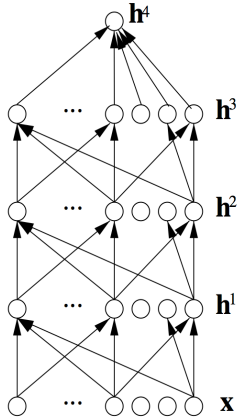
- Different energy functions and allowed values for the hidden and visible units:
  - Hinton et al 2006: binary-binary RBMs
  - Welling NIPS'2004: exponential family units
  - Ranzato & Hinton CVPR'2010: Gaussian RBM weaknesses (no conditional covariance), propose mcRBM
  - Ranzato et al NIPS'2010: mPoT, similar energy function
  - Courville et al ICML'2011: spike-and-slab RBM

Convolutionally Trained Spike & Slab RBMs Samples



Auto-Encoders & Variants: Learning a computational graph

Computational Graphs



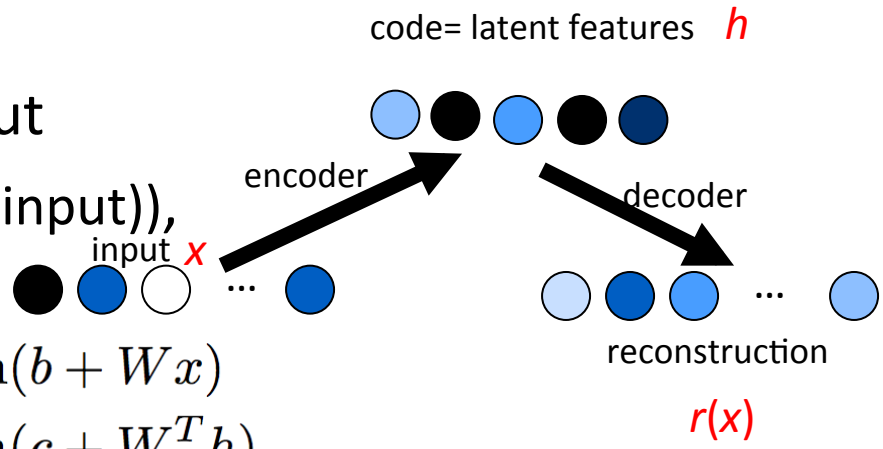
- Operations for particular task
- Neural nets' structure = computational graph for $P(y|\boldsymbol{x})$
- Graphical model's structure ≠ computational graph for inference
- Recurrent nets & graphical models

➔ **family of computational graphs sharing parameters**

- *Could we have a parametrized family of computational graphs defining "the model"?*

Simple Auto-Encoders

- MLP whose target output = input
- Reconstruction=decoder(encoder(input)), e.g.



$$
\begin{aligned}
h &= \tanh(b + Wx) \\
\text{reconstruction} &= \tanh(c + W^T h) \\
\text{Loss } L(x, \text{reconstruction}) &= ||\text{reconstruction} - x||^2
\end{aligned}
$$

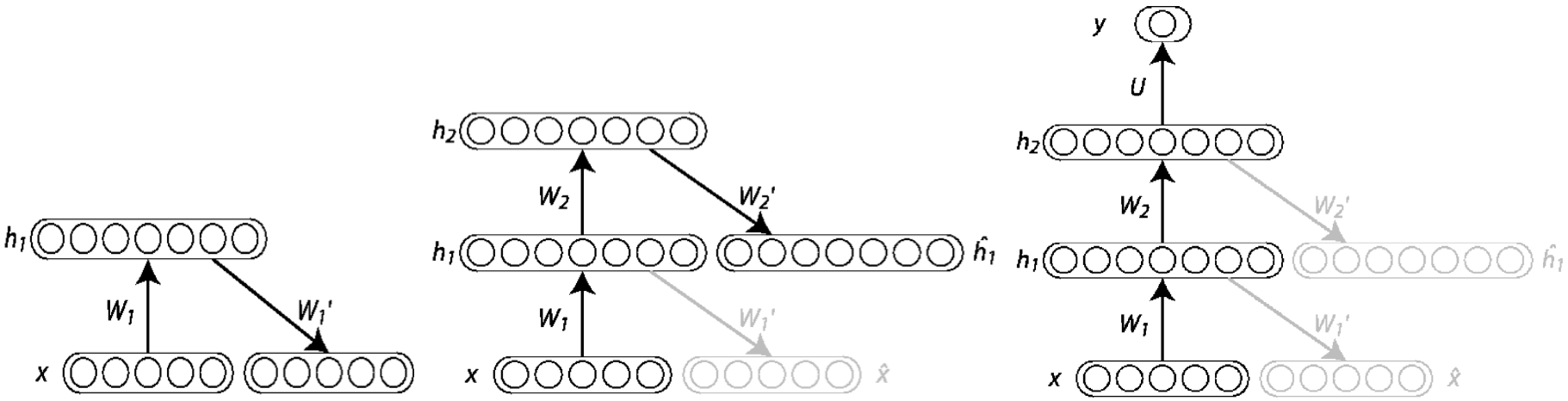
- With bottleneck, code = new coordinate system
- Encoder and decoder can have 1 or more layers
- Training deep auto-encoders notoriously difficult

I finally understand what auto-encoders do!

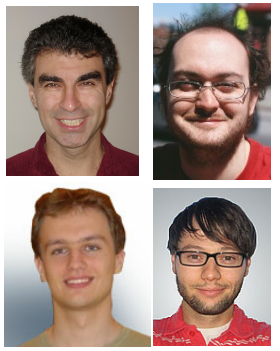
- Try to carve holes in $||r(x)-x||^2$ or $-\log P(x \mid h(x))$ at examples

- Vector $r(x)-x$ points in direction of increasing prob., i.e. estimate score = $d \log p(x) / dx$: learn **score** vector field = **local mean**
- Generalize (*valleys*) in between above holes to form *manifolds*
  - $d\, r(x) / dx$ estimates the **local covariance** and is linked to the Hessian $d^2 \log p(x) / dx^2$
- **A Markov Chain associated with AEs estimates the data-generating distribution (Bengio et al, NIPS'2013)**

Stacking Auto-Encoders



Auto-encoders can be stacked successfully (Bengio et al NIPS'2006) to form highly non-linear representations, which with fine-tuning overperformed purely supervised MLPs



(Auto-Encoder) Reconstruction Loss

- Discrete inputs: cross-entropy for binary inputs
  - $- \Sigma_i x_i \log r_i(x) + (1-x_i) \log(1-r_i(x))$ (with $0<r_i(x)<1$)

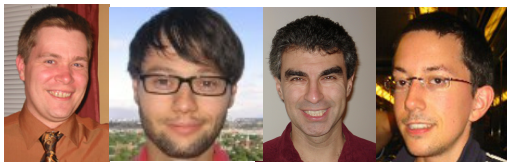
  or log-likelihood reconstruction criterion, e.g., for a multinomial (one-hot) input
  - $- \Sigma_i x_i \log r_i(x)$ (where $\Sigma_i r_i(x)=1$, summing over subset of inputs associated with this multinomial variable)

- In general: consider what are appropriate loss functions to predict each of the input variables,

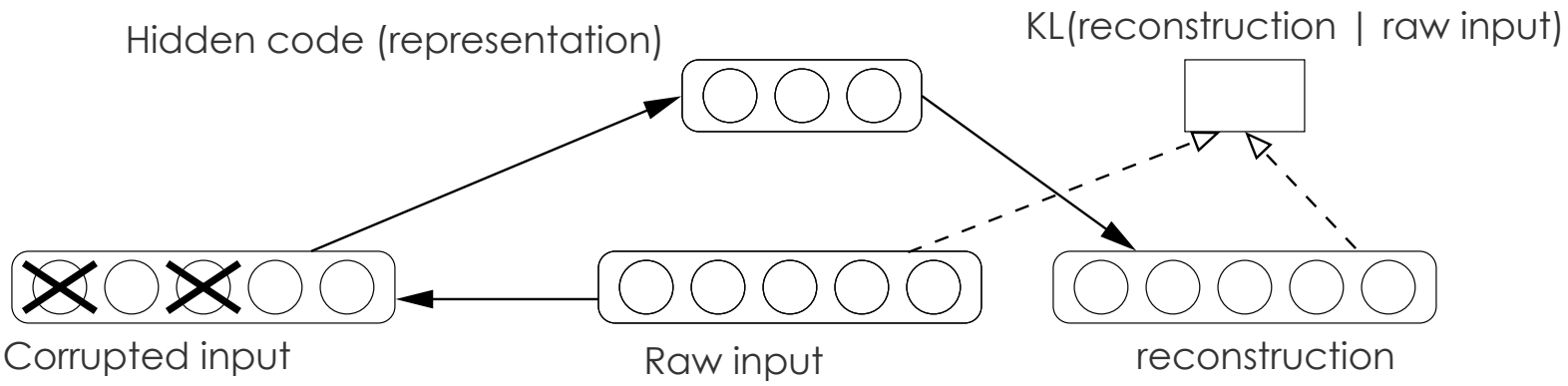
  typically, **reconstruction neg. log-likelihood $-\log P(x|h(x))$**

Denoising Auto-Encoder

(Vincent et al 2008)



- Corrupt the input during training only
- Train to reconstruct the uncorrupted input



- Encoder & decoder: any parametrization
- As good or better than RBMs for unsupervised pre-training

Denoising Auto-Encoder

- Learns a vector field pointing towards higher probability direction (Alain & Bengio 2013)

$$r(x)-x \propto d\log p(x)/dx$$

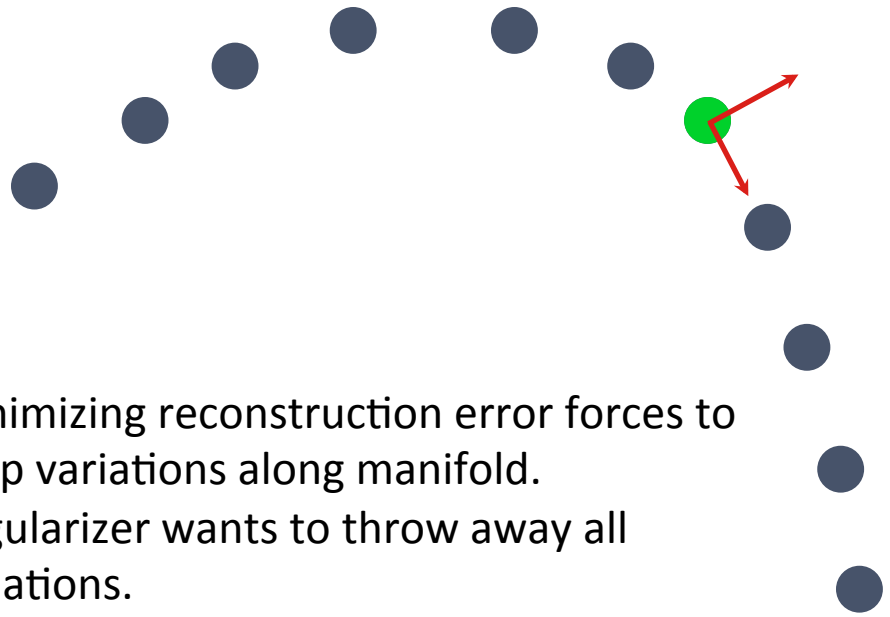
- Some DAEs correspond to a kind of Gaussian RBM with *regularized* Score Matching (Vincent 2011)

  [equivalent when noise→0]

- Compared to RBM:

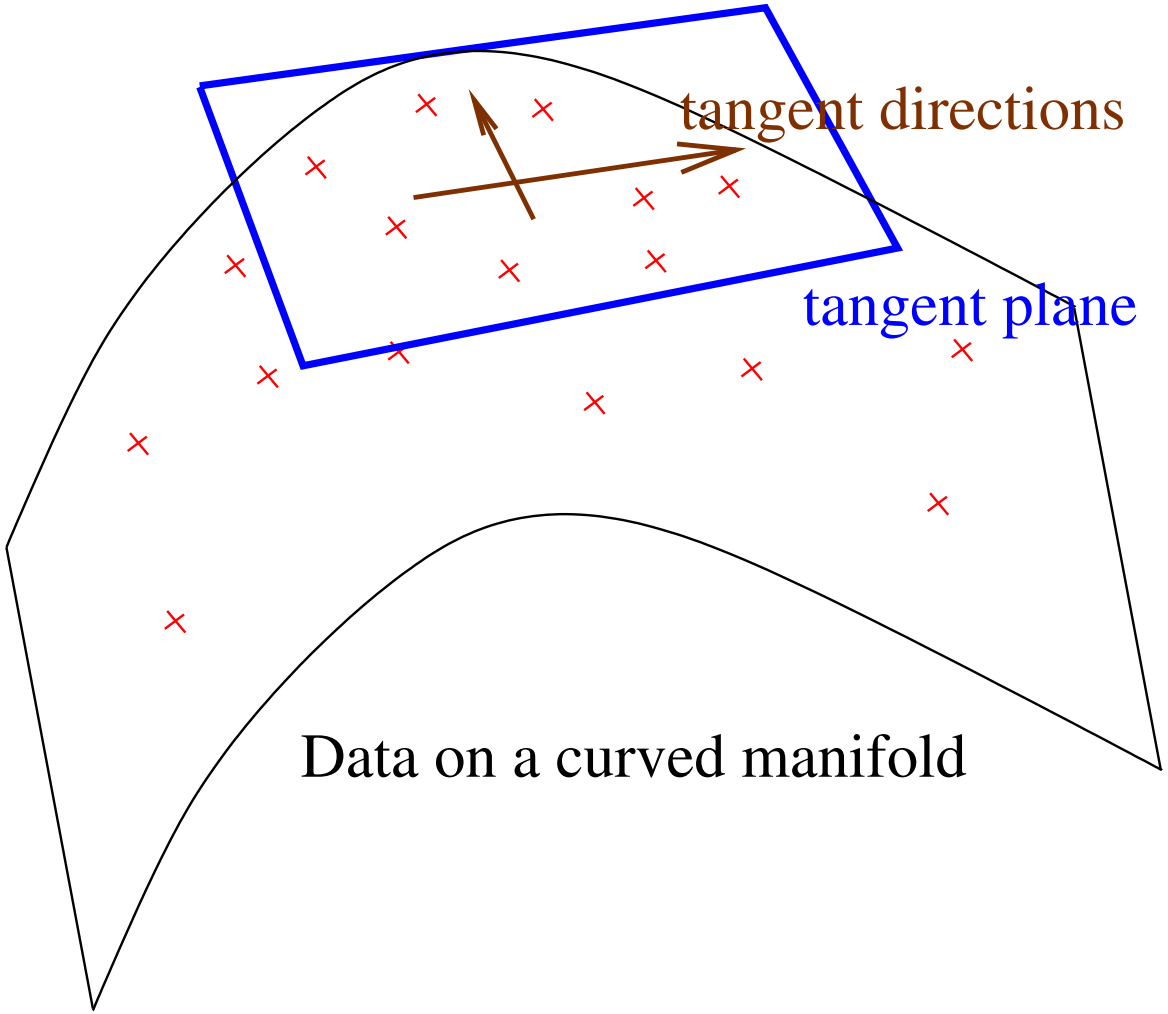
No partition function issue,
+ can measure training criterion

Auto-Encoders Learn Salient Variations, like a non-linear PCA

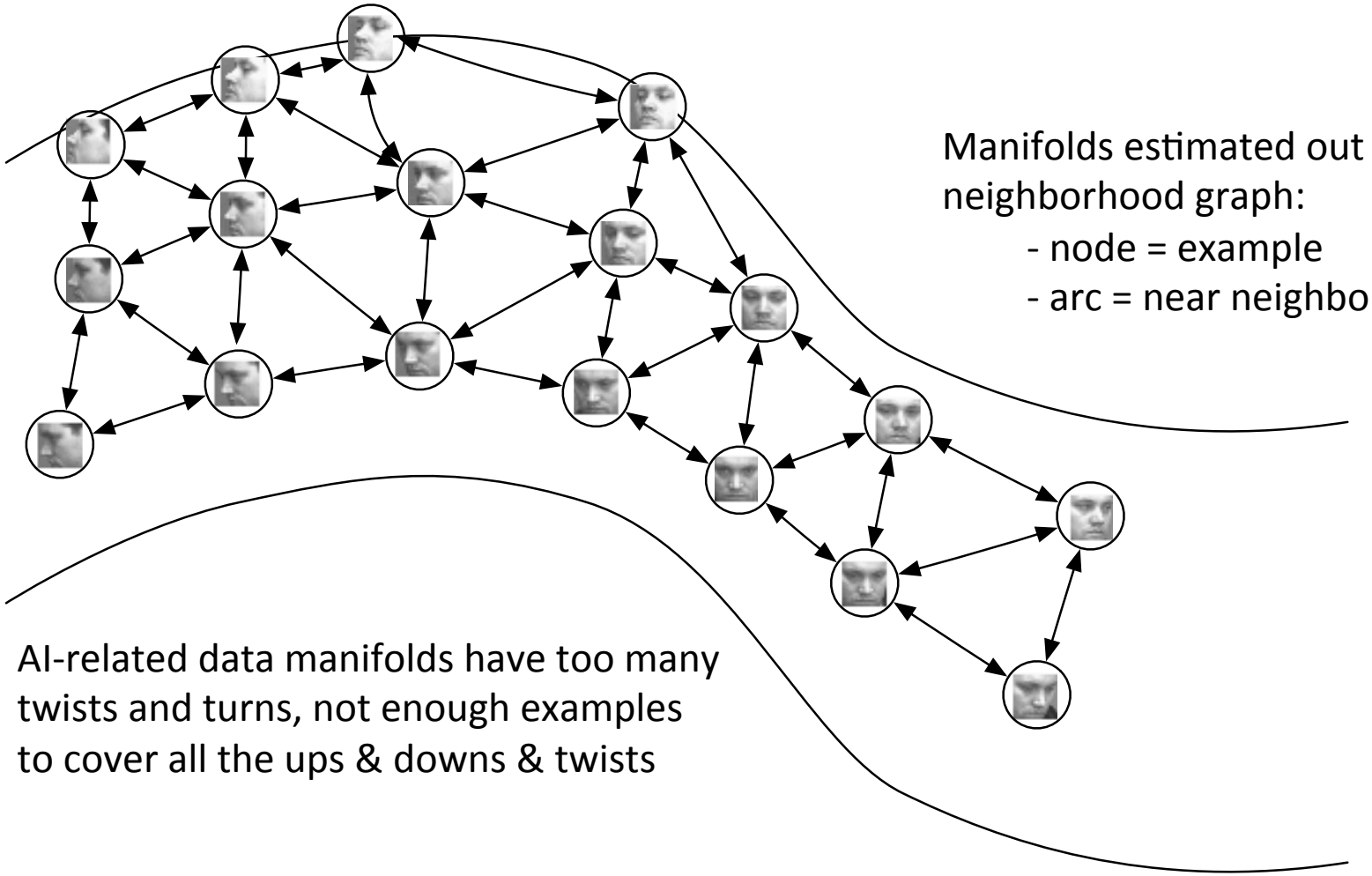


- Minimizing reconstruction error forces to keep variations along manifold.
- Regularizer wants to throw away all variations.
- With both: keep ONLY sensitivity to variations ON the manifold.

Manifold Learning = Representation Learning



Non-Parametric Manifold Learning: hopeless without powerful enough priors



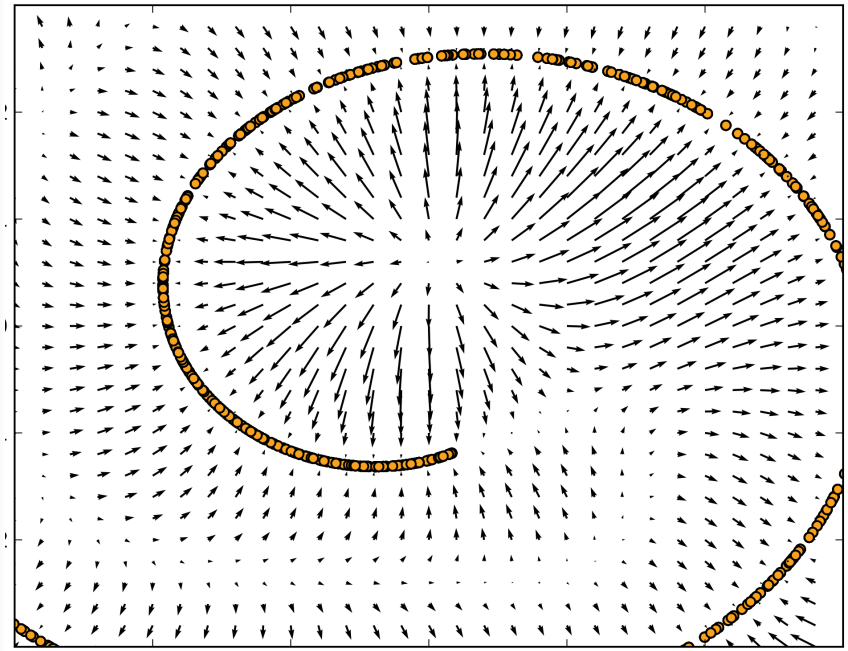
Manifolds estimated out of the neighborhood graph:

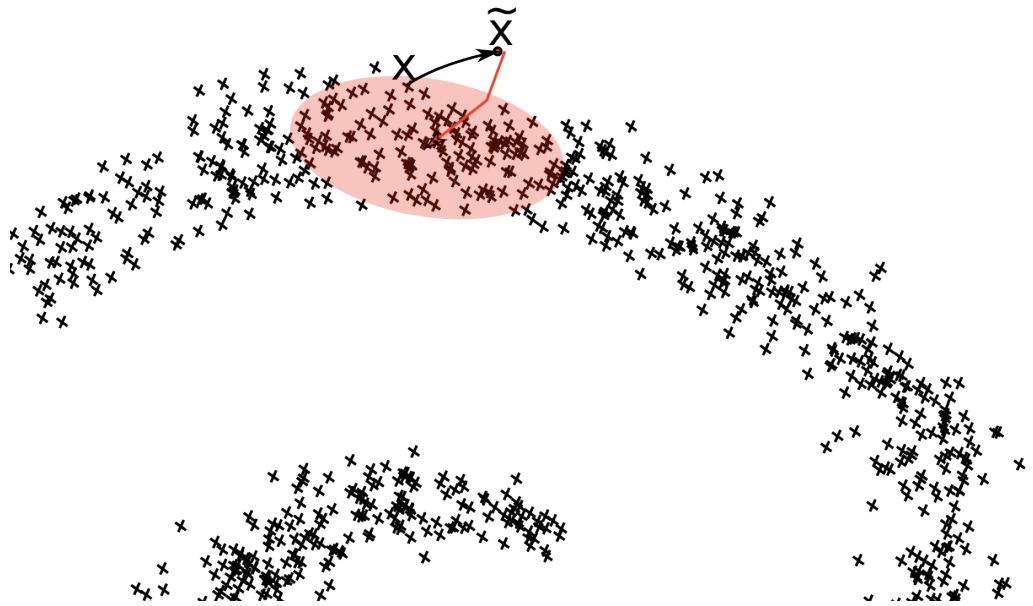
- node = example
- arc = near neighbor

AI-related data manifolds have too many twists and turns, not enough examples to cover all the ups & downs & twists

Regularized Auto-Encoders Learn a Vector Field or a Markov Chain Transition Distribution

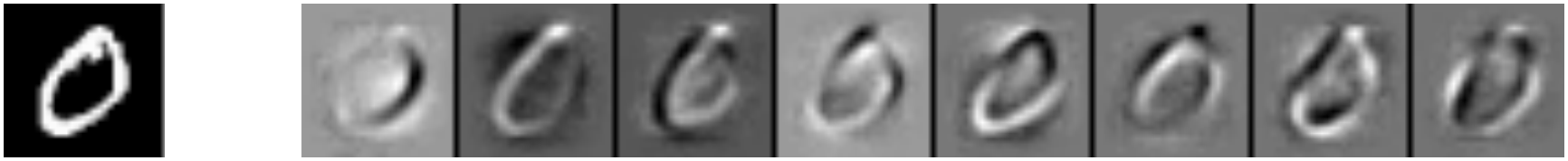
- (Bengio, Vincent & Courville, TPAMI 2013) review paper
- (Alain & Bengio ICLR 2013; Bengio et al, arxiv 2013)

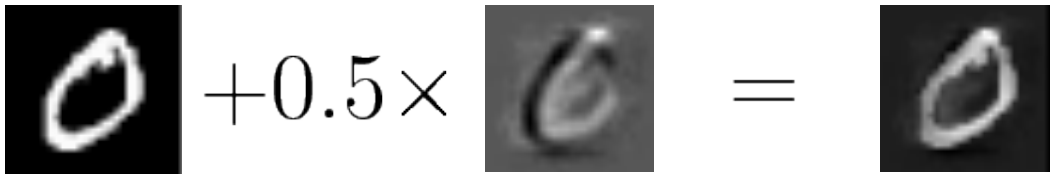




Input Point

Tangents

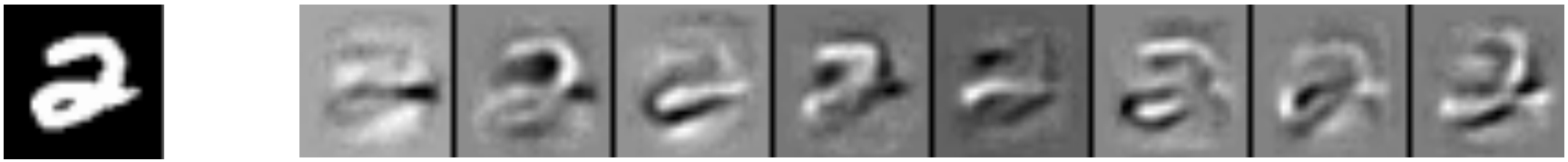




MNIST

Input Point

Tangents

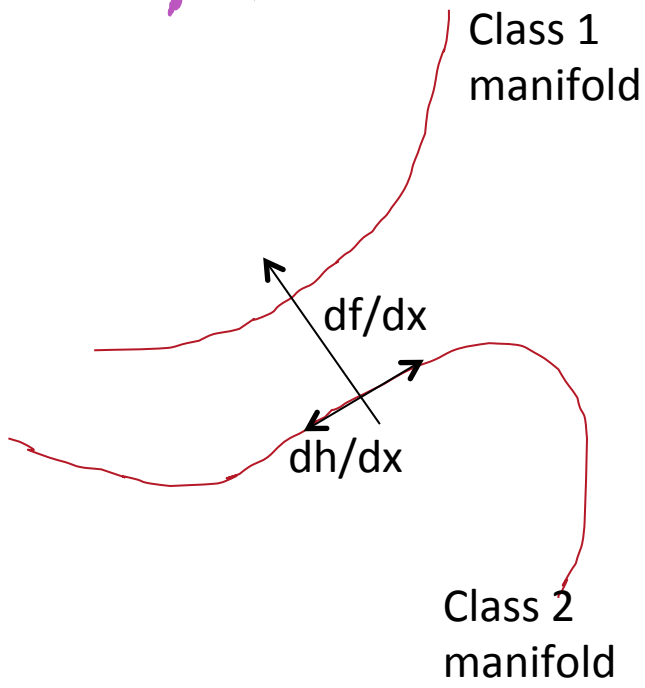


MNIST Tangents

Learned Tangent Prop: the Manifold Tangent Classifier

Makes classifier f(x) insensitive to variations on manifold at x

Tangent plane characterized by dh(x)/dx



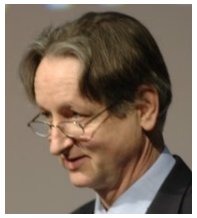
(Rifai et al NIPS'2012)

Deep Variants

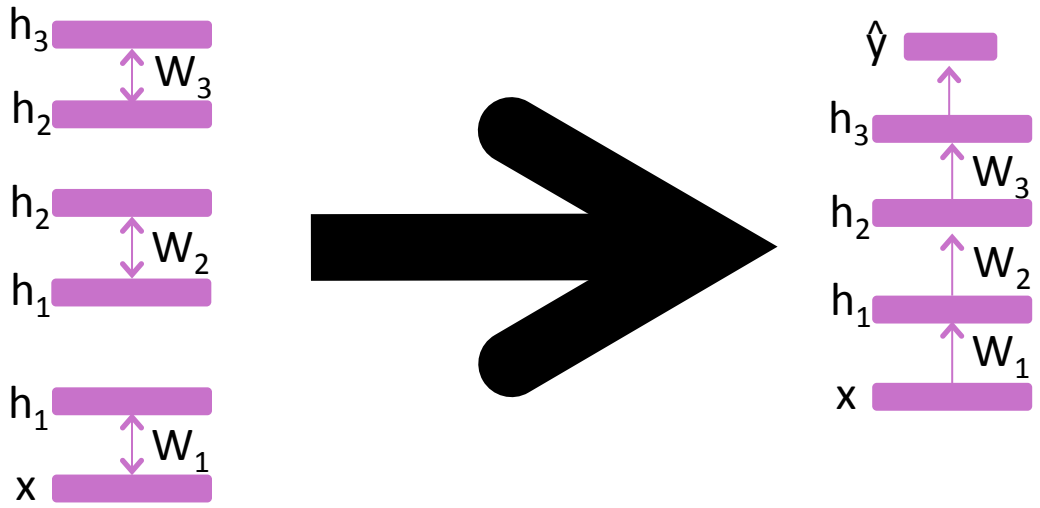
Level-Local Learning is Important

- Initializing each layer of an unsupervised deep Boltzmann machine helps a lot
- Initializing each layer of a supervised neural network as an RBM, auto-encoder, denoising auto-encoder, etc can help a lot
- Helps most the layers further away from the target
- Not just an effect of the unsupervised prior
- Jointly training all the levels of a deep architecture is difficult because of the increased non-linearity / non-smoothness
- Initializing using **a level-local learning algorithm** is a useful trick
- Providing intermediate-level targets can help tremendously (Gulcehre & Bengio ICLR 2013)

Stack of RBMs / AEs → Deep MLP



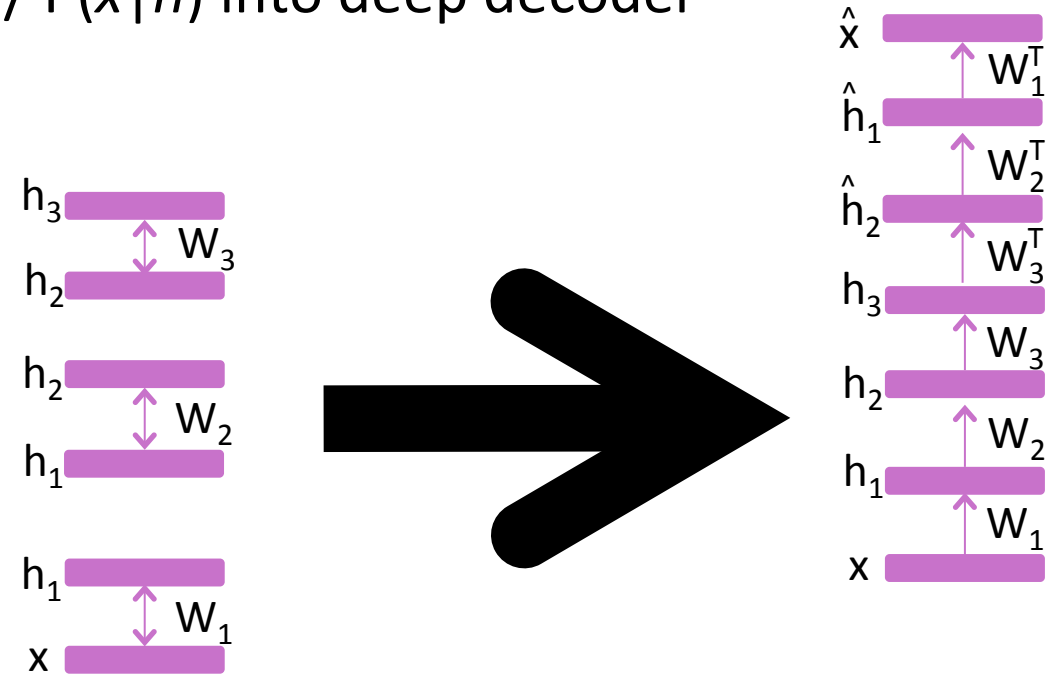
- Encoder or P(*h*|*v*) becomes MLP layer



Stack of RBMs / AEs → Deep Auto-Encoder

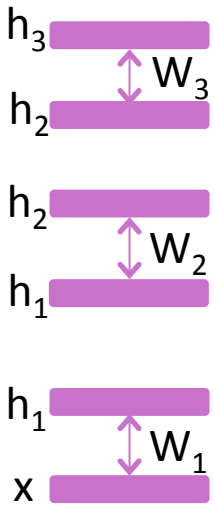
(Hinton & Salakhutdinov 2006)

- Stack encoders / P($h|x$) into deep encoder
- Stack decoders / P($x|h$) into deep decoder

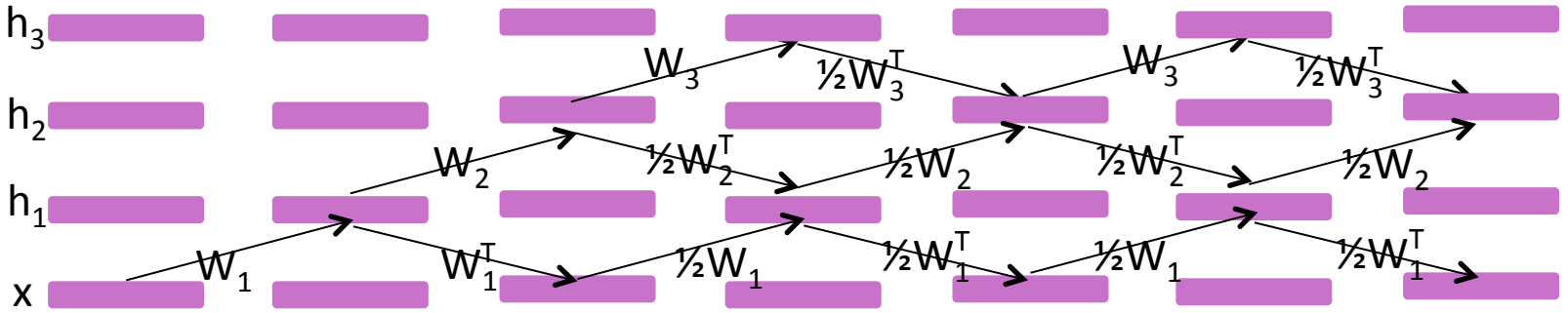


Stack of RBMs / AEs → Deep Recurrent Auto-Encoder

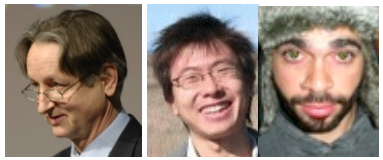
(Savard 2011)  (Bengio & Laufer, arxiv 2013)  



- Each hidden layer receives input from below and above
- Deterministic (mean-field) recurrent computation (Savard 2011)
- Stochastic (injecting noise) recurrent computation: Deep Generative Stochastic Networks (GSNs)
  (Bengio & Laufer arxiv 2013)

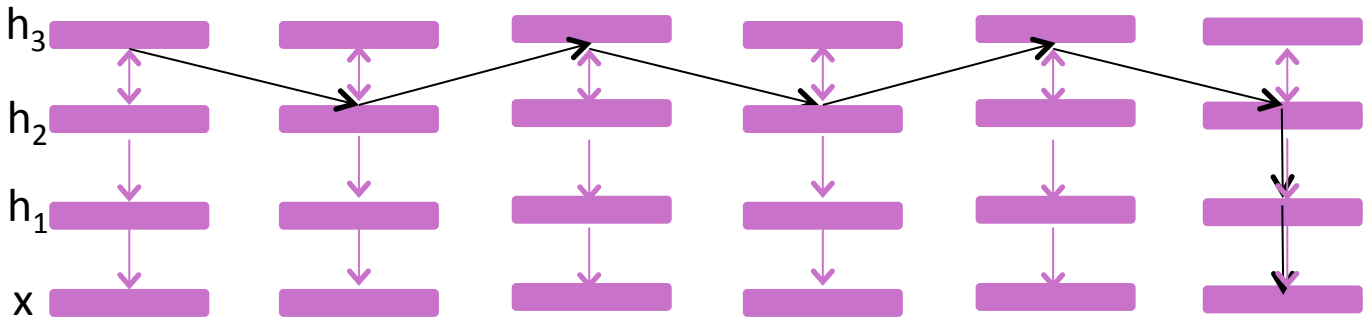


Stack of RBMs → Deep Belief Net



(Hinton et al 2006)

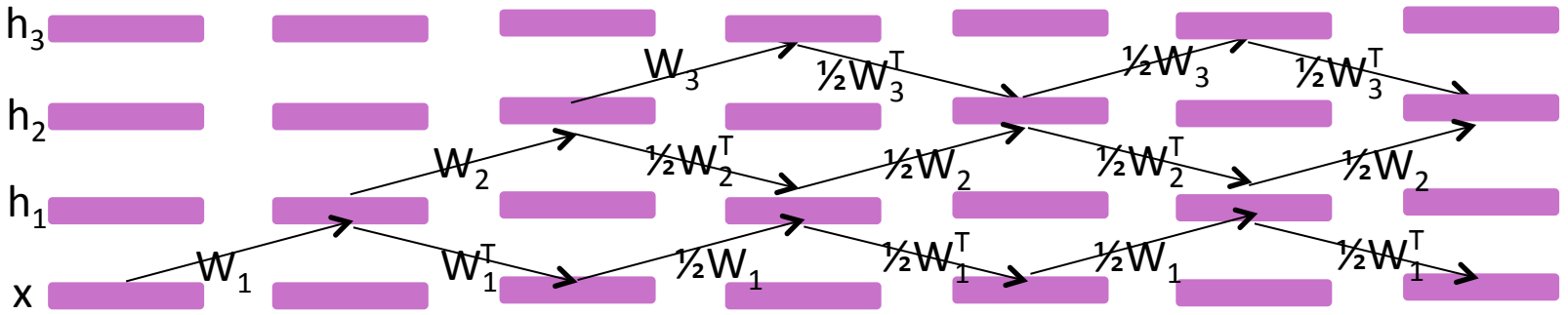
- Stack lower levels RBMs' P($x|h$) along with top-level RBM
- $P(x, h_1, h_2, h_3) = P(h_2, h_3)\, P(h_1|h_2)\, P(x \mid h_1)$
- Sample: Gibbs on top RBM, propagate down



Stack of RBMs → Deep Boltzmann Machine

(Salakhutdinov & Hinton AISTATS 2009)

- Halve the RBM weights because each layer now has inputs from below and from above
- Positive phase: (mean-field) variational inference = recurrent AE
- Negative phase: Gibbs sampling (stochastic units)
- train by SML/PCD

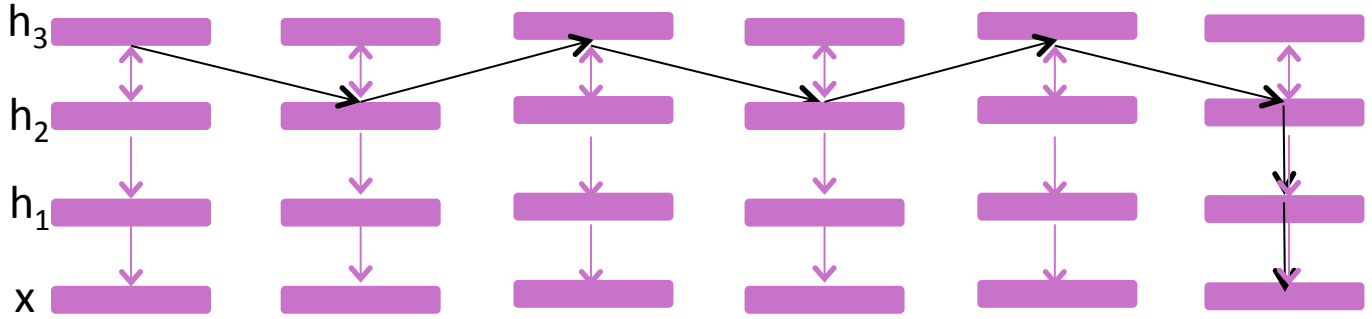


Stack of Auto-Encoders → Deep Generative Auto-Encoder

(Rifai et al ICML 2012)

- MCMC on top-level auto-encoder
  - h_{t+1} = encode(decode(h_t))+σ noise

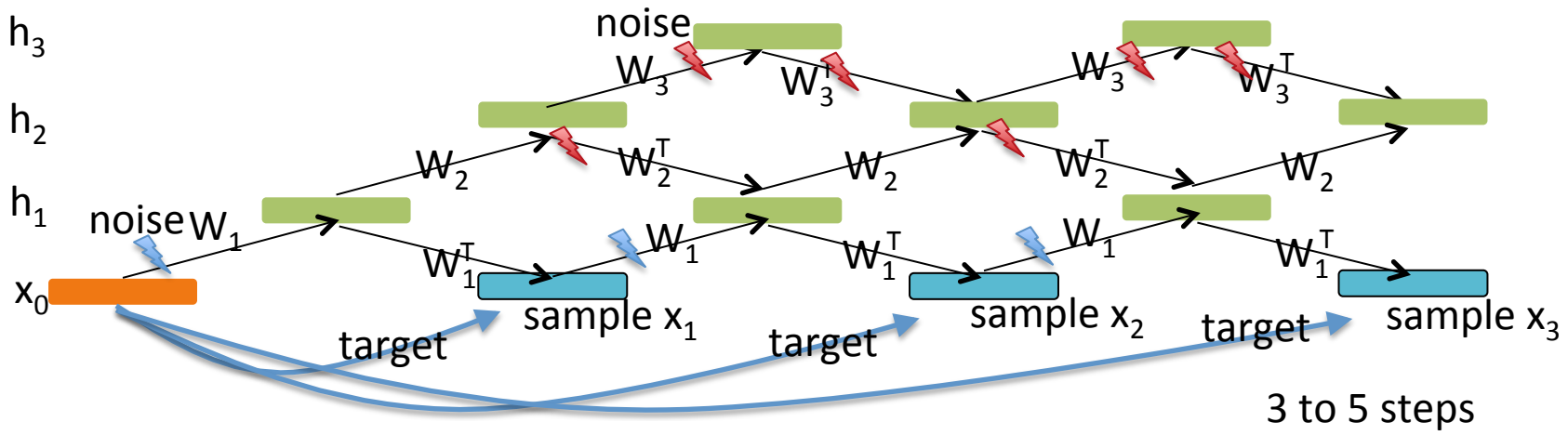
  where noise is Normal(0, d/dh encode(decode(h_t)))
- Then deterministically propagate down with decoders



Generative Stochastic Networks (GSN)

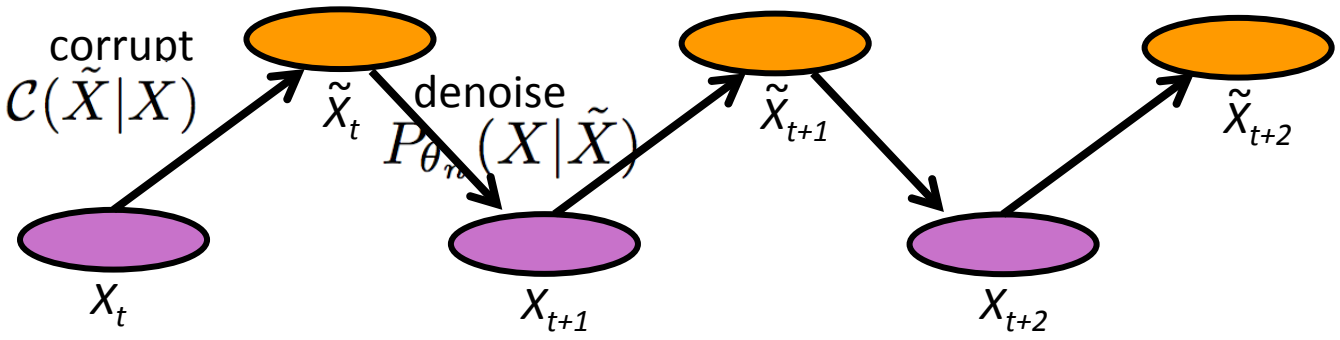
(Bengio, Yao, Alain & Vincent, arxiv 2013; Bengio & Laufer, arxiv 2013)

- **Recurrent parametrized stochastic computational graph that defines a transition operator for a Markov chain whose asymptotic distribution is implicitly estimated by the model**
- Noise injected in input and hidden layers
- Trained to max. reconstruction prob. of example at each step
- **Example** structure inspired from the DBM Gibbs chain:



Denoising Auto-Encoder Markov Chain

- $\mathcal{P}(X)$: true data-generating distribution
- $\mathcal{C}(\tilde{X}|X)$: corruption process
- $P_{\theta_n}(X|\tilde{X})$: denoising auto-encoder trained with *n* examples $X, \tilde{X}$ from $\mathcal{C}(\tilde{X}|X)\mathcal{P}(X)$, probabilistically "inverts" corruption
- T_n : Markov chain over *X* alternating $\tilde{X} \sim \mathcal{C}(\tilde{X}|X)$, $X \sim P_{\theta_n}(X|\tilde{X})$



New Theoretical Results (Bengio et al NIPS 2013)

- Denoising AE are consistent estimators of the data-generating distribution through their Markov chain, so long as they consistently estimate the conditional denoising distribution and the Markov chain converges.

$$\text{Making } P_{\theta_n}(X|\tilde{X}) \text{ match } \mathcal{P}(X|\tilde{X}) \text{ makes } \pi_n(X) \text{ match } \mathcal{P}(X)$$

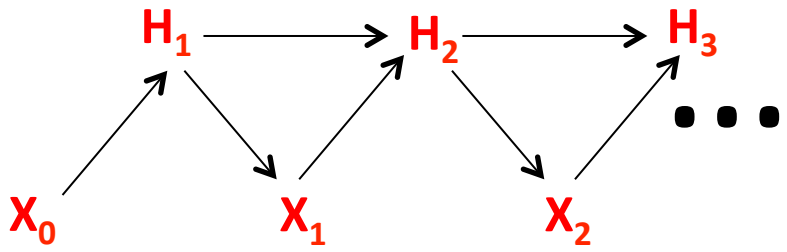
denoising distr. truth stationary distr. truth

Generative Stochastic Networks

Bengio et al, ICML 2014

- Generalizes the denoising auto-encoder training scheme
  - Introduce latent variables in the Markov chain (over X,H)
  - Instead of a fixed corruption process, have a deterministic function with parameters θ_1 and a noise source Z as input

$$H_{t+1} = f_{\theta_1}(X_t, Z_t, H_t)$$



$$H_{t+1} \sim P_{\theta_1}(H|H_t, X_t)$$
$$X_{t+1} \sim P_{\theta_2}(X|H_{t+1})$$

A Proper Generative Model for Dependency Networks, MP-DBMs, and efficient deep NADE sampling

- Dependency nets (Heckerman et al 2000) estimate $P_{\theta_i}(X_i \mid X_{-i})$ not guaranteed to be conditionals of a unique joint
- Heckerman et al's sampling iterates over i: not ergodic?
- Randomly choosing i: proper GSN
- Defines a unique joint distribution = stationary distr. of chain (which averages out over resampling orders)
- Generalized to estimators of P(subset(X) | X \ subset(X)) and justify efficient sampling schemes for MP-DBMs and deep NADE.

Applications

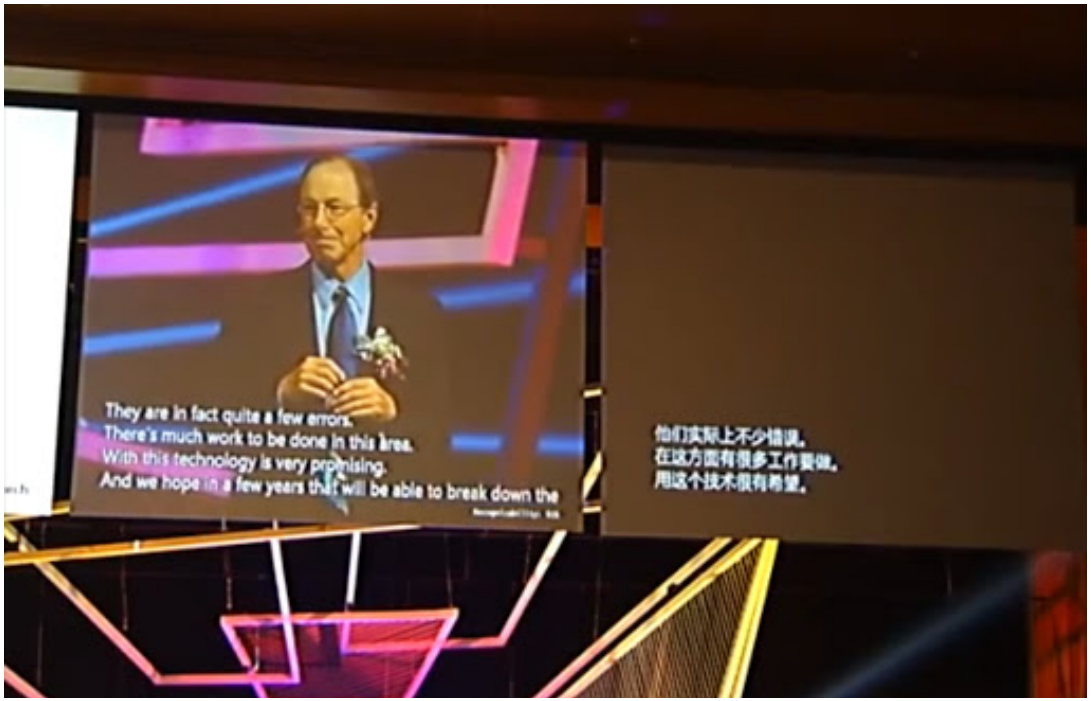
AI Tasks

- Perception
  - Vision
  - Speech
  - Multiple modalities
- Natural language understanding
- Reinforcement learning & control

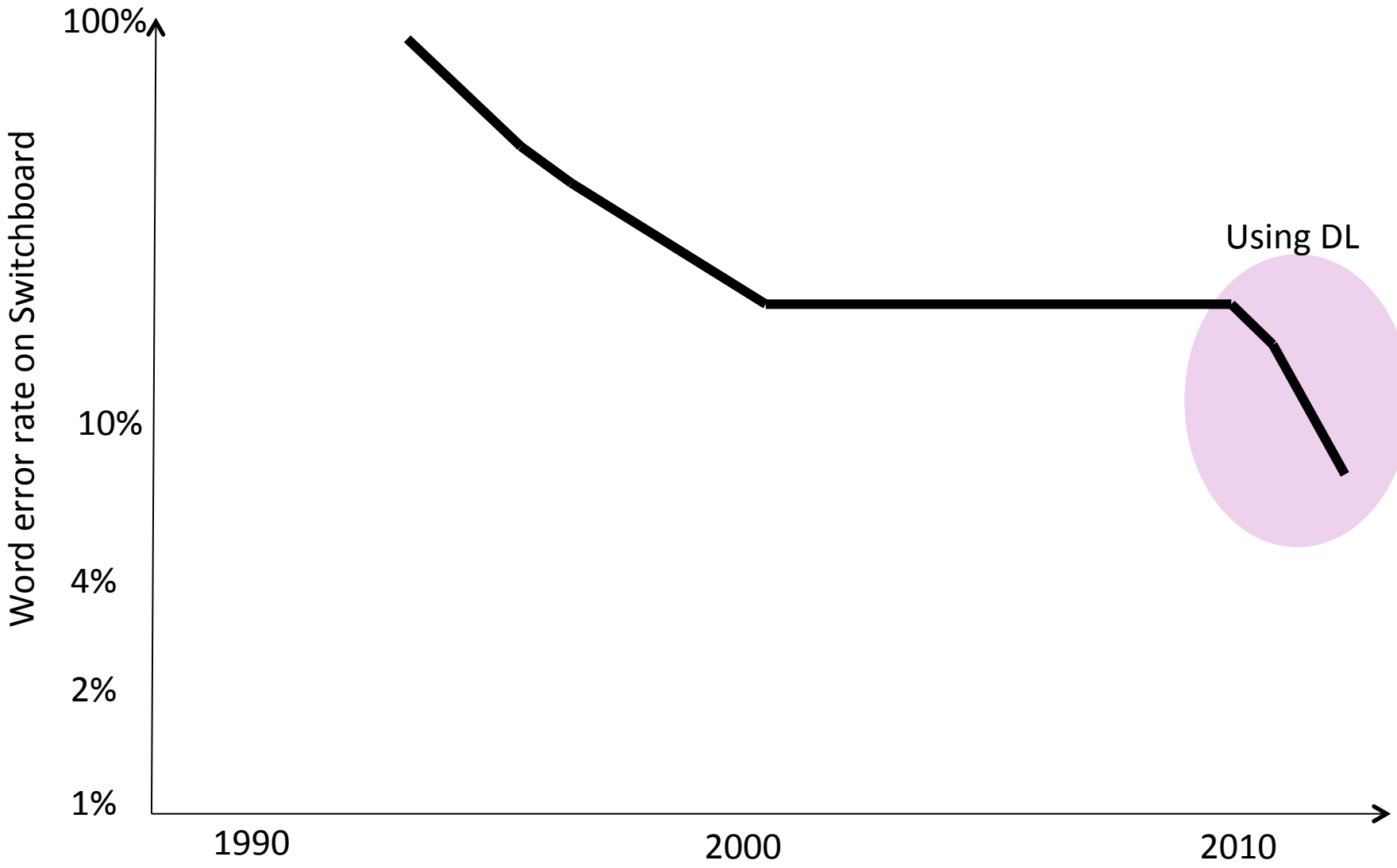
- COMPLEX HIGHLY-STRUCTURED DISTRIBUTION
- LOTS OF DATA (maybe mostly unlabeled)

2012: Industrial-scale success in speech recognition

- Google uses DL in their android speech recognizer (both server-side and on some phones with enough memory)
- Microsoft uses DL in their speech recognizer
- Error reductions on the order of 30%, a major progress



The dramatic impact of Deep Learning on Speech Recognition (according to Microsoft)



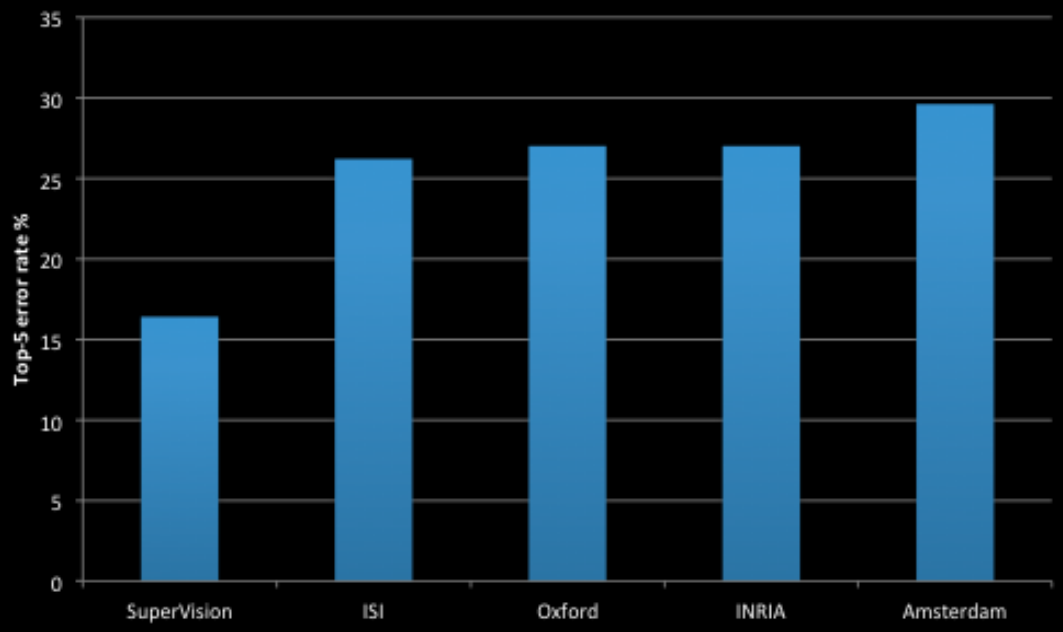
Deep Networks for Speech Recognition: results from Google, IBM, Microsoft

task	Hours of training data	Deep net+HMM	GMM+HMM same data	GMM+HMM more data
Switchboard	309	16.1	23.6	17.1 (2k hours)
English Broadcast news	50	17.5	18.8	
Bing voice search	24	30.4	36.2	
Google voice input	5870	12.3		16.0 (lots more)
Youtube	1400	47.6	52.3	

(numbers taken from Geoff Hinton's June 22, 2012 Google talk)

ImageNet Classification 2012

- Krizhevsky et al. -- 16.4% error (top-5)
- Next best (non-convnet) – 26.2% error



Slide from Rob Fergus, NIPS tutorial, 2012

Object Recognition Works

- Try it at http://deeplearning.cs.toronto.edu

Possible tags:

45%

39%

16% conv

Possible tags:

80% chimpanzee, chir

4% gorilla, Gorilla gorilla

4% ram, tup

3% hippopotamus, hippo, river horse

2% mask

Possible tags:

100% German shepherd,

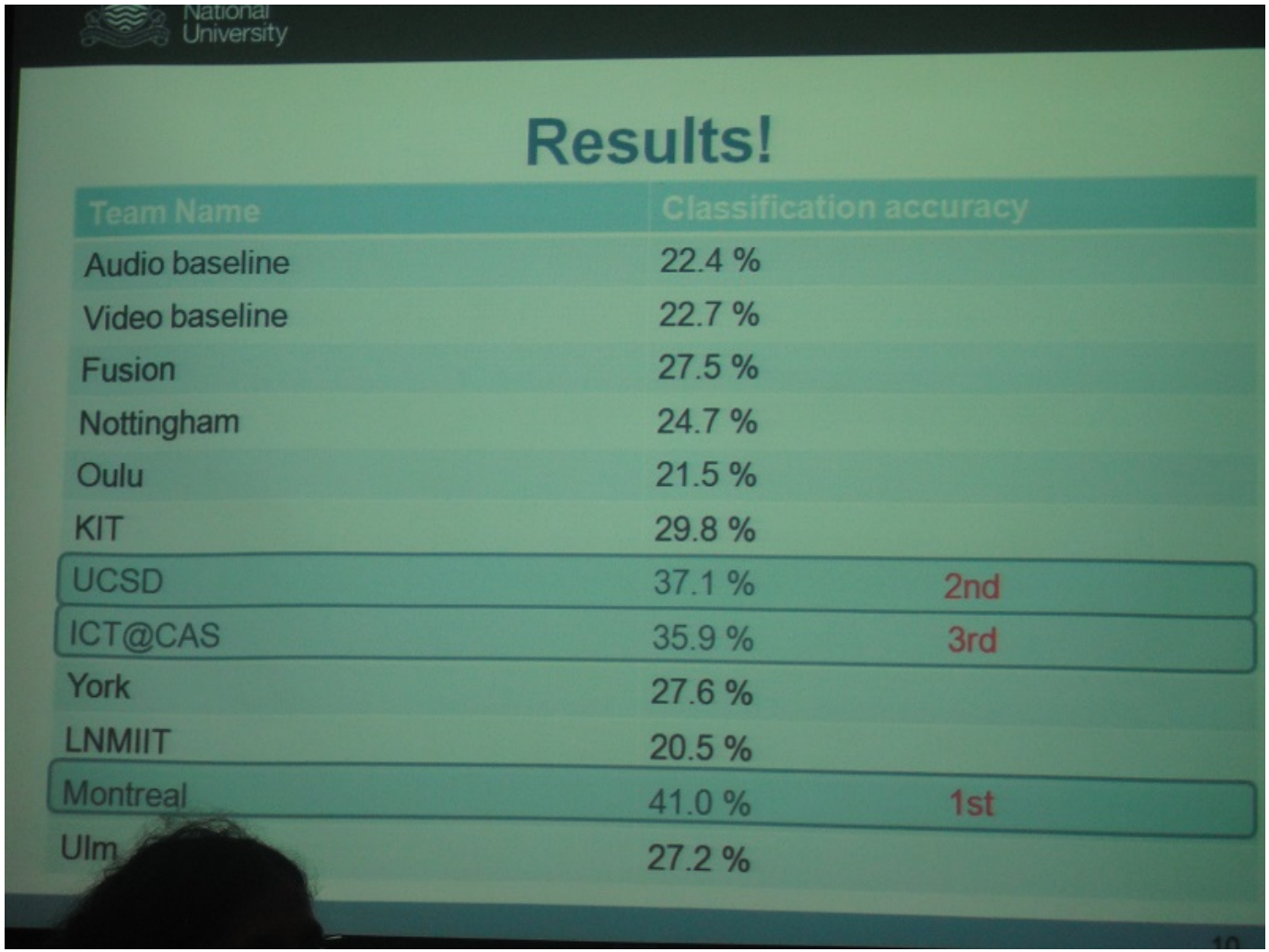
<1% dingo, warrigal, warragal

<1% Norwich terrier

<1% Airedale, Airedale terrier

Montreal Deep Nets Win Emotion Recognition in the Wild Challenge

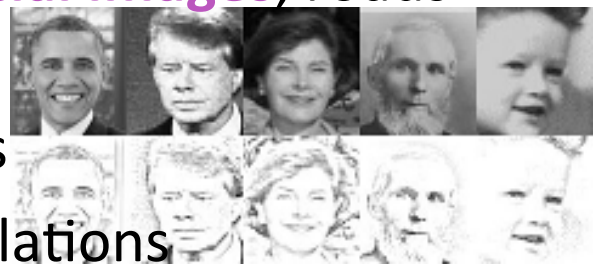
Predict emotional expression from video (using images + audio)



Dec. 9, 2013

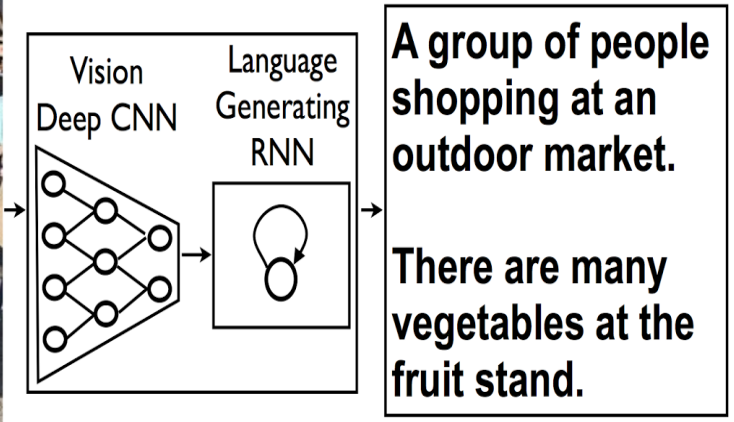
Some Applications of DL

- **Language Modeling** (Speech Recognition, Machine Translation)
- **Acoustic Modeling** (**speech recognition**, music modeling)
- **NLP syntactic/semantic tagging** (Part-Of-Speech, chunking, Named Entity Recognition, Semantic Role Labeling, Parsing)
- **NLP applications**: sentiment analysis, paraphrasing, question-answering, Word-Sense Disambiguation
- **Object recognition in images**: photo search and image search: handwriting recognition, document analysis, handwriting synthesis, **superhuman traffic sign classification**, street view house numbers, **emotion detection from facial images**, roads from satellites.
- **Personalization**/recommendation/fraud/ads
- **Molecular properties**: QSAR, quantum calculations



Generating Text from Images

- (Kiros *et al.*, 2014; Mao *et al.*, 2014; Donahue *et al.*, 2014; **Vinyals *et al.*, 2014**; Fang *et al.*, 2014; Chen and Zitnick, 2014; Karpathy and Li, 2014; Venugopalan *et al.*, 2014).
- Convolutional net → generative RNN



A close up of a child holding a stuffed animal

(GT: A young girl asleep on the sofa cuddling a stuffed bear.)

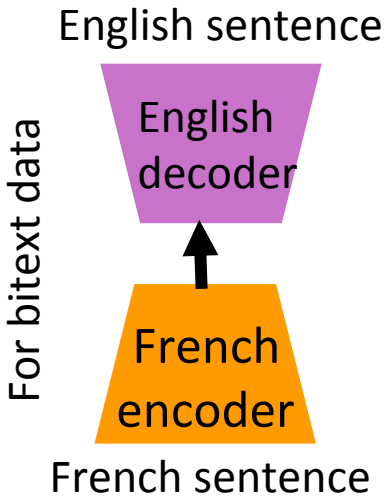
Two pizzas sitting on top of a stove top oven.

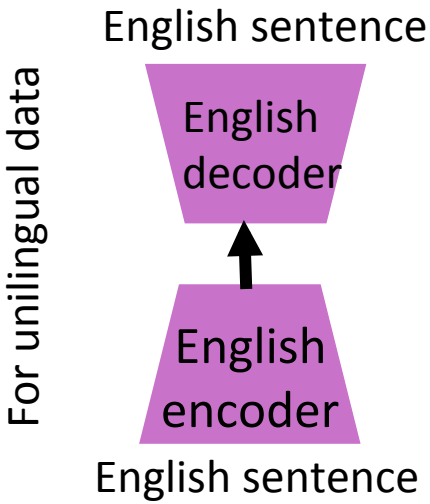
(GT: Three different types of pizza on top of a stove.)

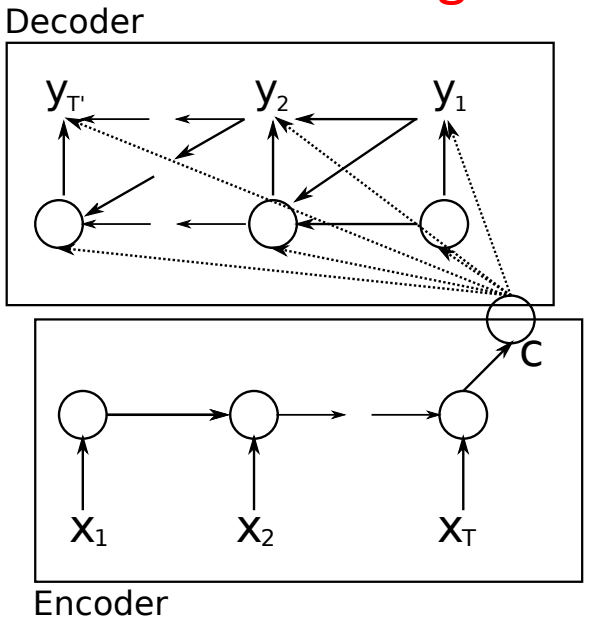
Breakthroughs in Machine Translation

- (Cho et al, EMNLP 2014) Learning Phrase Representations using RNN Encoder–Decoder for Statistical Machine Translation
- (Sutskever et al, NIPS 2014) Sequence to sequence learning with neural networks, 3 BLEU points improvement for English-French
- (Devlin et al, ACL 2014) Fast and Robust Neural Network Joint Models for Statistical Machine Translation

Best paper award, 6 BLEU points improvement for Arabic-English







More Successful Applications

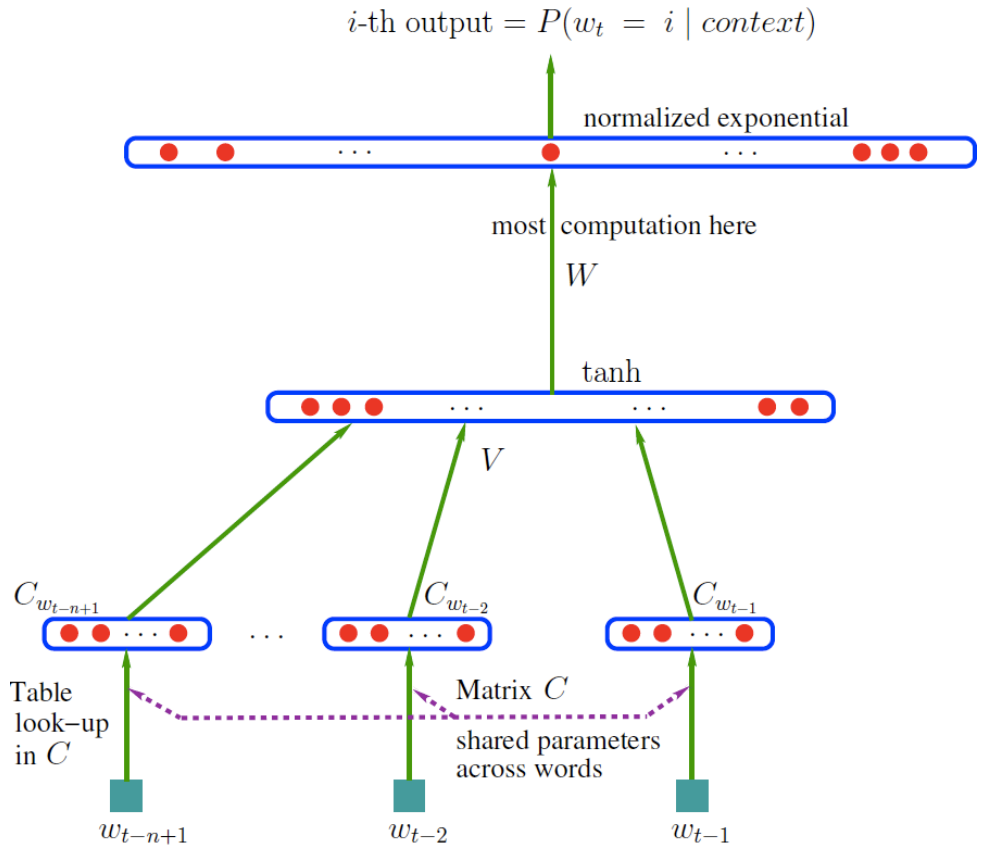
- Microsoft uses DL for speech rec. service (audio video indexing), based on Hinton/Toronto's DBNs (Mohamed et al 2012)
- Google uses DL in its Google Goggles service, using Ng/Stanford DL systems, and in its Google+ photo search service, using deep convolutional nets
- NYT talks about these: http://www.nytimes.com/2012/06/26/technology/in-a-big-network-of-computers-evidence-of-machine-learning.html?_r=1
- Substantially beating SOTA in language modeling (perplexity from 140 to 102 on Broadcast News) for speech recognition (WSJ WER from 16.9% to 14.4%) (Mikolov et al 2011) and translation (+1.8 BLEU) (Schwenk 2012)
- SENNA: Unsup. pre-training + multi-task DL reaches SOTA on POS, NER, SRL, chunking, parsing, with >10x better speed & memory (Collobert et al 2011)
- Recursive nets surpass SOTA in paraphrasing (Socher et al 2011)
- Denoising AEs substantially beat SOTA in sentiment analysis (Glorot et al 2011)
- Contractive AEs SOTA in knowledge-free MNIST (.8% err) (Rifai et al NIPS 2011)
- Le Cun/NYU's stacked PSDs most accurate & fastest in pedestrian detection and DL in top 2 winning entries of German road sign recognition competition

Already Many NLP Applications of DL

- Language Modeling (Speech Recognition, Machine Translation)
- Acoustic Modeling
- Part-Of-Speech Tagging
- Chunking
- Named Entity Recognition
- Semantic Role Labeling
- Parsing
- Sentiment Analysis
- Paraphrasing
- Question-Answering
- Word-Sense Disambiguation

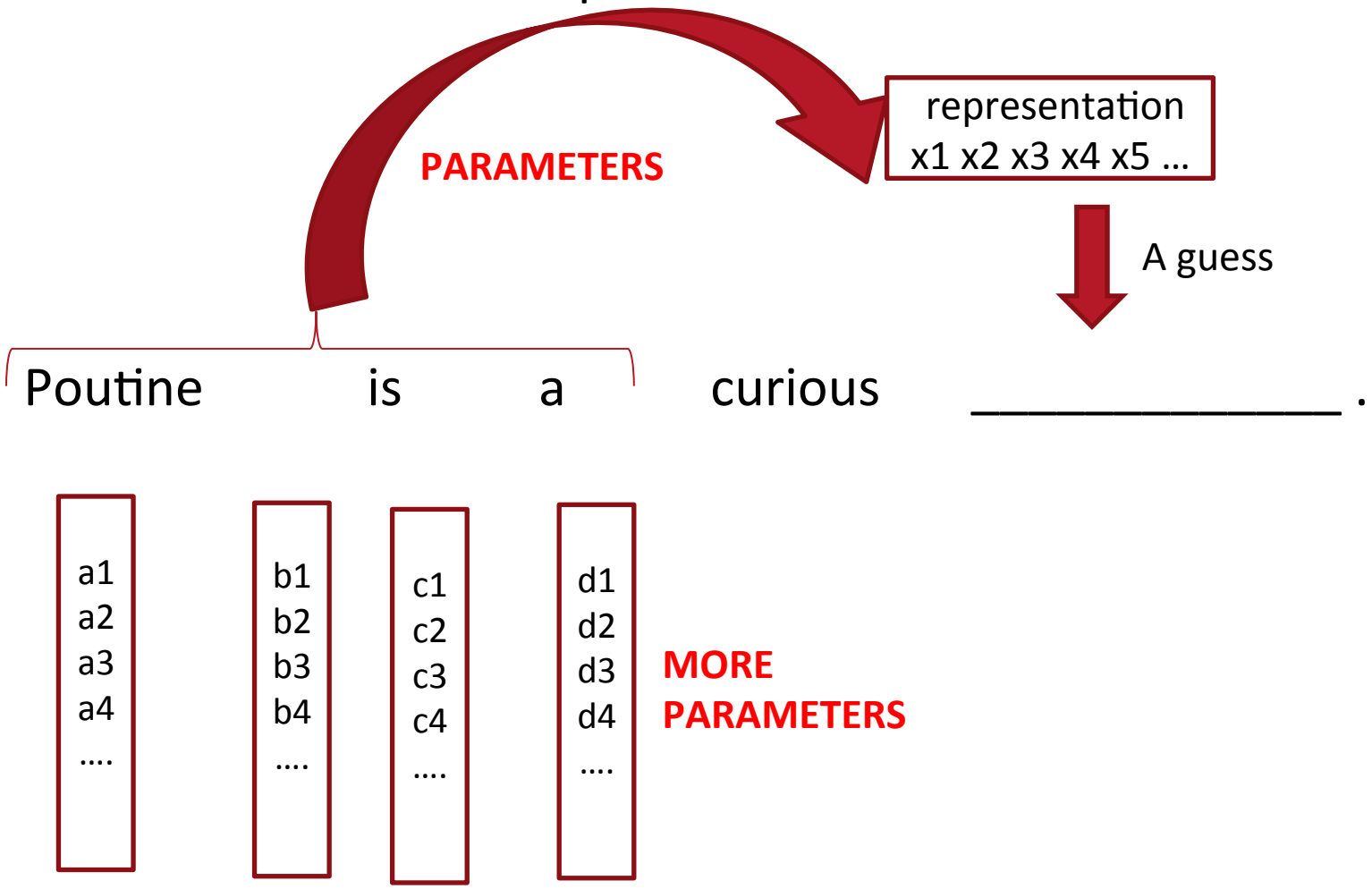
Neural Language Model

- *Bengio et al NIPS'2000 and JMLR 2003 "A Neural Probabilistic Language Model"*
  - Each word represented by a distributed continuous-valued code vector = embedding
  - Generalizes to sequences of words that are semantically similar to training sequences



Neural Language Models

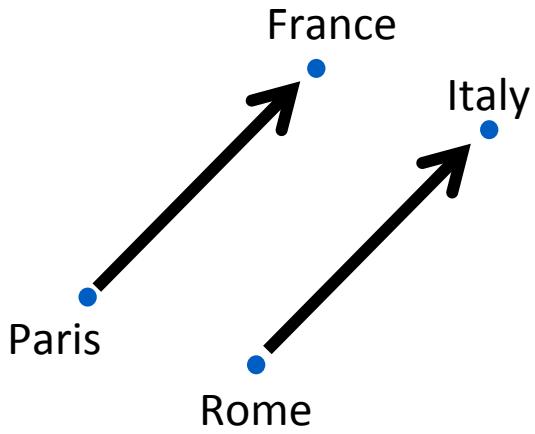
- Meanings and their combination all 'learned' together. Minimal structure imposed.



Neural word embeddings - visualization

Analogical Representations for Free (Mikolov et al, ICLR 2013)

- Semantic relations appear as linear relationships in the space of learned representations
- King – Queen ≈ Man – Woman
- Paris – France + Italy ≈ Rome



Practical Considerations

Deep Learning Tricks of the Trade

- Y. Bengio (2013), "Practical Recommendations for Gradient-Based Training of Deep Architectures"

  - Unsupervised pre-training
  - Stochastic gradient descent and setting learning rates
  - Main hyper-parameters
    - Learning rate schedule
    - Early stopping
    - Minibatches
    - Parameter initialization
    - Number of hidden units
    - L1 and L2 weight decay
    - Sparsity regularization
  - Debugging
  - How to efficiently search for hyper-parameter configurations

Stochastic Gradient Descent (SGD)

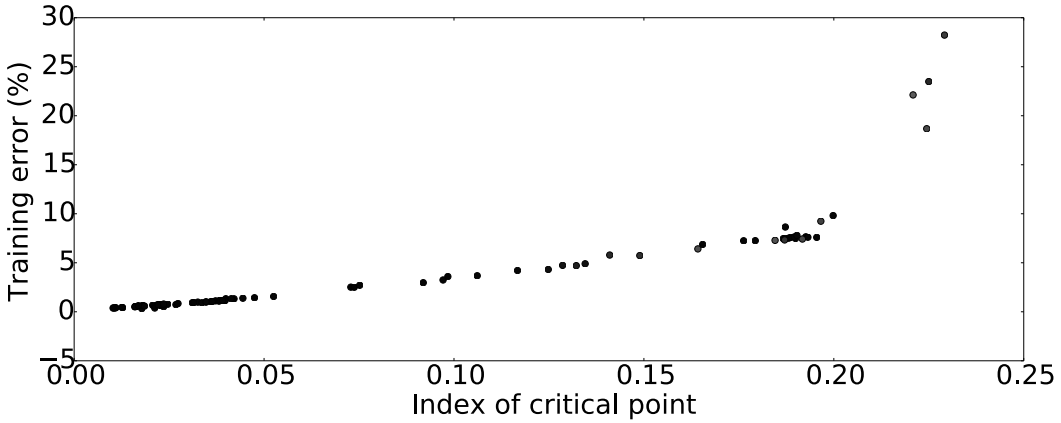
- Gradient descent uses total gradient over all examples per update, SGD updates after only 1 or few examples:

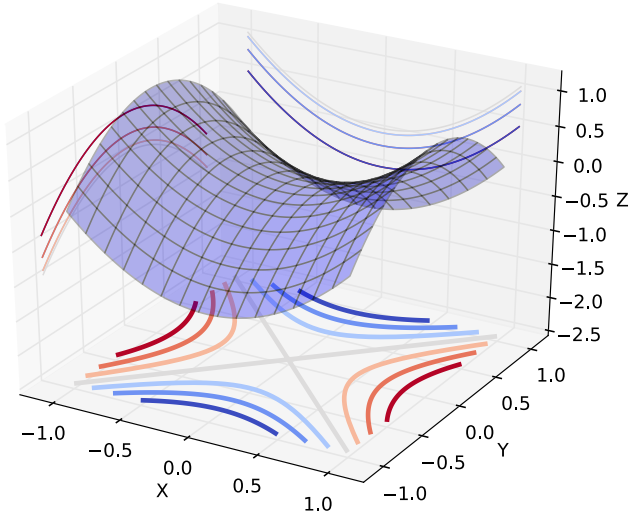
$$\theta^{(t)} \leftarrow \theta^{(t-1)} - \epsilon_t \frac{\partial L(z_t, \theta)}{\partial \theta}$$

- L = loss function, z_t = current example, θ = parameter vector, and ε_t = learning rate.
- Ordinary gradient descent is a batch method, very slow, should never be used. 2nd order batch method are being explored as an alternative but SGD with selected learning schedule remains the method to beat.

Saddle Points, not Local Minima

- Traditional thinking is that major obstacle for training deep nets is local minima
- Theoretical and empirical evidence suggest instead that saddle points are exponentially more prevalent critical points, and local minima tend to be of cost near that of global minimum
- (Dauphin et al NIPS'2014, Choromanska et al arxiv 2014)





Learning Rates

- Simplest recipe: keep it fixed and use the same for all parameters.
- Collobert scales them by the inverse of square root of the fan-in of each neuron
- Better results can generally be obtained by allowing learning rates to decrease, typically in O(1/t) because of theoretical convergence guarantees, e.g.,

$$\epsilon_t = \frac{\epsilon_0 \tau}{\max(t, \tau)}$$

with hyper-parameters ε_0 and τ.

- New papers on adaptive learning rates procedures (Schaul 2012, 2013), Adagrad (Duchi et al 2011), ADADELTA (Zeiler 2012)

Early Stopping

- Beautiful **FREE LUNCH** (no need to launch many different training runs for each value of hyper-parameter for #iterations)
- Monitor validation error during training (after visiting # of training examples = a multiple of validation set size)
- Keep track of parameters with best validation error and report them at the end
- If error does not improve enough (with some patience), stop.

Long-Term Dependencies

- In very deep networks such as **recurrent networks** (or possibly recursive ones), the gradient is a product of Jacobian matrices, each associated with a step in the forward computation. This can become very small or very large quickly [Bengio et al 1994], and the locality assumption of gradient descent breaks down.

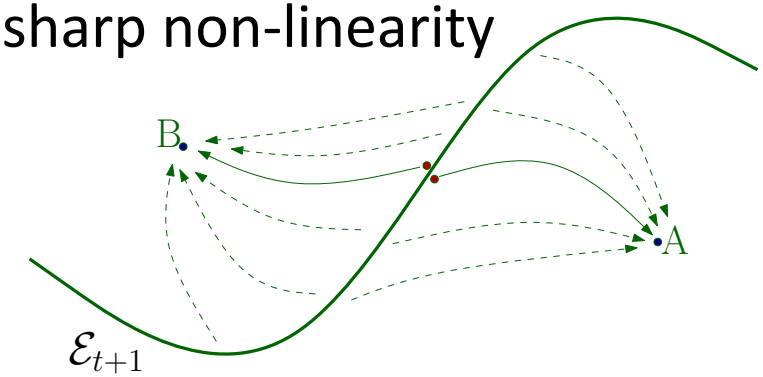
$$L = L(s_T(s_{T-1}(\ldots s_{t+1}(s_t, \ldots))))$$

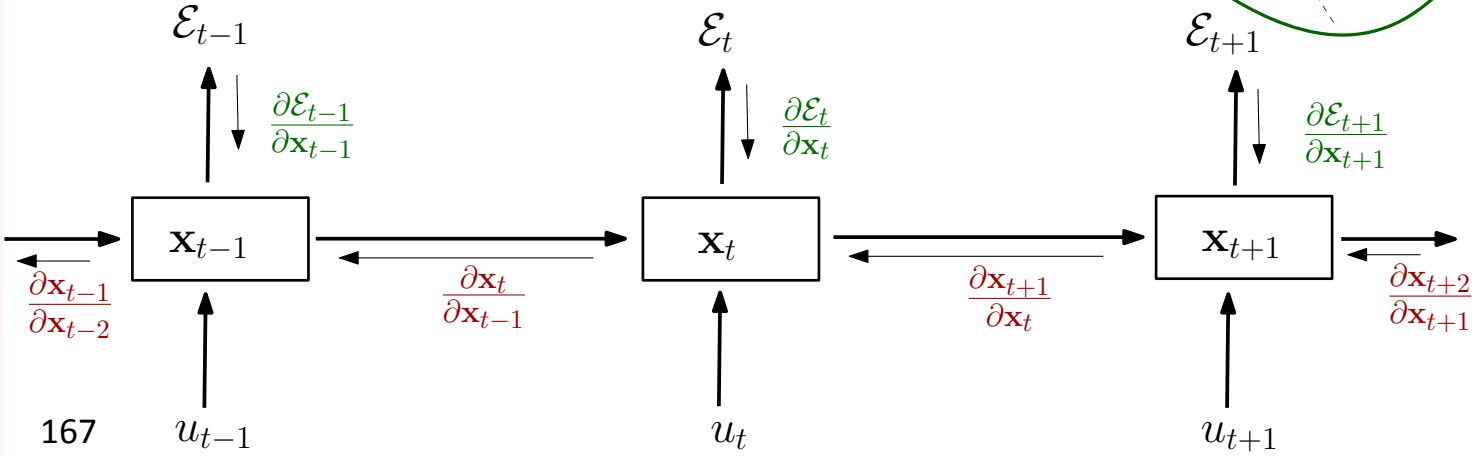
$$\frac{\partial L}{\partial s_t} = \frac{\partial L}{\partial s_T}\frac{\partial s_T}{\partial s_{T-1}}\cdots\frac{\partial s_{t+1}}{\partial s_t}$$

- Two kinds of problems:
  - sing. values of Jacobians > 1 → gradients explode
  - or sing. values < 1 → gradients shrink & vanish

The Optimization Challenge in Deep / Recurrent Nets

- Higher-level abstractions require highly non-linear transformations to be learned
- Sharp non-linearities are difficult to learn by gradient
- Composition of many non-linearities = sharp non-linearity
- Exploding or vanishing gradients

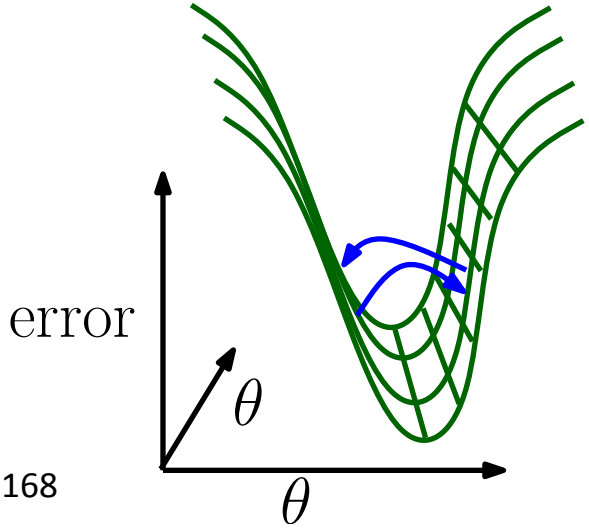


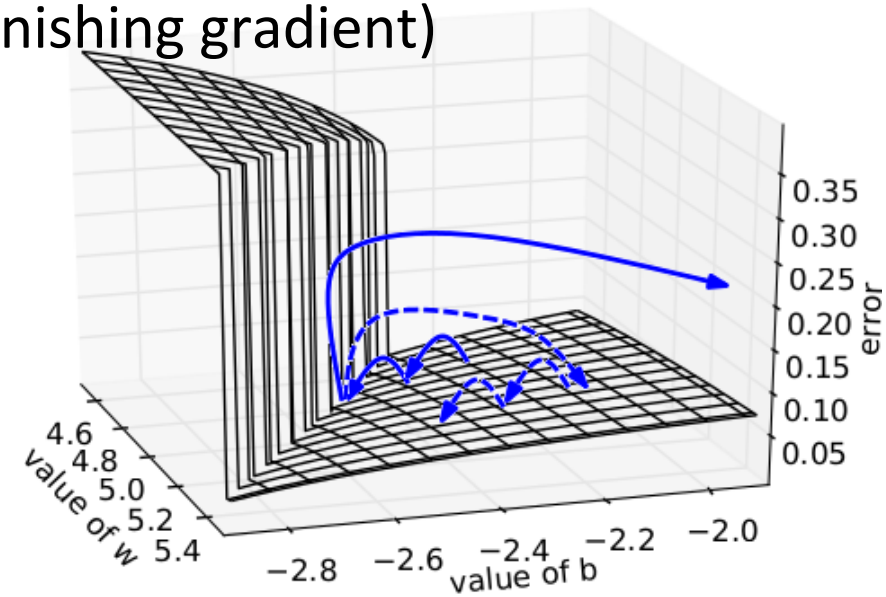


RNN Tricks

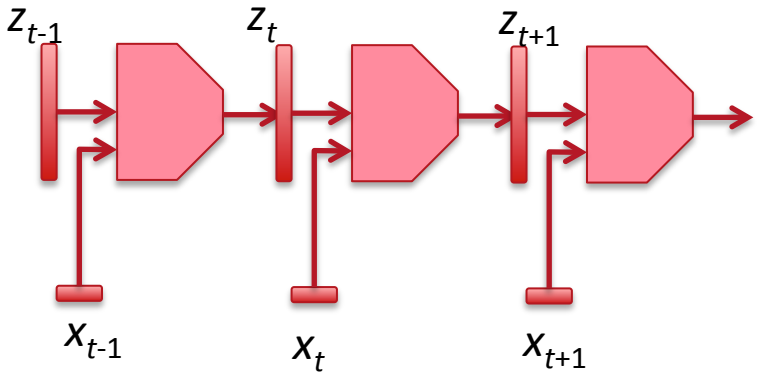
(Pascanu, Mikolov, Bengio, ICML 2013; Bengio, Boulanger & Pascanu, ICASSP 2013)

- **Clipping gradients** (avoid exploding gradients)
- Leaky integration (propagate long-term dependencies)
- Momentum (cheap 2nd order)
- **Initialization** (start in right ballpark avoids exploding/vanishing)
- Sparse Gradients (symmetry breaking)
- Gradient propagation regularizer (avoid vanishing gradient)
- **LSTM: gated self-loops** (avoid vanishing gradient)





Long-Term Dependencies and Clipping Trick



Trick first introduced by Mikolov is to clip gradients to a maximum NORM value.

Makes a big difference in Recurrent Nets (Pascanu et al ICML 2013)

Allows SGD to compete with HF optimization on difficult long-term dependencies tasks. Helped to beat SOTA in text compression, language modeling, speech recognition.

Gradient Norm Clipping

$$\hat{\mathbf{g}} \leftarrow \frac{\partial error}{\partial \theta}$$

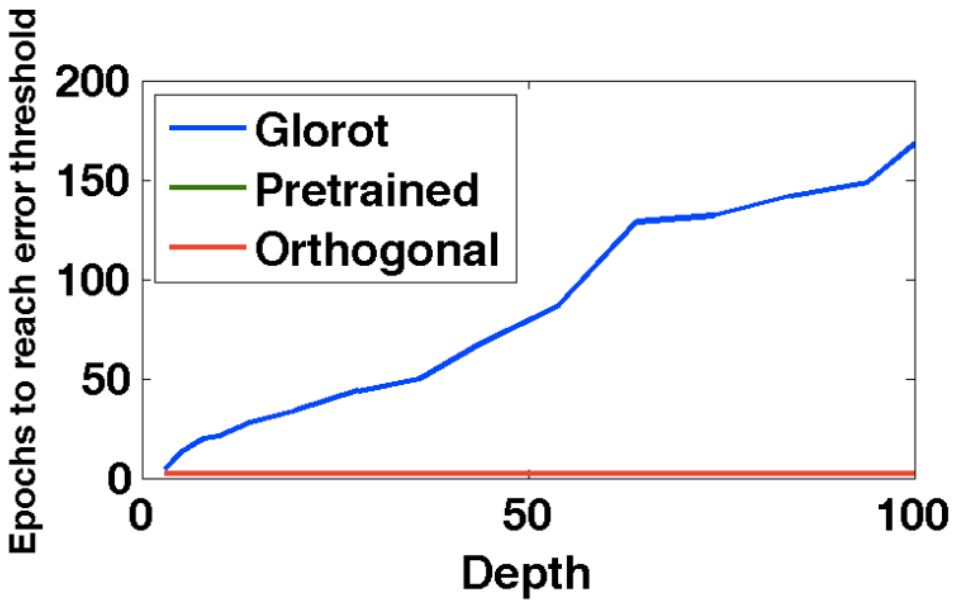
if $\|\hat{\mathbf{g}}\| \geq threshold$ **then**

$$\hat{\mathbf{g}} \leftarrow \frac{threshold}{\|\hat{\mathbf{g}}\|}\hat{\mathbf{g}}$$

end if

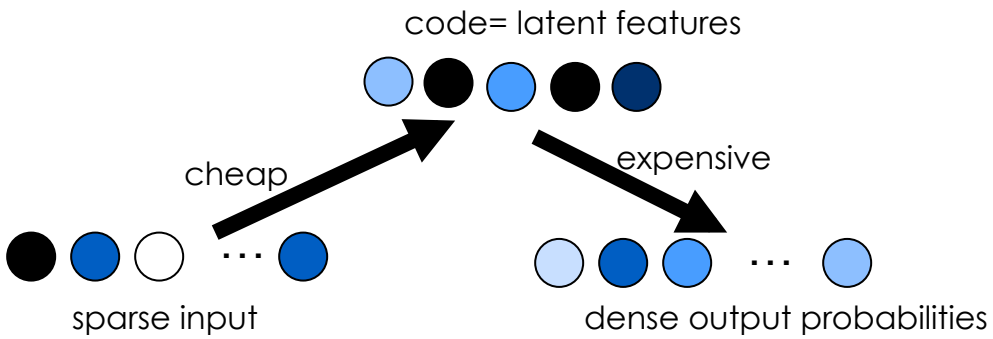
Orthogonal Initialization Works Even Better

- Auto-encoder pre-training tends to yield orthogonal W
- (Saxe, McClelland & Ganguli ICLR 2014) showed that **very deep** nets initialized with random orthogonal weights are much easier to train
- All singular values = 1

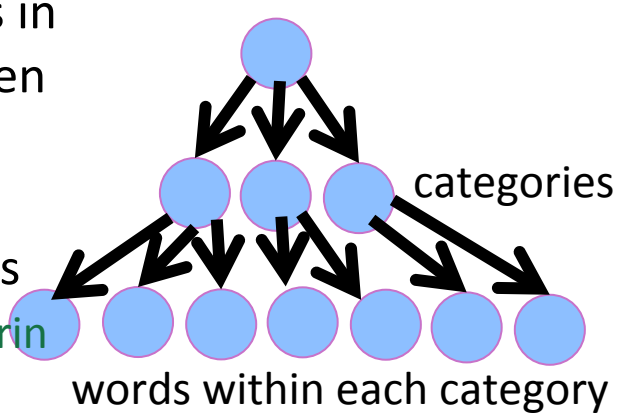


Handling Large Output Spaces

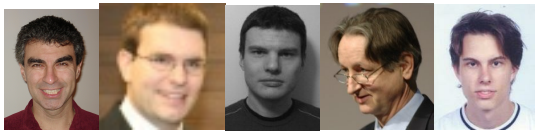
- Auto-encoders and RBMs reconstruct the input, which is sparse and high-dimensional; Language models have a huge output space (1 unit per word).



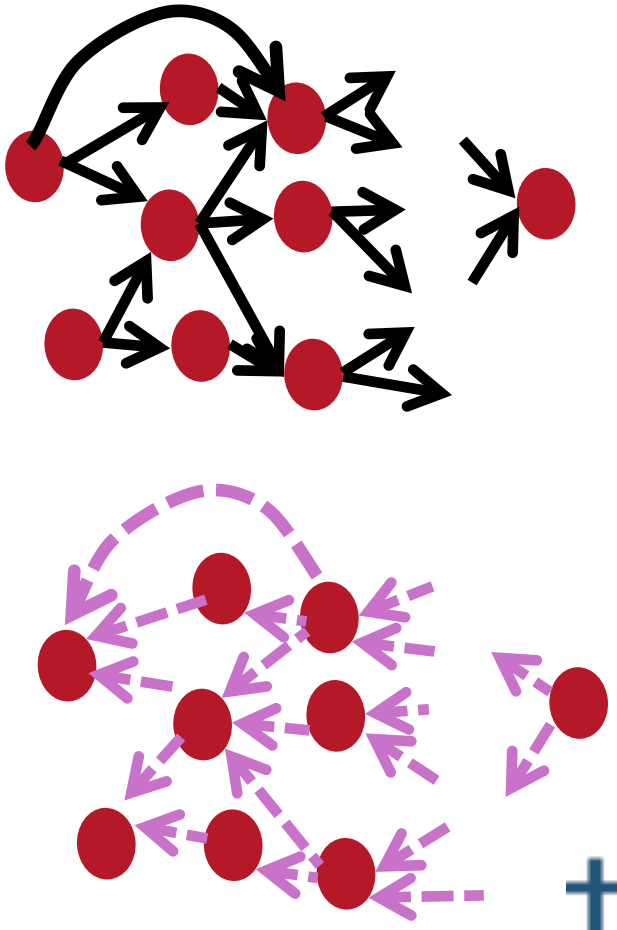
- (Dauphin et al, ICML 2011) Reconstruct the non-zeros in the input, and reconstruct as many randomly chosen zeros, + importance weights



- (Collobert & Weston, ICML 2008) sample a ranking loss
- Decompose output probabilities hierarchically (Morin & Bengio 2005; Blitzer et al 2005; Mnih & Hinton 2007,2009; Mikolov et al 2011)



Automatic Differentiation



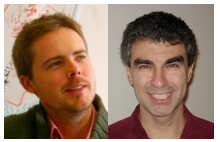
- Makes it easier to quickly and safely try new models.
- Theano Library (python) does it symbolically. Other neural network packages (Torch, Lush) can compute gradients for any given run-time value.

(Bergstra et al SciPy'2010)

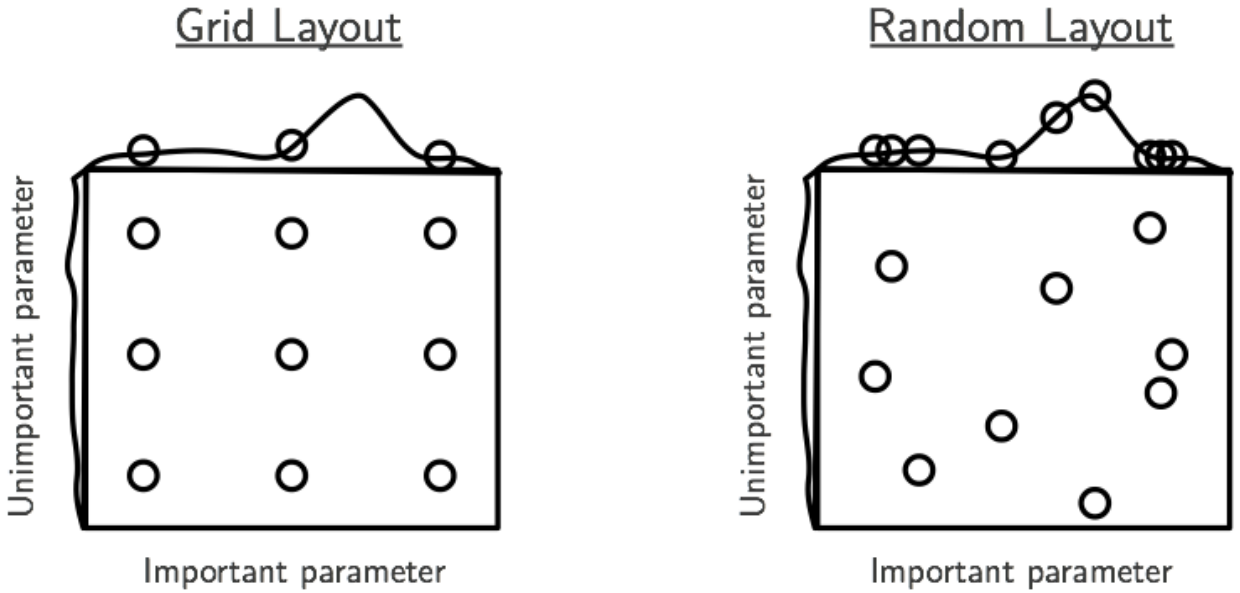
theano

Random Sampling of Hyperparameters

(Bergstra & Bengio 2012)

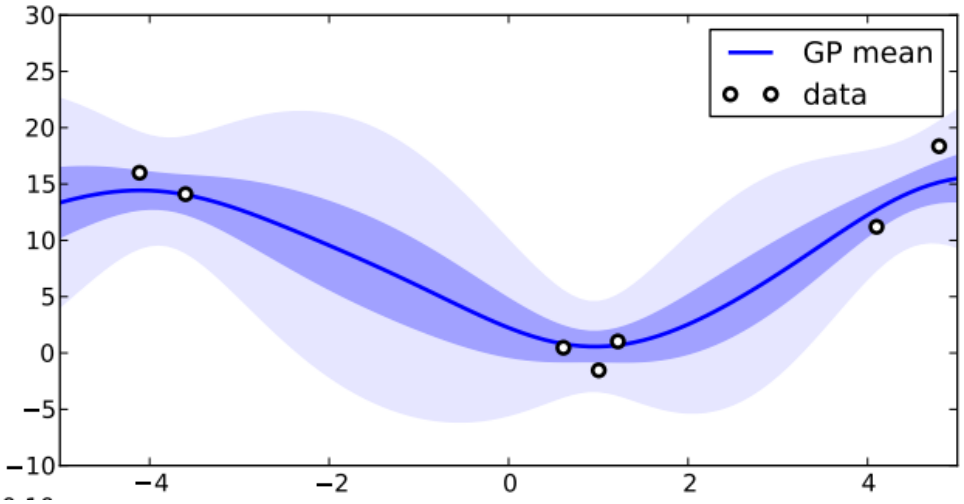


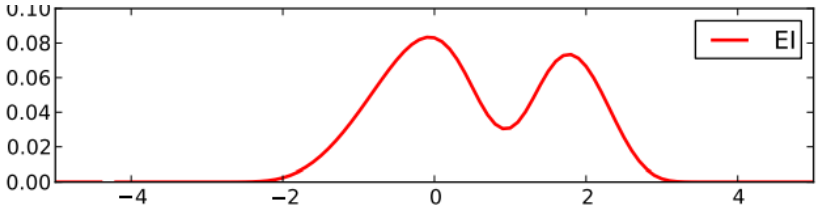
- Common approach: manual + grid search
- Grid search over hyperparameters: simple & wasteful
- Random search: simple & efficient
  - Independently sample each HP, e.g. l.rate~exp(U[log(.1),log(.0001)])
  - Each training trial is iid
  - If a HP is irrelevant grid search is wasteful
  - More convenient: ok to early-stop, continue further, etc.



Sequential Model-Based Optimization of Hyper-Parameters

- (Hutter et al JAIR 2009; Bergstra et al NIPS 2011; Thornton et al arXiv 2012; Snoek et al NIPS 2012)
- Iterate
- Estimate P(valid. err | hyper-params config x, D)
- choose optimistic x, e.g. $\max_x$ P(valid. err < current min. err | x)
- train with config x, observe valid. err. v, D ← D U {(x,v)}





Part 4

Challenges & Questions

Deep Learning Challenges (Bengio, arxiv 1305.0445 Deep learning of representations: looking forward)

- Computational Scaling
- Optimization & Underfitting
- Intractable Marginalization, Approximate Inference & Sampling
- Disentangling Factors of Variation
- Reasoning & One-Shot Learning of Facts

Deep Learning Challenges
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Challenge: Computational Scaling

- Recent breakthroughs in speech, object recognition and NLP hinged on faster computing, GPUs, and large datasets

- In speech, vision and NLP applications we tend to find that

*as **Ilya Sutskever** would say*

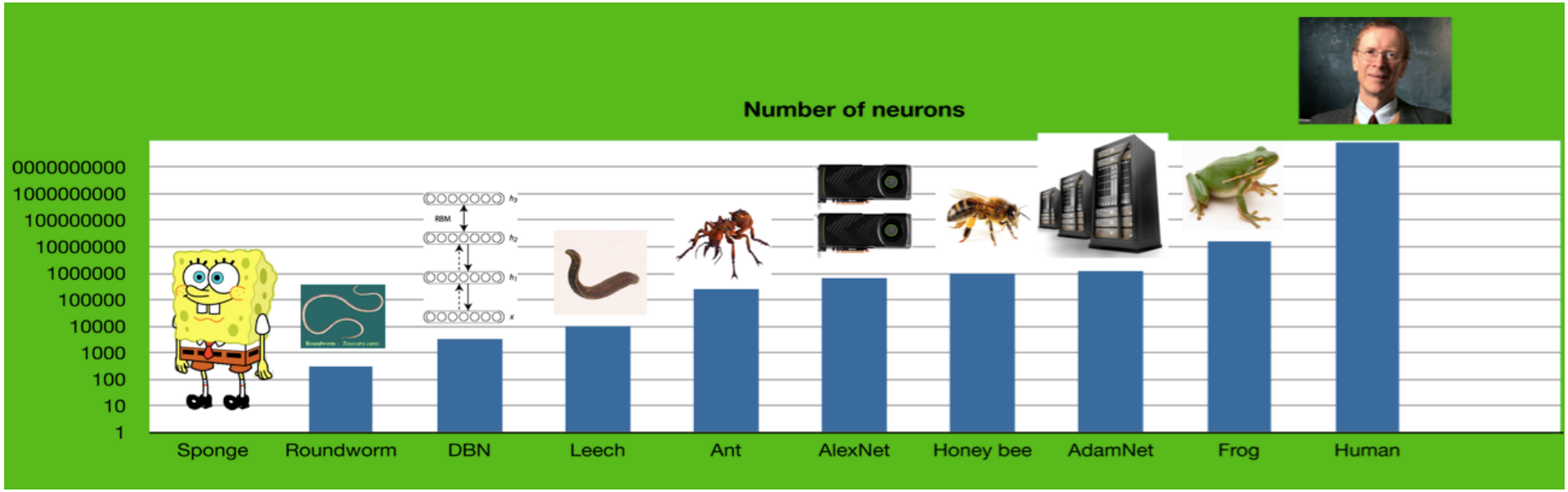
BIGGER IS BETTER

Because deep learning is

EASY TO REGULARIZE while

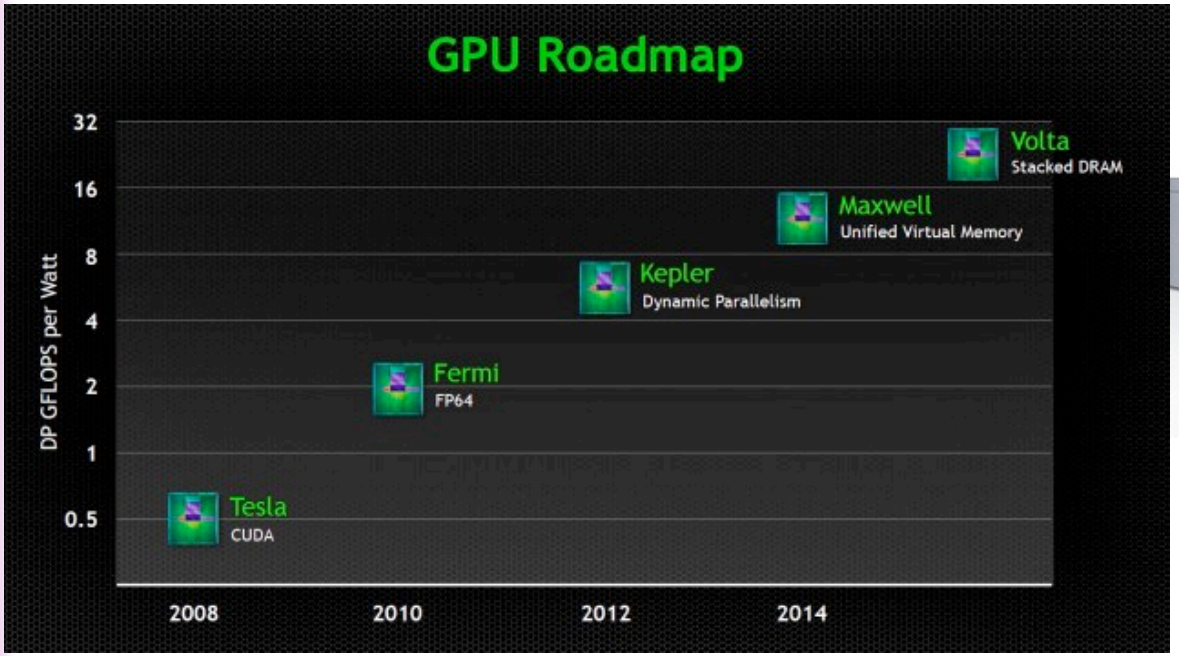
it is MORE DIFFICULT TO AVOID UNDERFITTING

We still have a long way to go in raw computational power

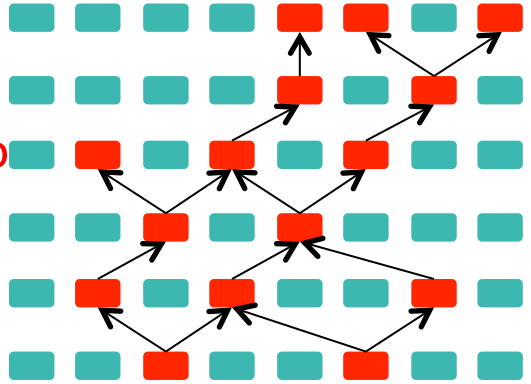


Challenge: Computational Scaling

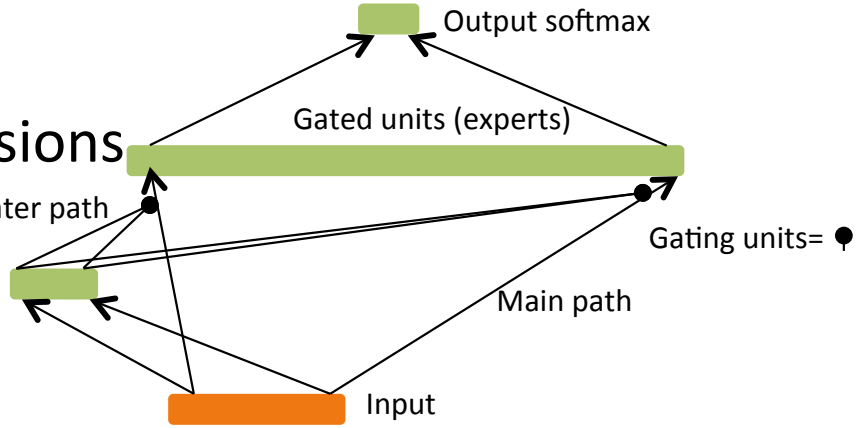
- Recent breakthroughs in speech, object recognition and NLP hinged on faster computing, GPUs, and large datasets
- A 100-fold speedup is possible without waiting another 10 yrs?
  - Challenge of distributed training
  - Challenge of conditional computation

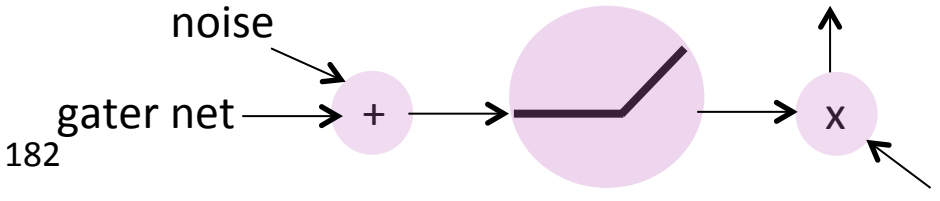


Conditional Computation: only visit a small fraction of parameters / example



- Deep nets vs decision trees
- Hard mixtures of experts (Collobert, Bengio & Bengio 2002)
- Conditional computation for deep nets: sparse distributed gaters selecting combinatorial subsets of a deep net
- Challenges:
  - Credit assignment for hard decisions
  - Gated architectures exploration
- Noisy rectifiers work well





Distributed Training

- Minibatches
- Large minibatches + 2nd order & natural gradient methods
- Asynchronous SGD (Bengio et al 2003, Le et al ICML 2012, Dean et al NIPS 2012)
  - Bottleneck: sharing weights/updates among nodes, to avoid node-models to move too far from each other
- Ideas forward:
  - Low-resolution sharing only where needed
  - Specialized conditional computation (each computer specializes in updates to some cluster of gated experts, and prefers examples which trigger these experts)

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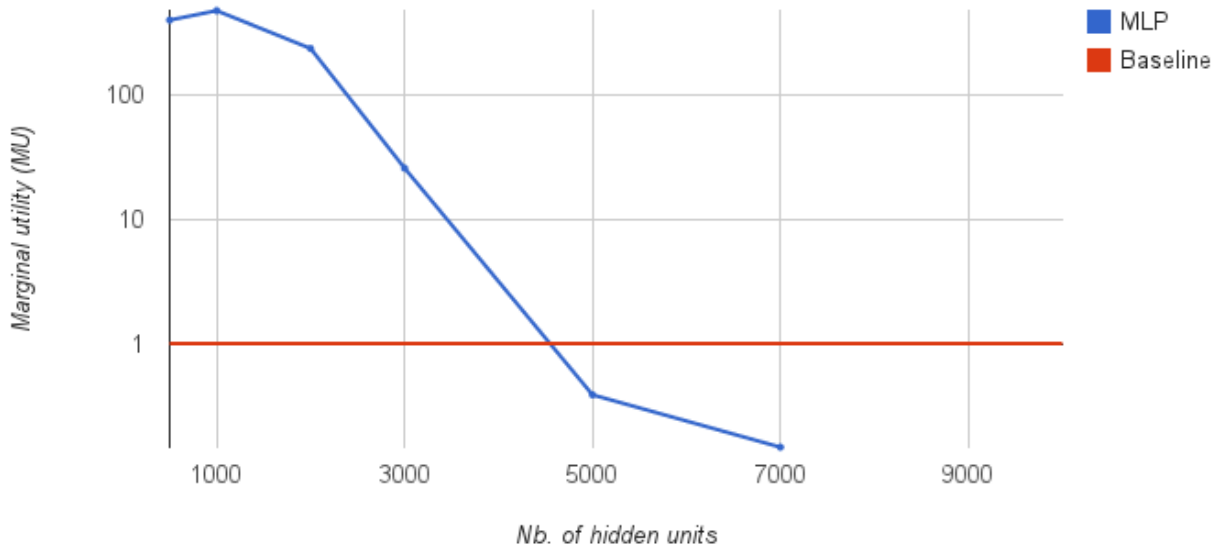
Optimization & Underfitting

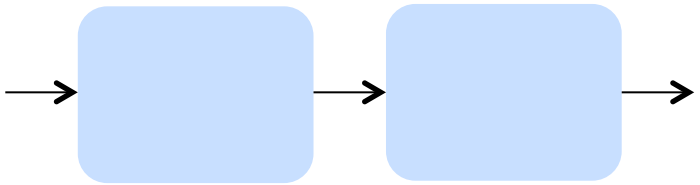
- On large datasets, major obstacle is underfitting
- **Marginal utility** of wider MLPs decreases quickly below memorization baseline



- Current limitations: local minima, ill-conditioning or else?

Guided Training, Intermediate Concepts

- In (Gulcehre & Bengio ICLR'2013) we set up a task that seems almost impossible to learn by shallow nets, deep nets, SVMs, trees, boosting etc
- Breaking the problem in two sub-problems and pre-training each module separately, then fine-tuning, nails it
- *Need prior knowledge to decompose the task*
- Guided pre-training allows to find much better solutions, escape effective local minima



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Basic Challenge with Probabilistic Models: marginalization

- Joint and marginal likelihoods involve intractable sums over configurations of random variables (inputs x, latent h, outputs y) e.g.

$$P(x) = \sum_h P(x,h)$$

$$P(x,h) = e^{-\text{energy}(x,h)} / Z$$

$$Z = \sum_{x,h} e^{-\text{energy}(x,h)}$$

- MCMC methods can be used for these sums, by sampling from a chain of x's (or of (x,h) pairs) approximately from P(x,h)

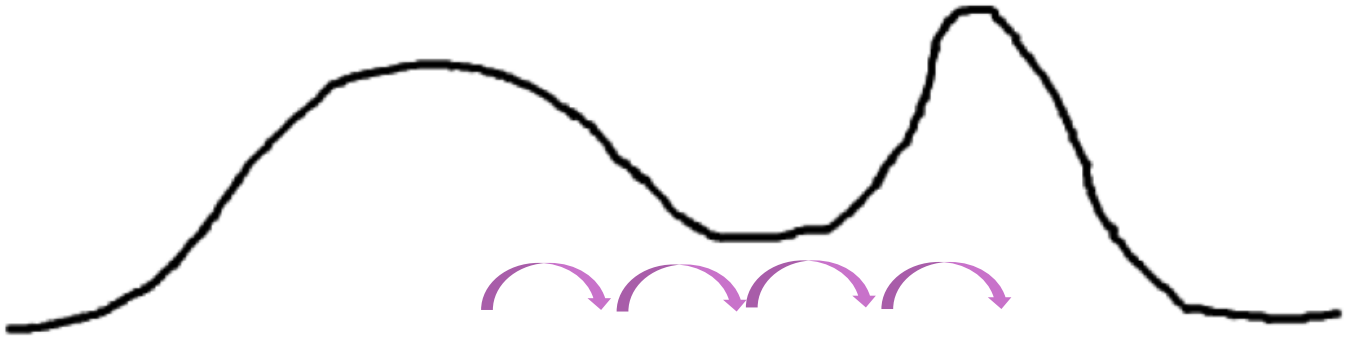
Two Fundamental Problems with Probabilistic Models with Many Random Variables

1. MCMC mixing between modes
   (manifold hypothesis)

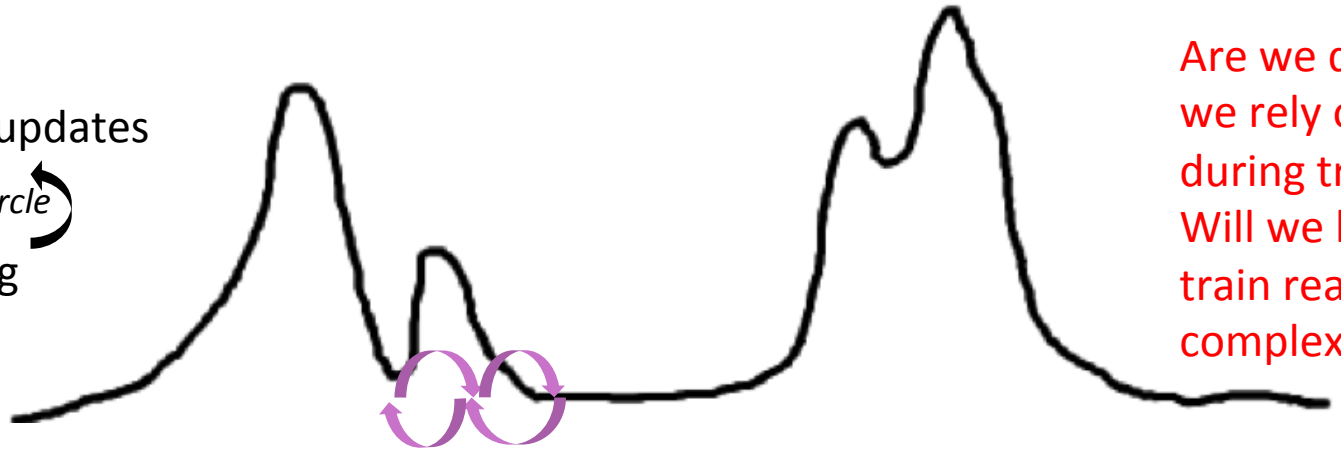
2. Many non-negligeable modes
   (both in posterior & joint distributions)

For gradient & inference: More difficult to mix with better trained models

- Early during training, density smeared out, mode bumps overlap



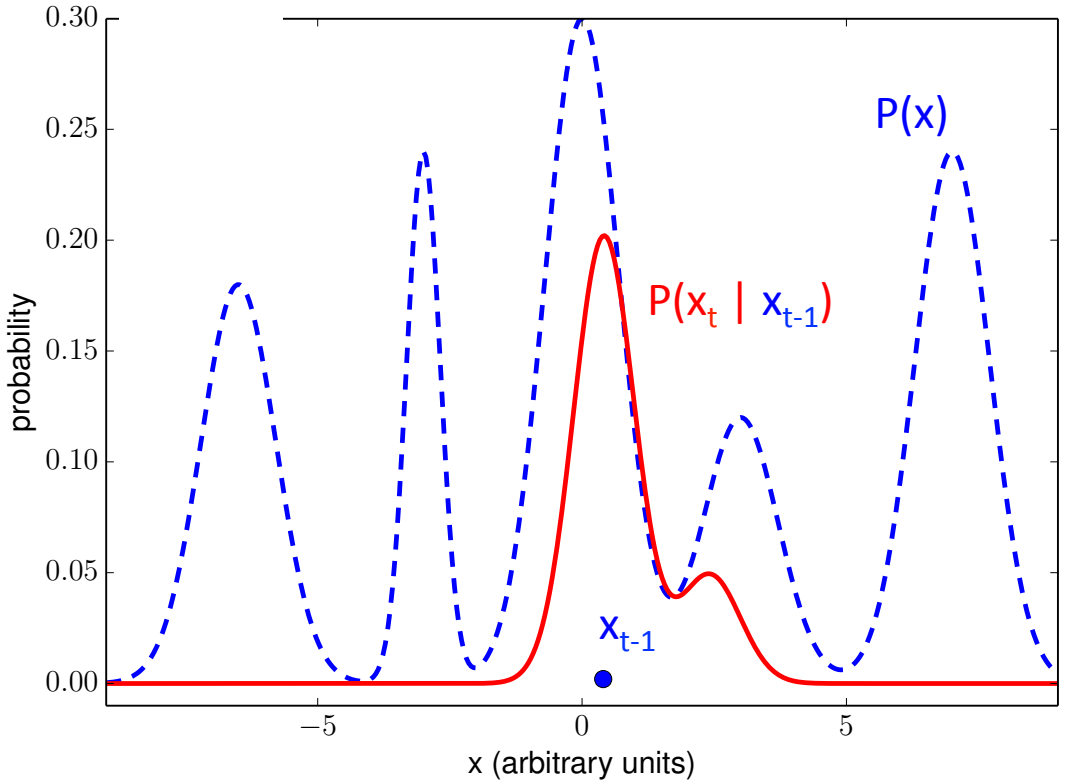
- Later on, hard to cross empty voids between modes



Are we doomed if we rely on MCMC during training? Will we be able to train really large & complex models?

Many Modes Challenge: Instead of learning P(x) directly, learn Markov chain operator $P(x_t \mid x_{t-1})$

- P(x) may have many modes, making the normalization constant intractable, and MCMC approximations poor
- Partition fn of $P(x_t \mid x_{t-1})$ much simpler because most of the time a local move, might even be well approximated by unimodal

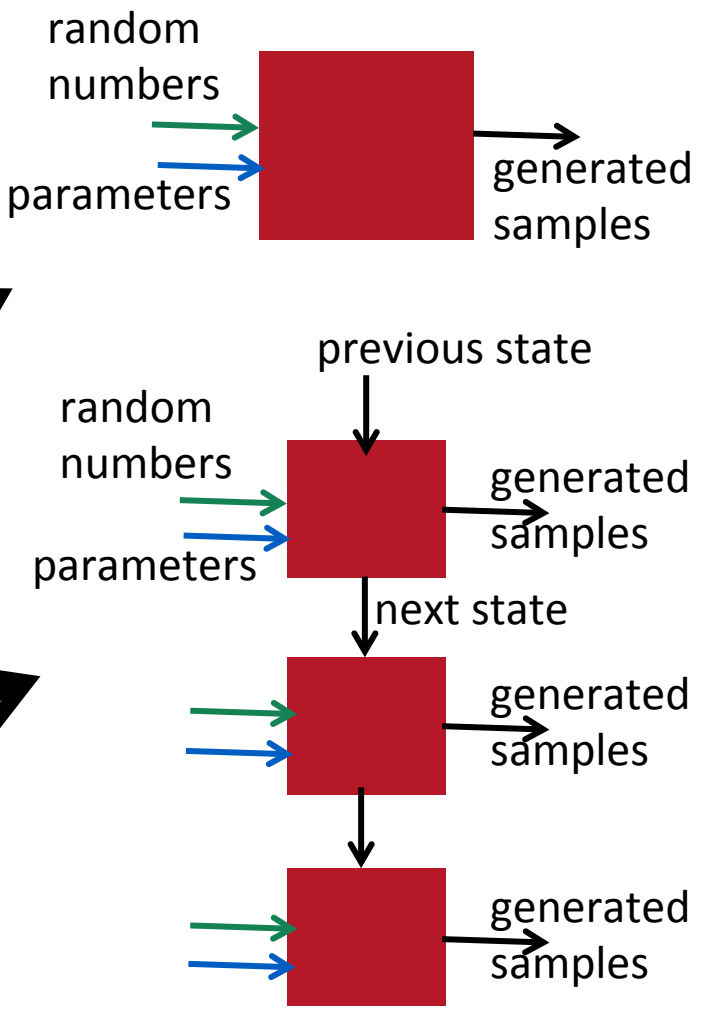


Bypassing Normalization Constants with Generative Black Boxes

- **Instead of parametrizing p(x), parametrize a machine which generates samples**

- (Goodfellow et al, NIPS 2014, Generative adversarial nets) for the case of ancestral sampling in a deep generative net. Variational auto-encoders are closely related.

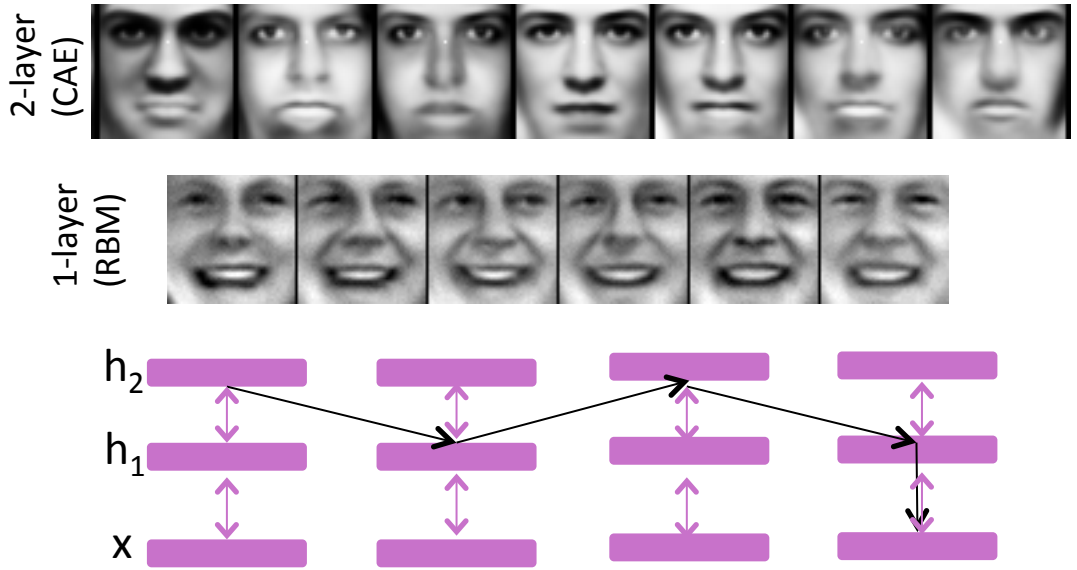
- (Bengio et al, ICML 2014, Generative Stochastic Networks), learning the transition operator of a Markov chain that generates the data.



Poor Mixing: Depth to the Rescue

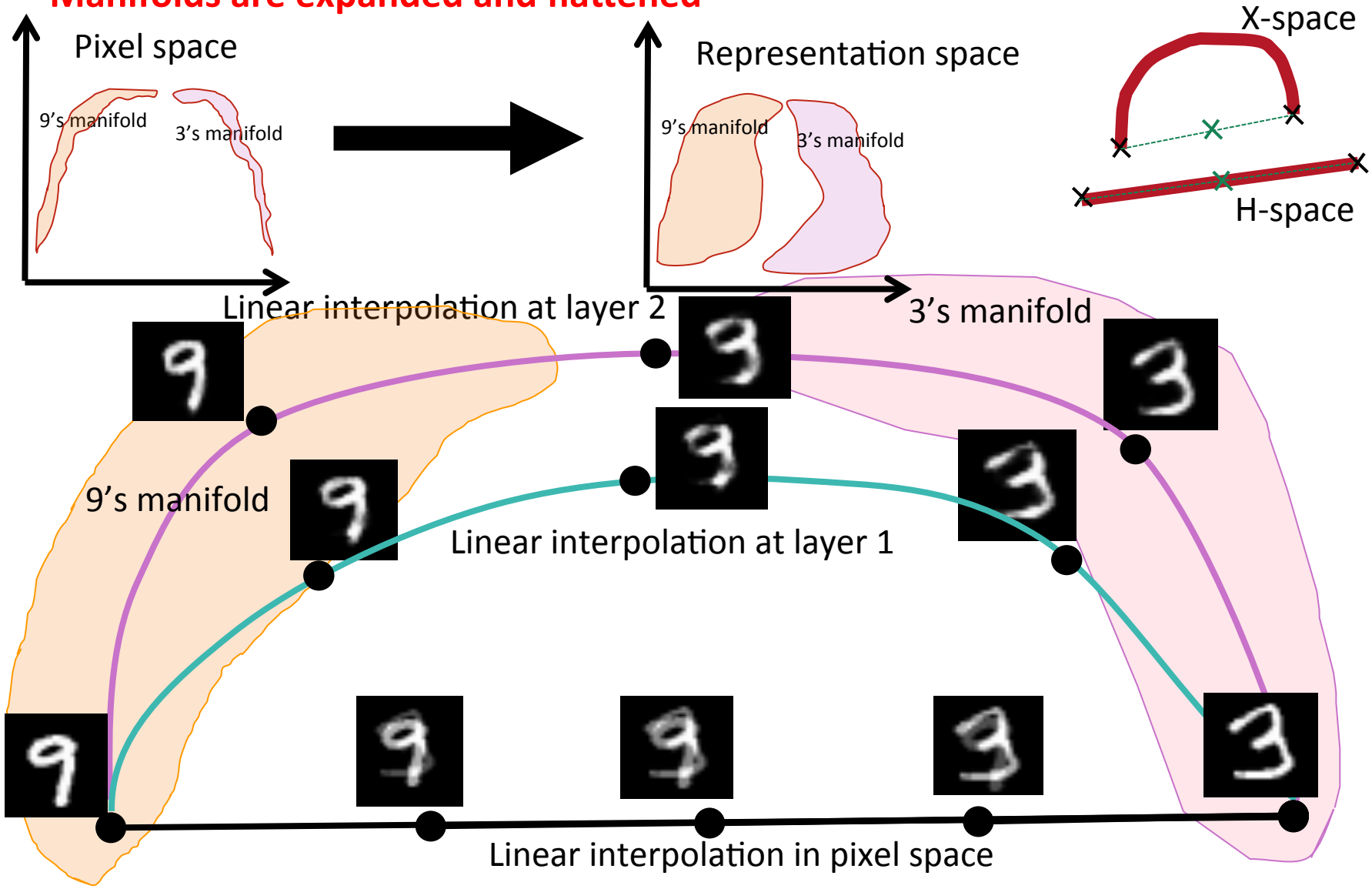
(Bengio et al ICML 2013)

- Sampling from DBNs and stacked Contractive Auto-Encoders:
  1. MCMC sampling from top layer model
  2. Propagate top-level representations to input-level repr.
- Deeper nets visit more modes (classes) faster



Space-Filling in Representation-Space

- **Deeper representations → abstractions → disentangling**
- **Manifolds are expanded and flattened**



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Disentangling the Underlying Factors

- How could a learner disentangle the unknown underlying factors of variation?
  - Statistical structure present in the data
  - Hints = priors

- Good disentangling →

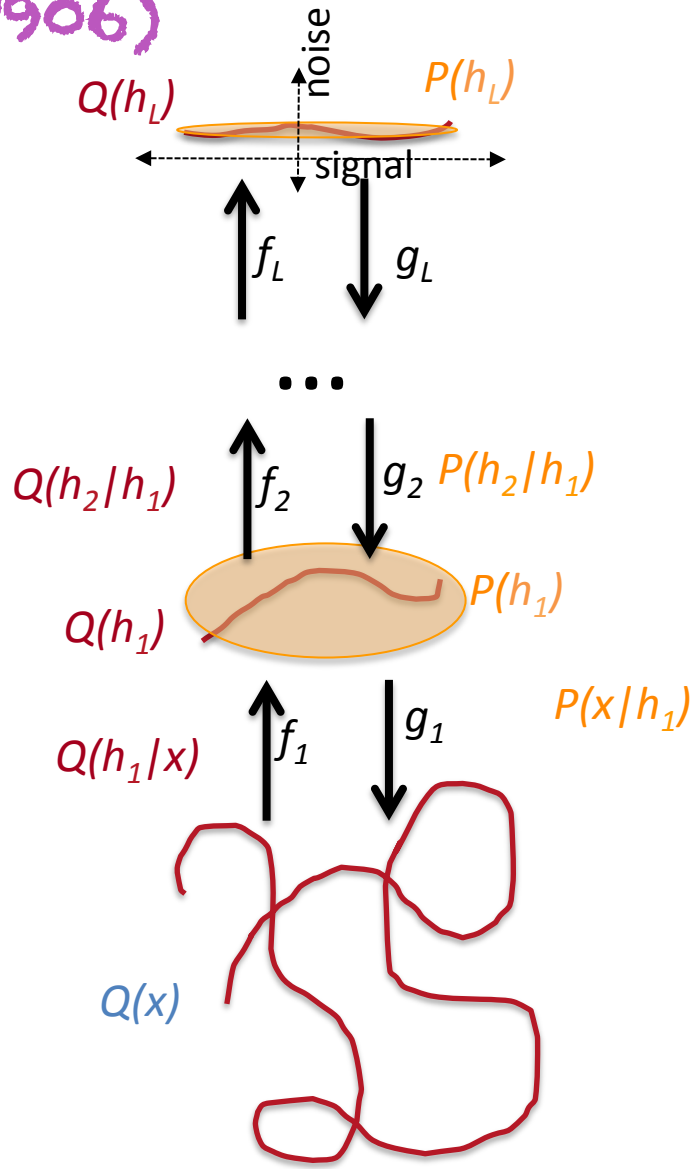
  avoid the curse of dimensionality

Extracting Structure By Gradual Disentangling and Manifold Unfolding (Bengio 2014, arXiv 1407.7906)

Each level transforms the data into a representation in which it is easier to model, unfolding it more, contracting the noise dimensions and mapping the signal dimensions to a factorized (uniform-like) distribution.

$$\min KL(Q(x,h)||P(x,h))$$

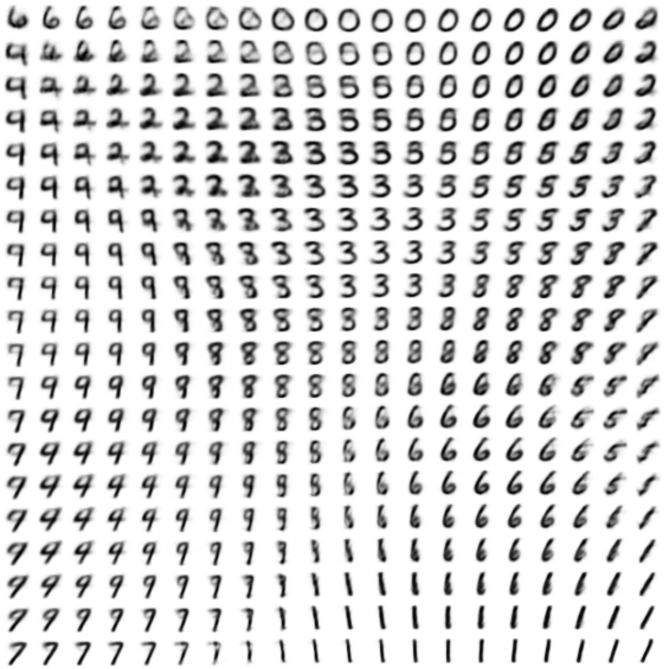
for each intermediate level h



Variational Auto-Encoder: Random Sampling at Top Level

- Models trained with the KL(Q||P) or VAE training objective
- Randomly sample from 2-D top-level h (Gaussian), project down:

(from Kingma & Welling ICLR 2014)



Deep Directed Generative AEs

(Ozair & Bengio 2014, arXiv 1410.0630)

- log P(x) >= log P(x|h=f(x)) + log P(h=f(x))

= bound that is maximized and becomes tight as training progresses

- Stacking such auto-encoders yields representations that become sparser and with less correlation between features

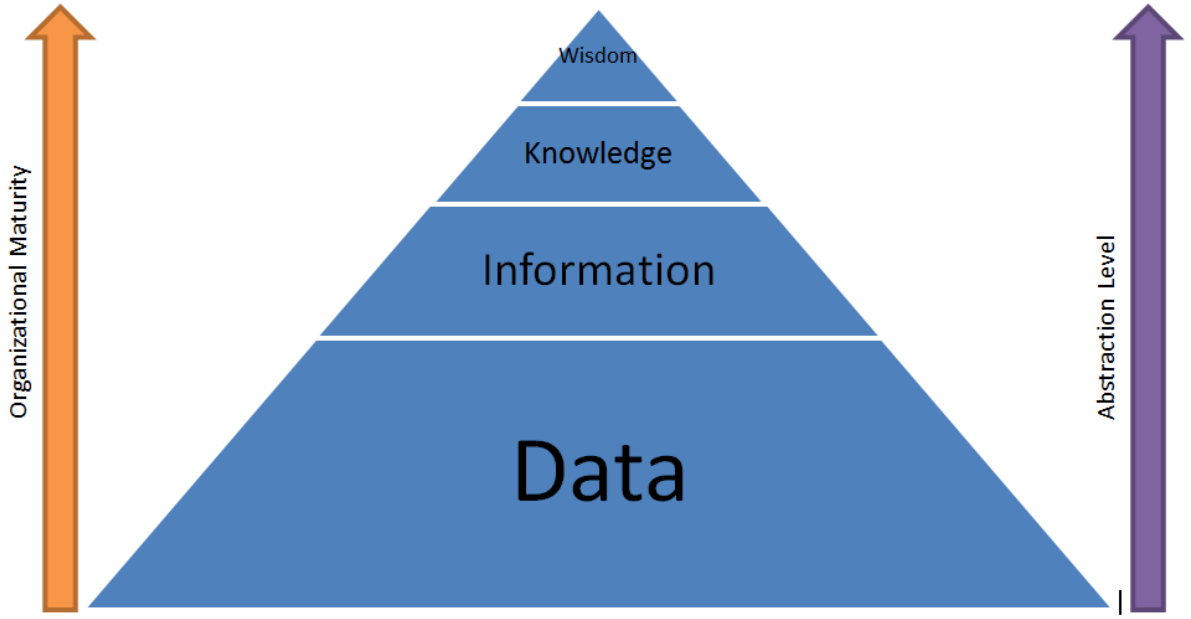
Samples	Entropy	Avg # active bits	$\|\|Corr - diag(Corr)\|\|_F$
Data (X)	297.6	102.1	63.5
Output of 1^{st} encoder $(f_1(X))$	56.9	20.1	11.2
Output of 2^{nd} encoder $(f_2(f_1(X)))$	47.6	17.4	9.4

Broad Priors as Hints to Disentangle the Factors of Variation

- *Multiple factors*: distributed representations
- Multiple levels of abstraction: *depth*
- *Semi-supervised* learning: Y is one of the factors explaining X
- *Multi-task* learning: different tasks share some factors
- *Manifold* hypothesis: probability mass concentration
- Natural *clustering*: class = manifold, well-separated manifolds
- Temporal and spatial *coherence*
- *Sparsity*: most factors irrelevant for particular X
- *Simplicity* of factor dependencies (in the right representation)

Conclusion: Learning Multiple Levels of Abstraction

- The big payoff of deep learning is to allow learning higher levels of abstraction
- Higher-level abstractions disentangle the factors of variation, which allows much easier generalization and transfer



Conclusions

- Deep Learning has matured
  - Int. Conf. on Learning Representation 2013 & 2014 a huge success!
- Industrial applications (Google, Microsoft, Baidu, Facebook, …)

- Room for improvement:
  - Scaling computation
  - Optimization
  - Bypass intractable marginalizations
  - More disentangled abstractions
  - Reason from incrementally added facts

Additional pointers

Related Tutorials

- Deep Learning (MIT Press book in preparation): http://www.iro.umontreal.ca/~bengioy/dlbook/
- Deep Learning tutorials (python): http://deeplearning.net/tutorials
- Stanford deep learning tutorials with simple programming assignments and reading list http://deeplearning.stanford.edu/wiki/
- IPAM 2012 Summer school on Deep Learning http://www.iro.umontreal.ca/~bengioy/talks/deep-learning-tutorial-aaai2013.html
- **More reading: references in my upcoming Deep Learning book**

Software

- Theano (Python CPU/GPU) mathematical and deep learning library http://deeplearning.net/software/theano
  - Can do automatic, symbolic differentiation
  - On top of Theano: Pylearn2
    - http://deeplearning.net/software/pylearn2
- Torch ML Library (C++ + Lua) http://www.torch.ch/
- Senna: for NLP tasks
  - by Collobert et al. http://ronan.collobert.com/senna/
  - State-of-the-art performance on many tasks
  - 3500 lines of C, extremely fast and using very little memory

LISA team: Merci! Questions?