UNSUPERVISED LEARNING

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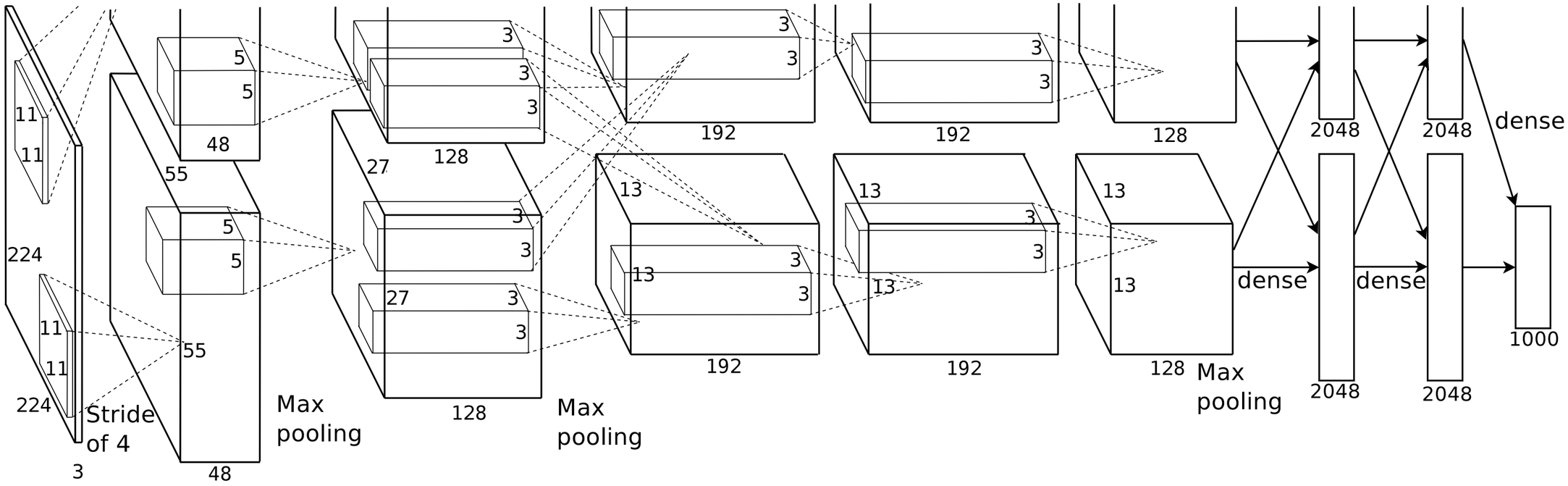
Deep Learning for Computer Vision Tutorial @ CVPR 2014
Columbus, OH

Motivation

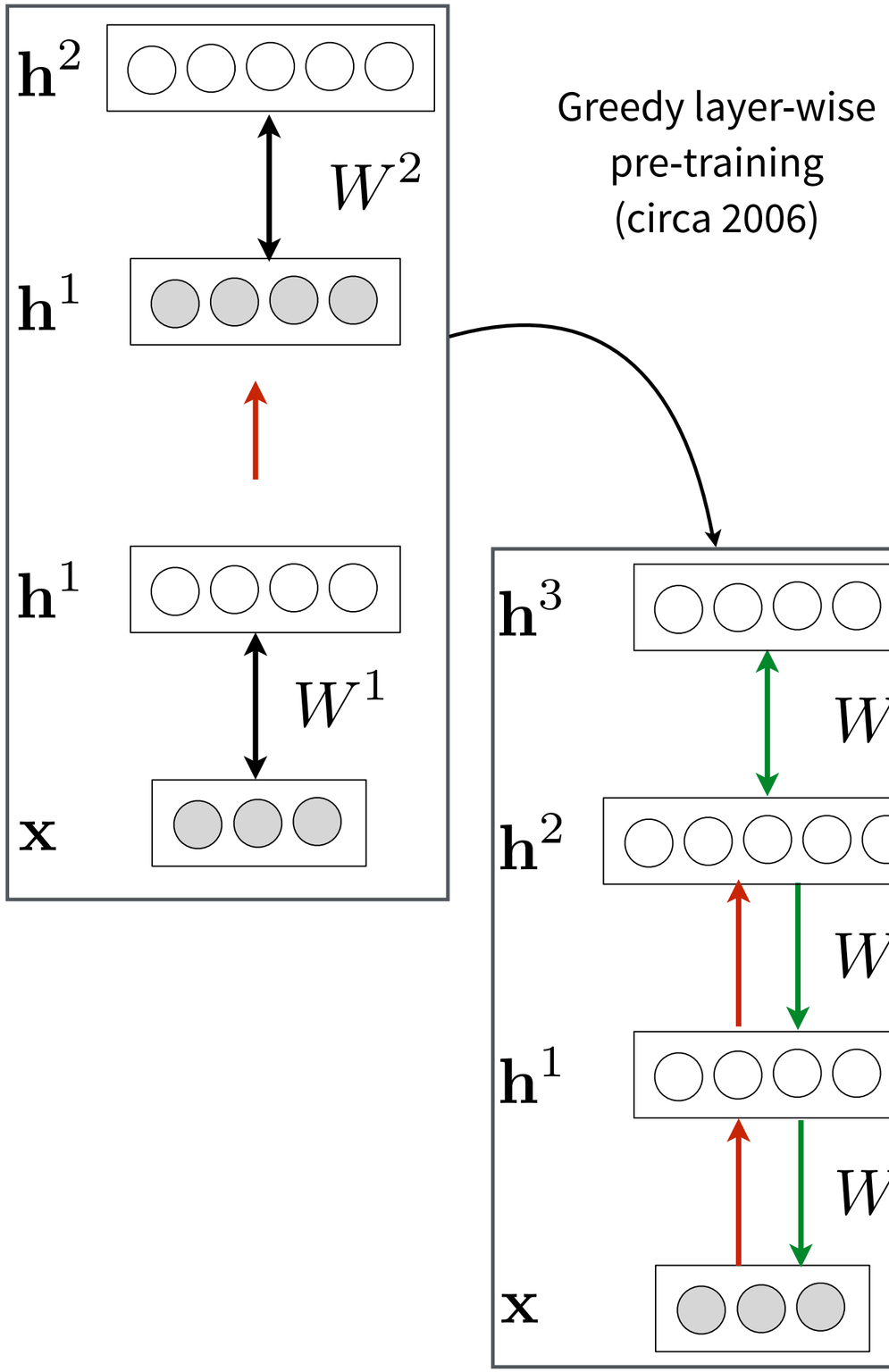


- Most impressive results in deep learning have been obtained with purely supervised learning methods (see previous talk)
- In vision, typically classification (e.g. object recognition)
- Though progress has been slower, it is likely that unsupervised learning will be important to future advances in DL

Image: Krizhevsky (2012) - AlexNet, the “hammer” of DL

An Interesting Historical Fact

- Unsupervised learning was the catalyst for the present DL revolution that started around 2006
- Now we can train deep supervised neural nets without “pre-training”, thanks to
  - Algorithms (nonlinearities, regularization)
  - More data
  - Better computers (e.g. GPUs)
- Should we still care about unsupervised learning?



Why Unsupervised Learning?

<u>Reason 1:</u>

We can exploit unlabelled data; much more readily available and often free.

Why Unsupervised Learning?

Reason 2:

We can capture enough information about the observed variables so as to ask new questions about them; questions that were not anticipated at training time.

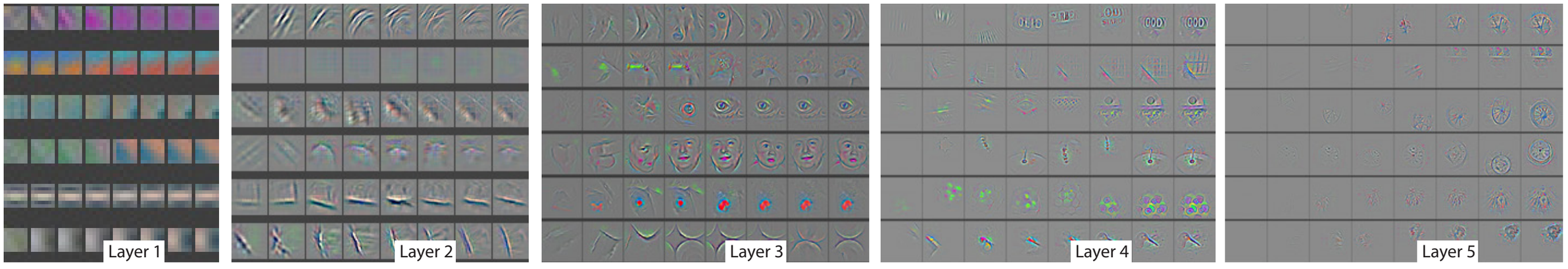


Image: Features from a convolutional net (Zeiler and Fergus, 2013)

Why Unsupervised Learning?

Reason 3:

Unsupervised learning has been shown to be a good regularizer for supervised learning; it helps generalize.

This advantage shows up in practical applications:

- transfer learning, domain adaptation
- unbalanced classes
- zero-shot, one-shot learning

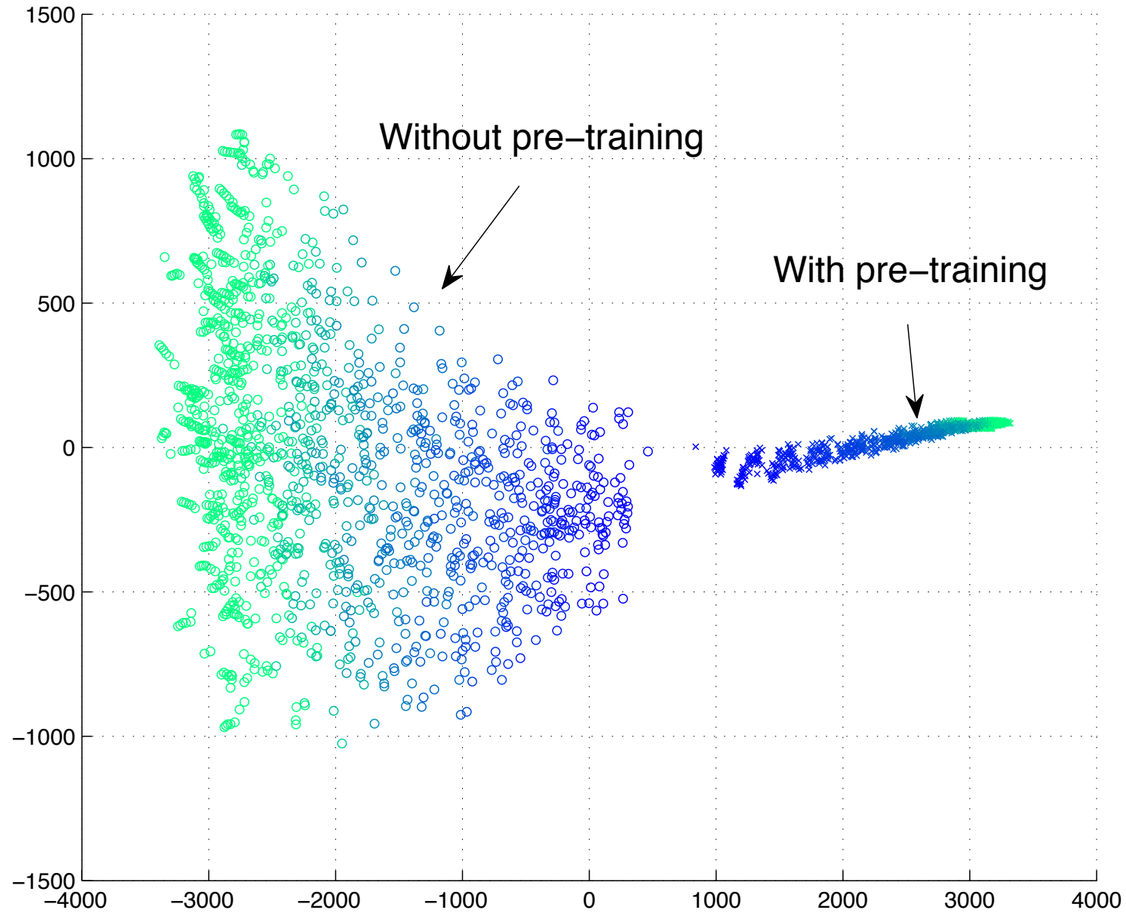
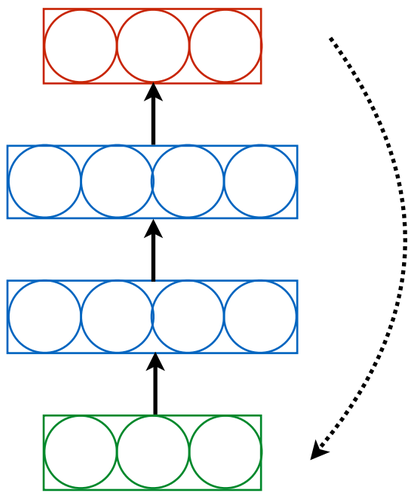


Image: ISOMAP embedding of functions represented by 50 networks w and w/o pre training (Erhan et al., 2010)

Why Unsupervised Learning?

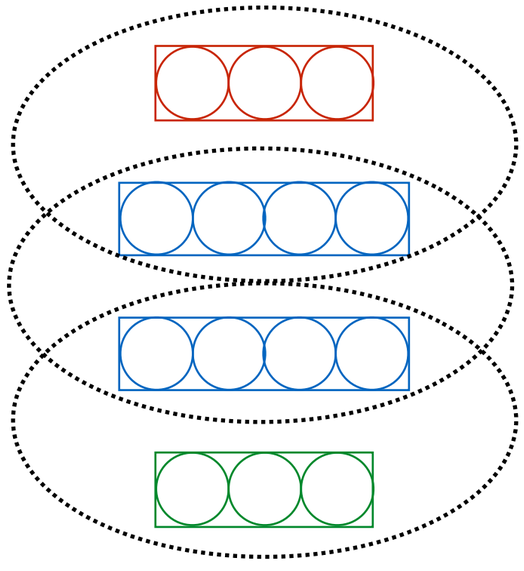
Reason 4:

There is evidence that unsupervised learning can be achieved mainly through a level-local training signal; compare this to supervised learning where the only signal driving parameter updates is available at the output and gets backpropagated.



Propagate credit

Supervised learning

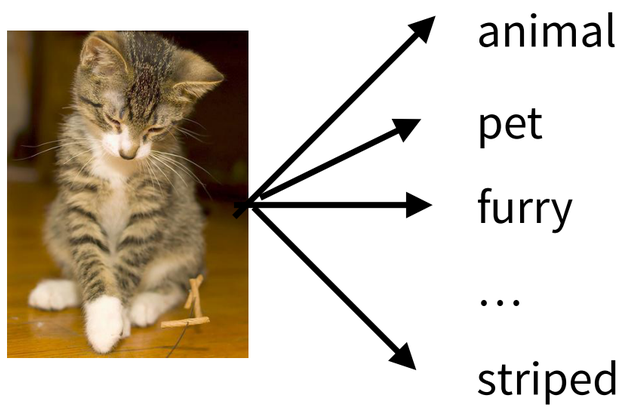


Local learning

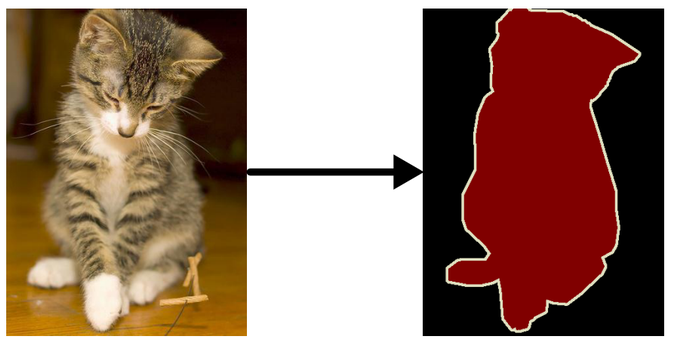
Why Unsupervised Learning?

Reason 5:

A recent trend in machine learning is to consider problems where the output is high-dimensional and has a complex, possibly multi-modal joint distribution. Unsupervised learning can be used in these "structured output" problems.



Attribute Prediction



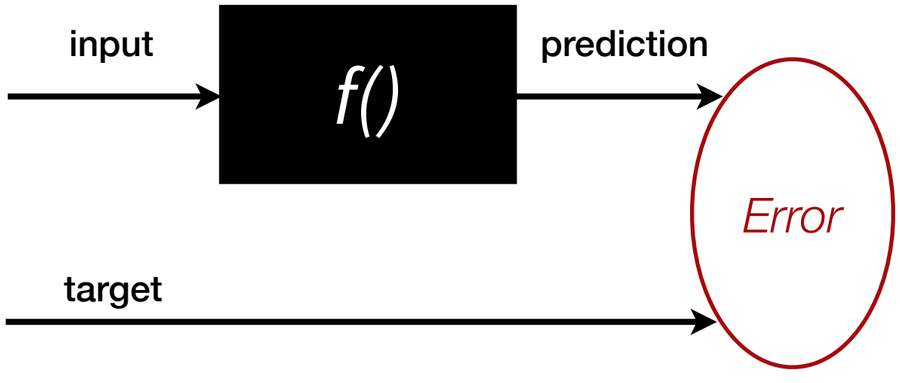
Segmentation

Learning Representations

- "Concepts" or "Abstractions" that help us make sense of the variability in data
- Often hand-designed to have desirable properties: e.g. sensitive to variables we want to predict, less sensitive to other factors explaining variability
- DL has leveraged the ability to learn representations
  - these can be task-specific or task-agnostic

Supervised Learning of Representations

- Learn a representation with the objective of selecting one that is best suited for predicting targets given input



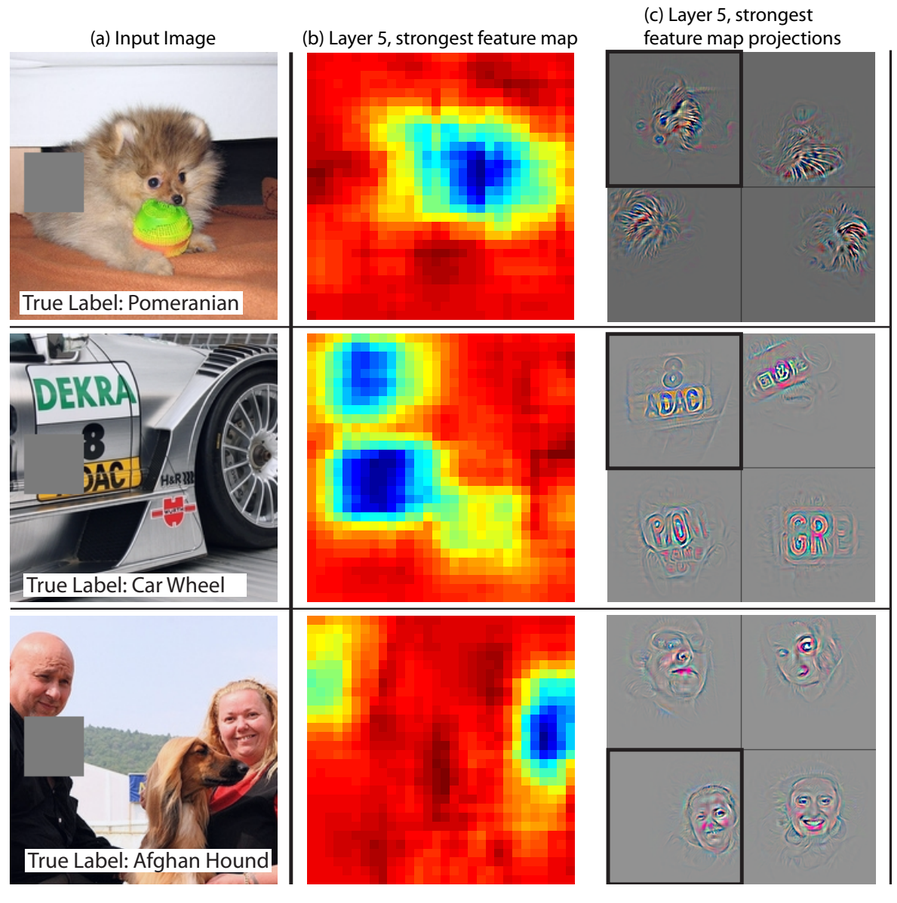
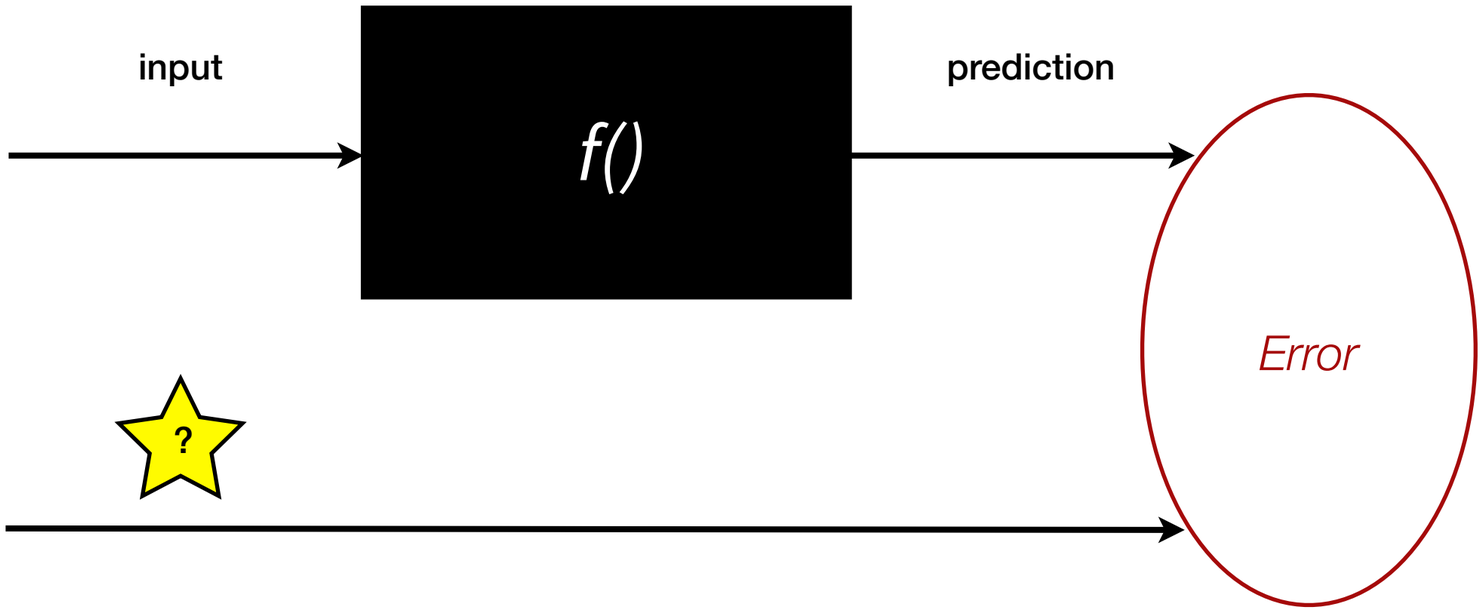


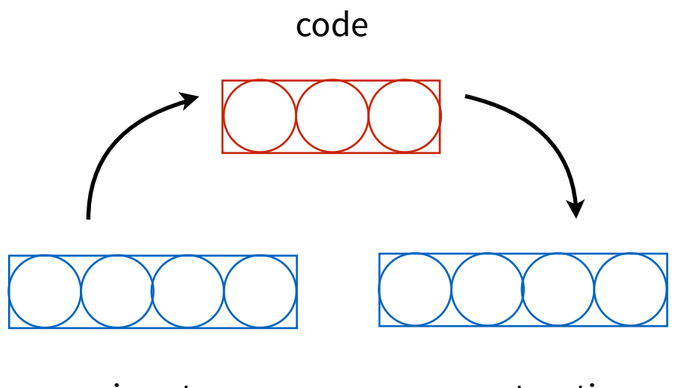
Image: Features from a convolutional net (Zeiler and Fergus, 2013)

Unsupervised Learning of Representations



Unsupervised learning of representations

- What is the objective?
  - reconstruction error?
  - maximum likelihood?
  - disentangle factors of variation?



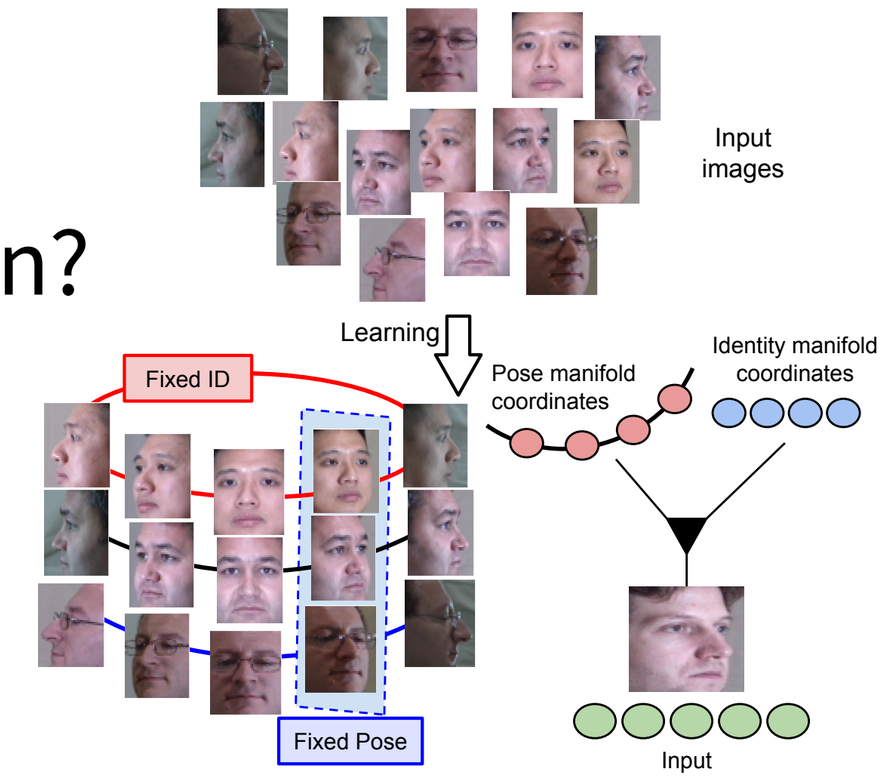


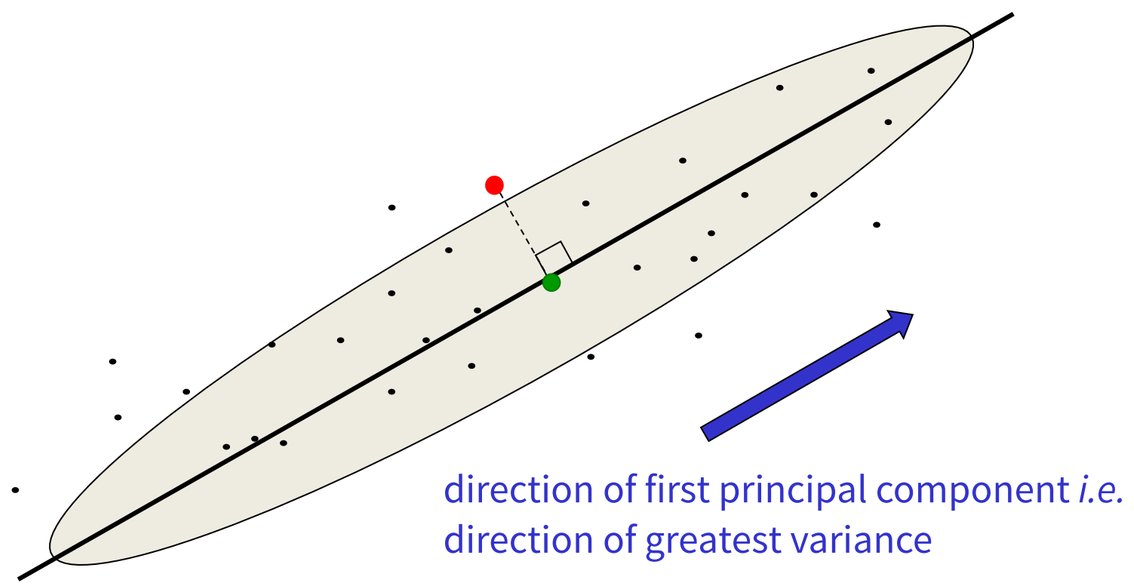
Image: Lee et al. 2014

Overview (for the remainder of the talk)

- Unsupervised building blocks of Deep Learning
  - Auto-encoders
  - Restricted Boltzmann Machines
- Their use in Deep Architectures (how/why?)
- Practical considerations

Principal Components Analysis

- PCA works well when the data is near a linear manifold in high-dimensional space
- Project the data onto this subspace spanned by principal components
- In dimensions orthogonal to the subspace the data has low variance

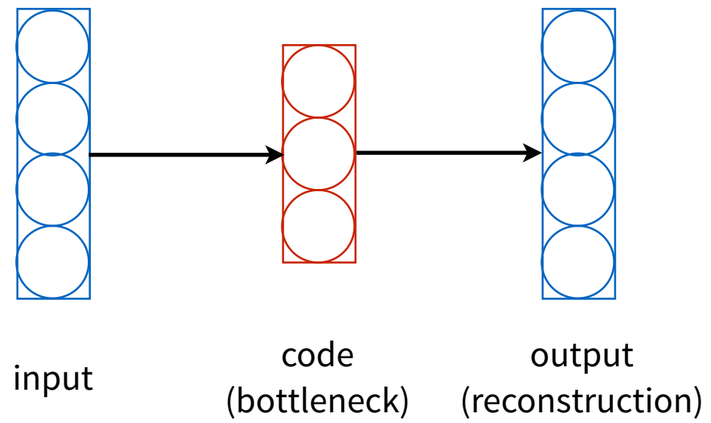


Credit: Geoff Hinton

An inefficient way to fit PCA

- Train a neural network with a “bottleneck” hidden layer

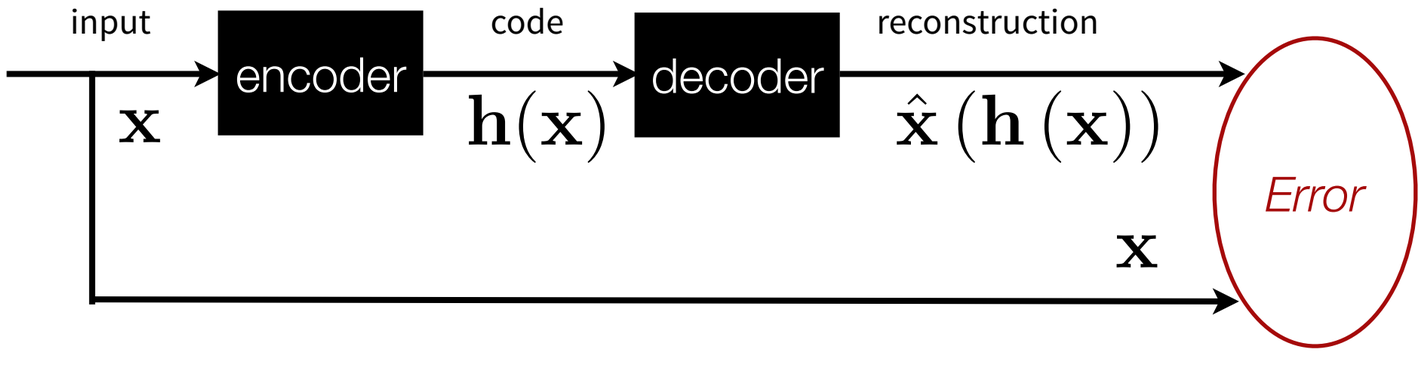
- Try to make the output the same as the input



- If the hidden and output layers are linear, and we minimize squared reconstruction error:
  - The M hidden units will span the same space as the first M principal components
  - But their weight vectors will not be orthogonal
  - And they will have approximately equal variance

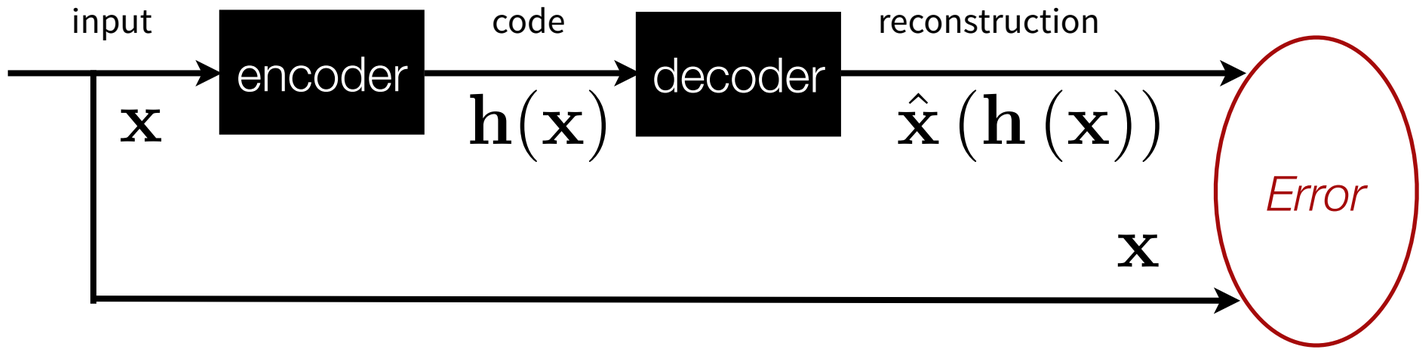
Credit: Geoff Hinton

Why fit PCA inefficiently?



- With nonlinear layers before and after the code, it should be possible to represent data that lies on or near a nonlinear manifold
  - the encoder maps from data space to co-ordinates on the manifold
  - the decoder does the inverse transformation
- The encoder/decoder can be rich, multi-layer functions

Auto-encoder

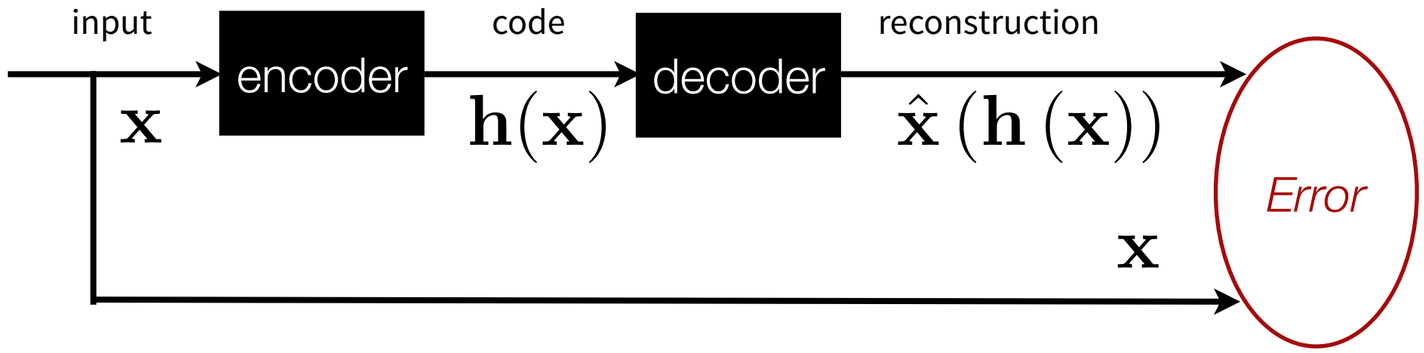


- Feed-forward architecture

- Trained to minimize reconstruction error

  - bottleneck or regularization essential

Auto-encoder



- Feed-forward architecture
- Trained to minimize reconstruction error
  - bottleneck or regularization essential

Example: real-valued data

Encoder

$$h_j(\mathbf{x}) = \sigma\left(\sum_i w_{ji} x_i\right)$$

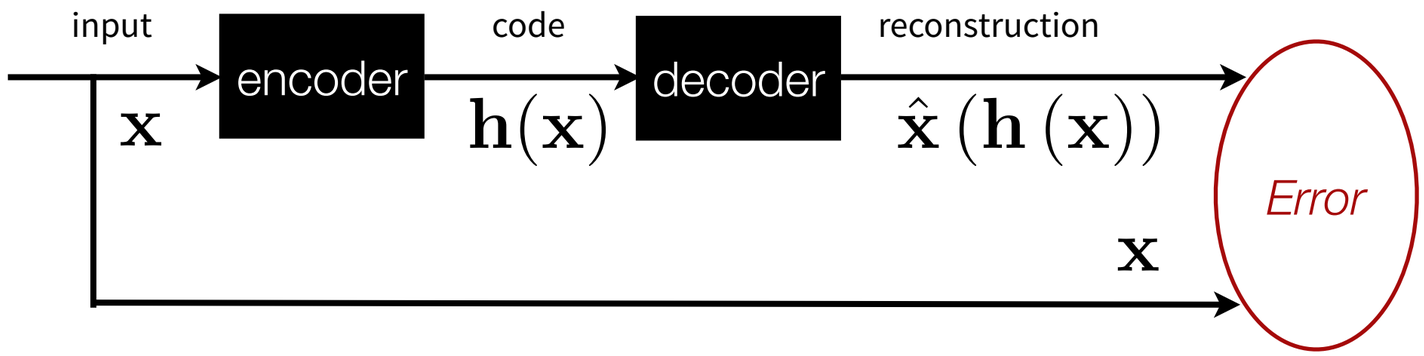
Decoder

$$\hat{x}_i(\mathbf{h}(\mathbf{x})) = \sum_j w_{ji} h_j(\mathbf{x})$$

Error

$$E = \sum_\alpha \left(\hat{\mathbf{x}}(\mathbf{h}(\mathbf{x}^\alpha)) - \mathbf{x}^\alpha\right)^2$$

Regularized Auto-encoders



- Permit code to be higher-dimensional than the input

- Capture structure of the training distribution due to predictive opposition b/w reconstruction distribution and regularizer

- Regularizer tries to make enc/dec as simple as possible

Simple?

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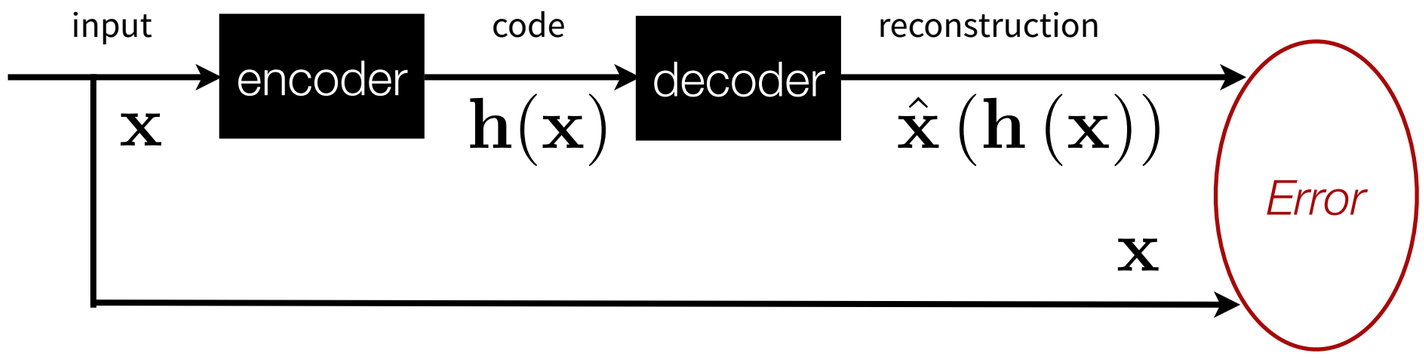
  (sparse auto-encoders)
- Add noise to the input or code and reconstruct the cleaned-up version
  (denoising auto-encoders)
- Reconstruct the input from the code and make the code insensitive to the input (contractive auto-encoders)

Sparse Auto-encoders



$$\mathcal{L}_{\mathrm{SAE}} = \mathbb{E}[l(\mathbf{x}, \hat{\mathbf{x}}(\mathbf{h}(\mathbf{x})))] + \beta \sum_j \mathrm{KL}(\rho || \hat{\rho}_j)$$

$$\hat{\rho}_j = \frac{1}{N} \sum_i^N h_j(\mathbf{x}_i) \text{ : mean activation}$$

ρ : target activation (small)

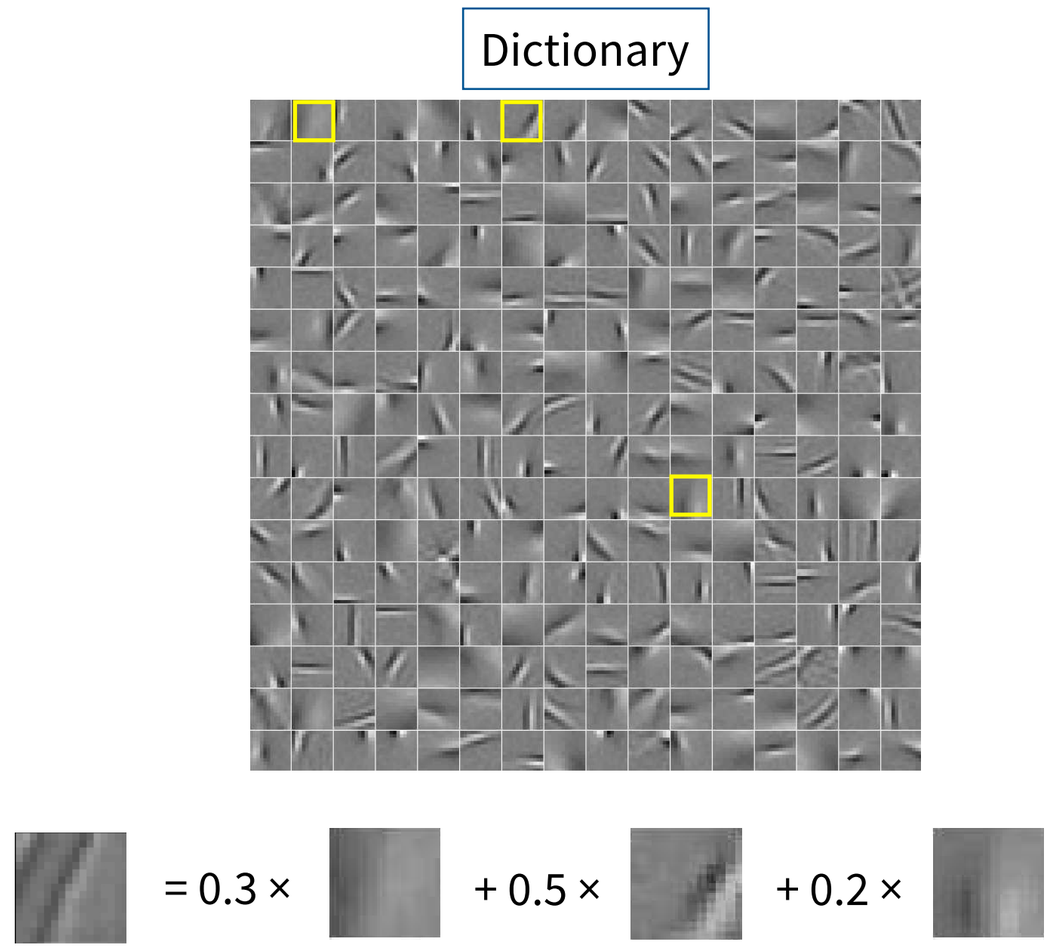
- Apply a sparsity penalty to the hidden activations
- Also see Predictive Sparse Decomposition (Kavukcuoglu et al. 2008)

Diversion: Sparse Coding

- Inputs as sparse linear combinations of basis elements

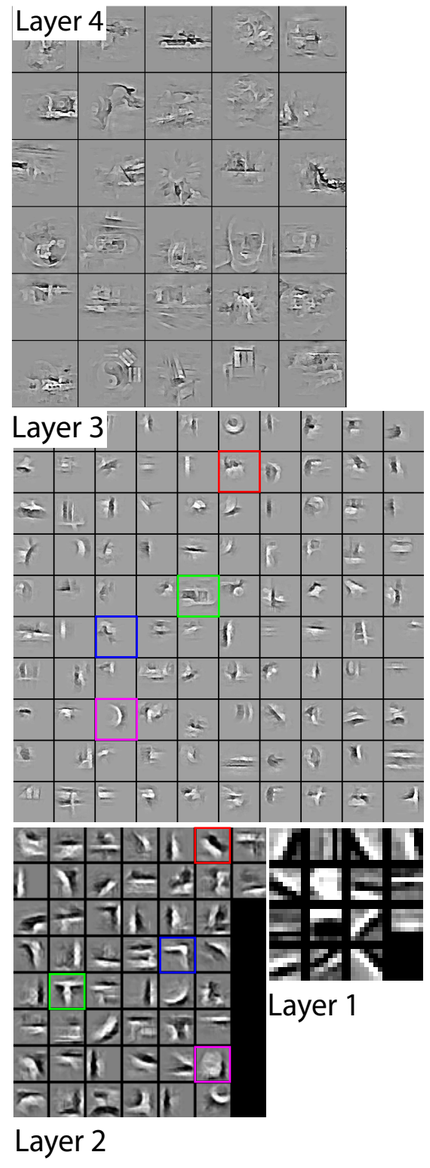
- Linear decoder, no encoder

  - relies on optimization for inference



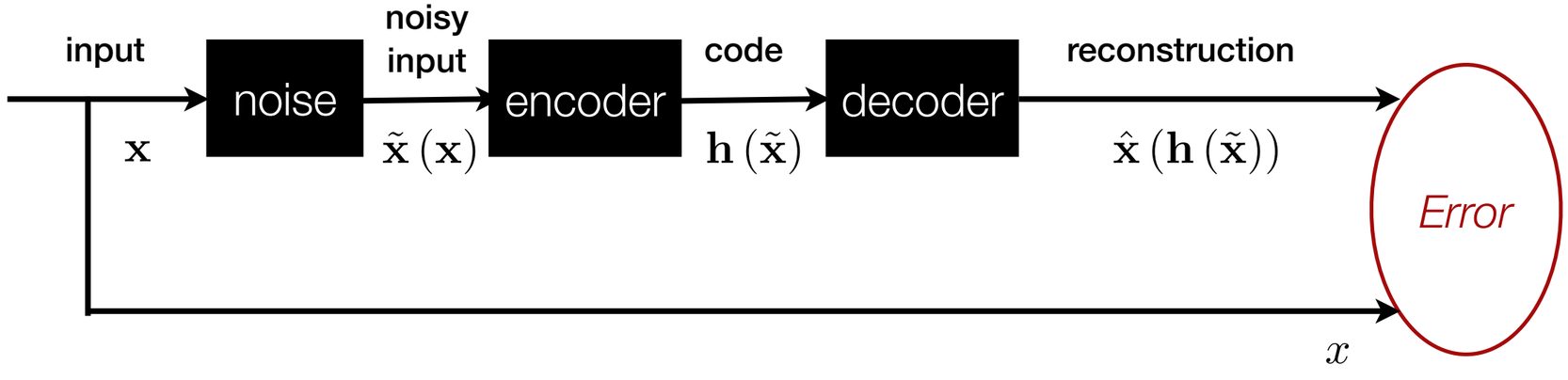
Deconvolutional Networks

- Deep convolutional sparse coding
- Trained to reconstruct the input from any layer
- Fast approximate inference
- Recently used to visualize features learned by convolutional nets (Zeiler and Fergus 2013)



(Vincent et al. 2008)

Denoising Auto-encoders



$$\mathcal{L}_{\mathrm{DAE}} = \mathbb{E}\left[l\left(\mathbf{x}, \hat{\mathbf{x}}\left(\mathbf{h}\left(\tilde{\mathbf{x}}\right)\right)\right)\right]$$

$$\tilde{\mathbf{x}}(\mathbf{x}) = \mathbf{x} + \epsilon$$

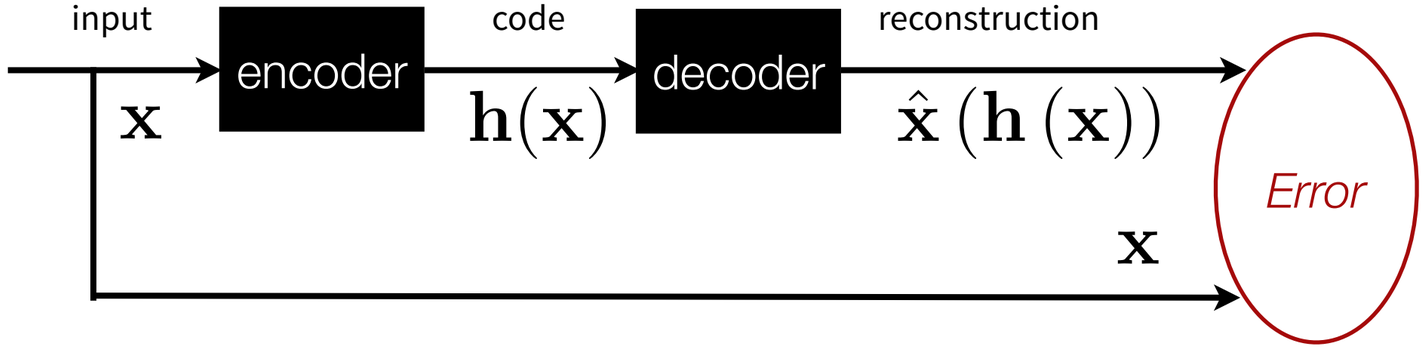
$$\epsilon \sim \mathcal{N}\left(\mathbf{0}, \sigma^2 I\right)$$

only one possible choice of noise model

- The code can be viewed as a lossy compression of the input
- Learning drives it to be a good compressor for training examples (and hopefully others as well) but not arbitrary inputs

(Rifai et al. 2011)

Contractive Auto-encoders



$$\mathcal{L}_{\mathrm{CAE}} = \mathbb{E}\left[l\left(\mathbf{x}, \hat{\mathbf{x}}\left(\mathbf{h}\left(\mathbf{x}\right)\right)\right) + \lambda \left|\left| \frac{\partial \mathbf{h}\left(\mathbf{x}\right)}{\partial \mathbf{x}} \right|\right|^2 \right]$$

$$\mathbf{h}\left(\mathbf{x}\right) = \mathrm{sigmoid}\left(W\mathbf{x} + b\right)$$

$$\hat{\mathbf{x}}\left(\mathbf{h}\left(\mathbf{x}\right)\right) = \mathrm{sigmoid}\left(W^T\mathbf{h} + c\right)$$

- Learn good models of high-dimensional data (Bengio et al. 2013)
- Can obtain good representations for classification
- Can produce good quality samples by a random walk near the manifold of high density (Rifai et al. 2012)

What do Denoising Auto-encoders Learn?

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- The reconstruction function locally characterizes the data generating density (Alain and Bengio 2013)
    - derivative of the log-density (score) with respect to the input
    - second derivative of the density
    - other local properties

What do Denoising Auto-encoders Learn?

- The reconstruction function locally characterizes the data generating density (Alain and Bengio 2013)
  - derivative of the log-density (score) with respect to the input
  - second derivative of the density
  - other local properties
- Bengio et al. (2013) generalized this result to arbitrary variables (discrete, continuous, or both), arbitrary corruption, arbitrary loss function

Advanced Autoencoders

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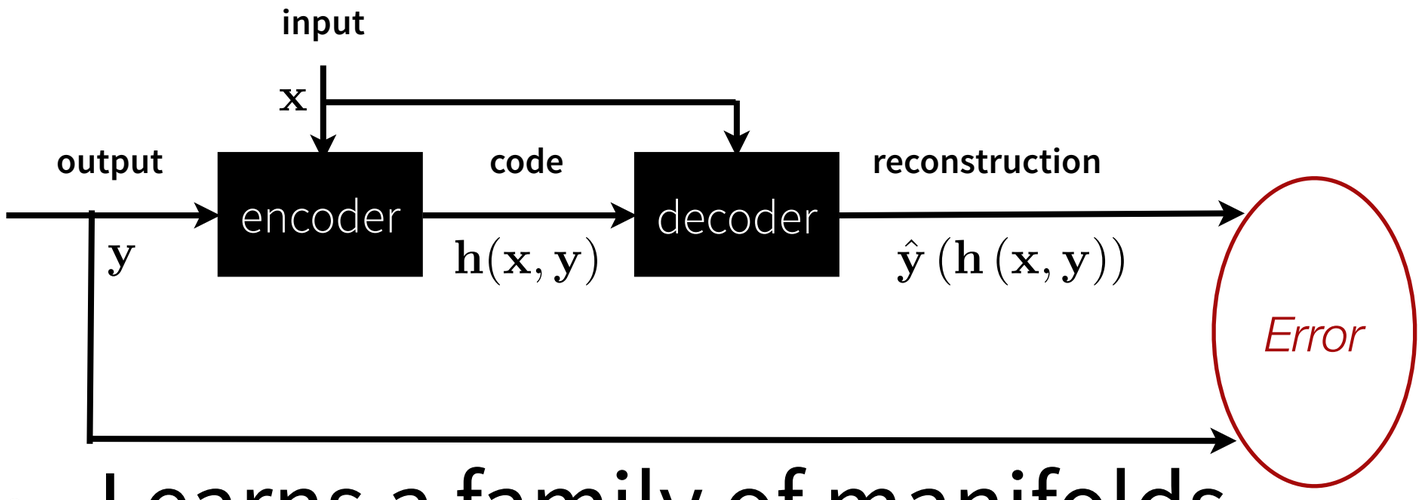
- (Kamyshanska and Memisivec 2013) demonstrate a way to score data under an autoencoder

Advanced Autoencoders

- (Bengio et al. 2013) also showed a way to sample from an autoencoder by running a Markov chain that alternately adds noise and denoises
- (Kamyshanska and Memisivec 2013) demonstrate a way to score data under an autoencoder
- Generative Stochastic Networks (Bengio et al. 2013) are an intriguing recent generalization of DAEs

Relational Autoencoders

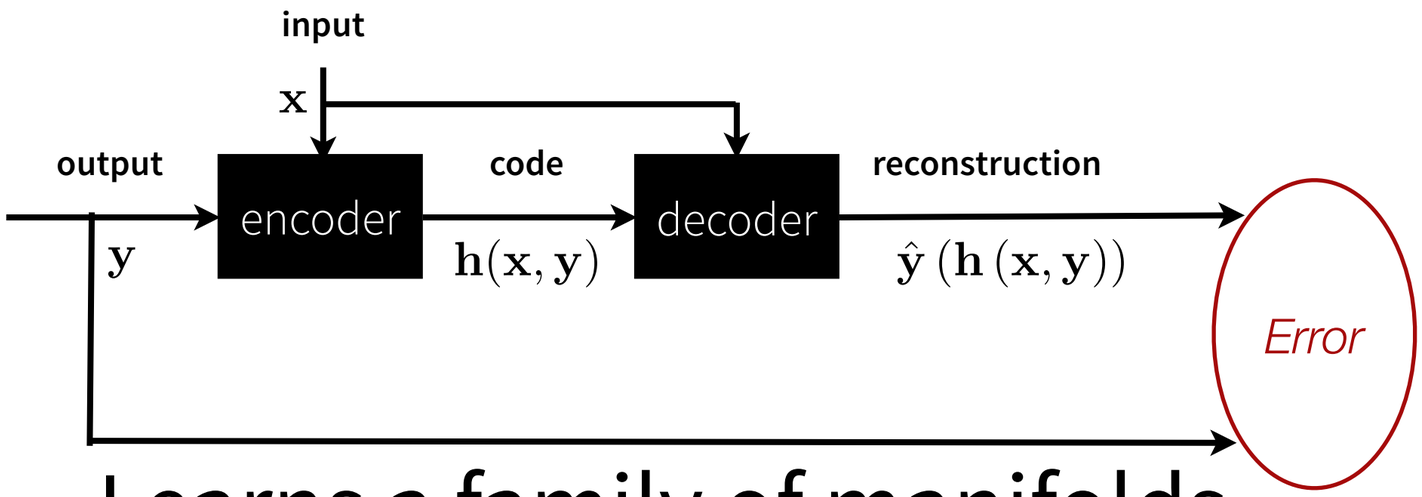


- Learns a family of manifolds (Memisevic 2011)

- Can be viewed as AE whose weights are modulated by input vector $w_{kj}(\mathbf{x}) = \sum_i \hat{w}^i_{kj} x_i$

- Used for modelling image transformations, extracting spatio-temporal features

Relational Autoencoders



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Example: real-valued data

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Decoder

$$\hat{y}_j\left(\mathbf{h}\left(\mathbf{x};\mathbf{y}\right)\right) = \sum_{ki} \hat{w}^i_{kj} x_i h_k(\mathbf{x};\mathbf{y})$$

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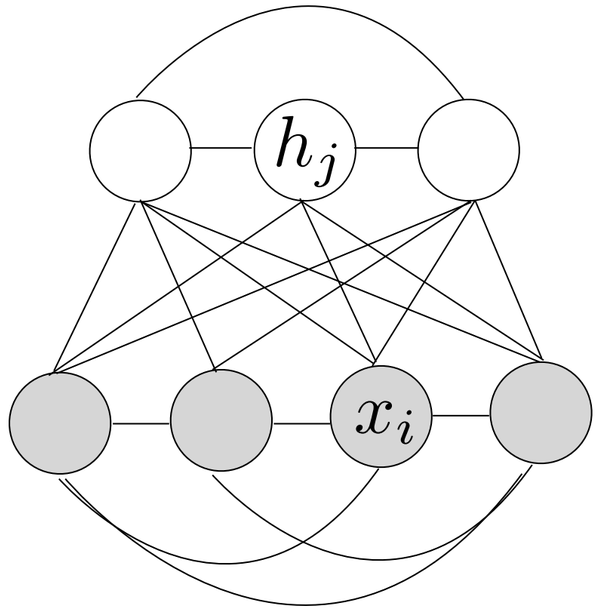
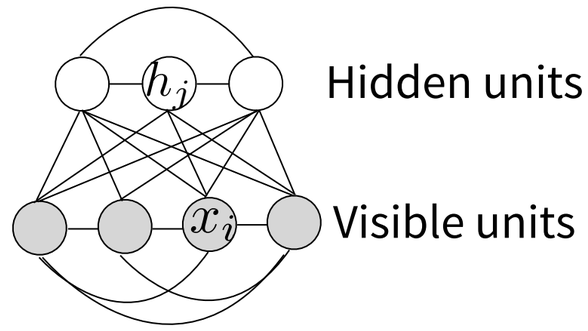
Boltzmann Machines

- Stochastic Hopfield Networks with hidden units
- Both visible and hidden units are binary
- Make the states of the hidden units form interpretations of the perceptual input presented at the visible units



Energy Function

- Energy-based model: negative energy assigns a "goodness" to every joint configuration



$E(\mathbf{x}, \mathbf{h})$ Energy function

- Can convert negative energies to probabilities by normalizing

$$p(\mathbf{x}, \mathbf{h}) = \frac{1}{Z} e^{-E(\mathbf{x}, \mathbf{h})}$$

$$p(\mathbf{x}) = \frac{1}{Z} \sum_{\mathbf{h}} e^{-E(\mathbf{x}, \mathbf{h})}$$

Inference in a Boltzmann Machine

- The binary stochastic units make biased random decisions
- Probability of activating is a function of an “energy gap”

$$p(h_k = 1|\mathbf{x}, \{h_l\}\forall l \neq k) = \frac{1}{1 + e^{-\Delta E_k}}$$

- The number of possible hidden configurations is exponential so we need MCMC to sample from the posterior (this is slow!)

$$\Delta E_k = E(h_k = 0) - E(h_k = 1) = b_k + \sum_i x_i w_{ik} + \sum_l h_l w_{kl}$$

Learning in a Boltzmann Machine

- Goal: maximize the product of the probabilities that the Boltzmann machine assigns to the binary vectors in the training set
- Everything that one weight needs to know about the other weights and the data is contained in the difference of two correlations

$$\frac{\partial \log p(\mathbf{x})}{\partial w_{ij}} = \langle s_i s_j \rangle_{\mathbf{x}} - \langle s_i s_j \rangle_{\text{model}}$$

$$\Delta w_{ij} \propto \langle s_i s_j \rangle_{\mathbf{x}} - \langle s_i s_j \rangle_{\text{model}}$$

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Derivative of log prob of one training vector, **v**, under the model

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Expected value of product of states at thermal equilibrium when **v** is clamped on the visible units (positive phase)

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Derivative of log prob of one training vector, **v**, under the model

Expected value of product of states at thermal equilibrium when **v** is clamped on the visible units (positive phase)

Expected value of product of states at thermal equilibrium with no clamping (negative phase)

$$\Delta w_{ij} \propto \langle s_i s_j \rangle_{\mathbf{x}} - \langle s_i s_j \rangle_{\text{model}}$$

Credit: Geoff Hinton

Why do we need a negative phase?

$$p(\mathbf{x}) = \frac{\sum_{\mathbf{h}} e^{-E(\mathbf{x},\mathbf{h})}}{\sum_{\mathbf{u}} \sum_{\mathbf{g}} e^{-E(\mathbf{u},\mathbf{g})}}$$

Credit: Geoff Hinton

Why do we need a negative phase?

The positive phase finds hidden configurations that work well with **x** and lowers their energies

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The positive phase finds hidden configurations that work well with **x** and lowers their energies

The negative phase finds the joint configurations that are the best competitors and raises their energies

Credit: Geoff Hinton

How to inefficiently collect stats

Positive phase

- Clamp a data vector on the visible units and set the hidden units to random binary states

  - Update the hidden units one at a time until the network reaches “thermal equilibrium”

  - Sample $\langle s_i s_j \rangle$ for every connected pair of units

  - Repeat for all data vectors in the training set and average

Credit: Geoff Hinton

How to inefficiently collect stats

Positive phase

- Clamp a data vector on the visible units and set the hidden units to random binary states
  - Update the hidden units one at a time until the network reaches “thermal equilibrium”
  - Sample $\langle s_i s_j \rangle$ for every connected pair of units
  - Repeat for all data vectors in the training set and average

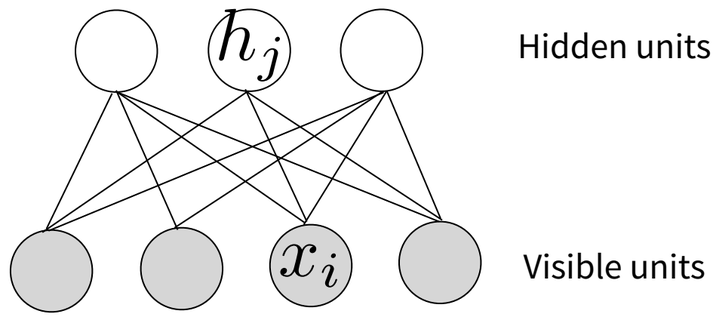
Negative phase

- Set all the units to random states
  - Update all the units one at a time until the network reaches thermal equilibrium
  - Sample $\langle s_i s_j \rangle$ for every connected pair of units
  - Repeat many times and average to get good estimates

Credit: Geoff Hinton

Restricted Boltzmann Machines

- We restrict the connectivity to make inference and learning easier.
  - Only one layer of hidden units.
  - No connections between hidden units.

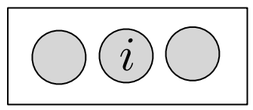


- In an RBM it only takes one step to reach thermal equilibrium when the visible units are clamped
  - So we can quickly get the exact value of $\langle x_i h_j \rangle_{\mathbf{x}}$

$$p(h_j = 1|\mathbf{x}) = \frac{1}{1 + e^{-(b_j + \sum_{i \in \text{vis}} x_i w_{ij})}}$$

Credit: Geoff Hinton

The Boltzmann Machine Learning Algorithm - RBMs



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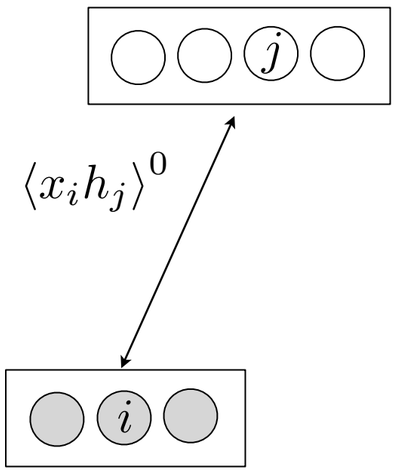
Credit: Geoff Hinton

The Boltzmann Machine Learning Algorithm - RBMs



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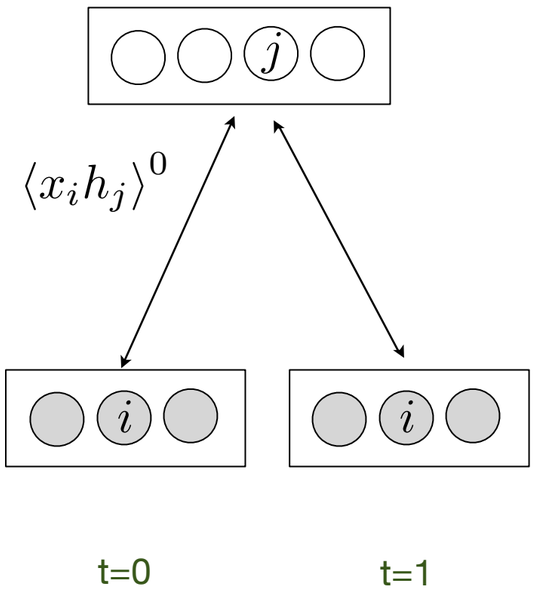
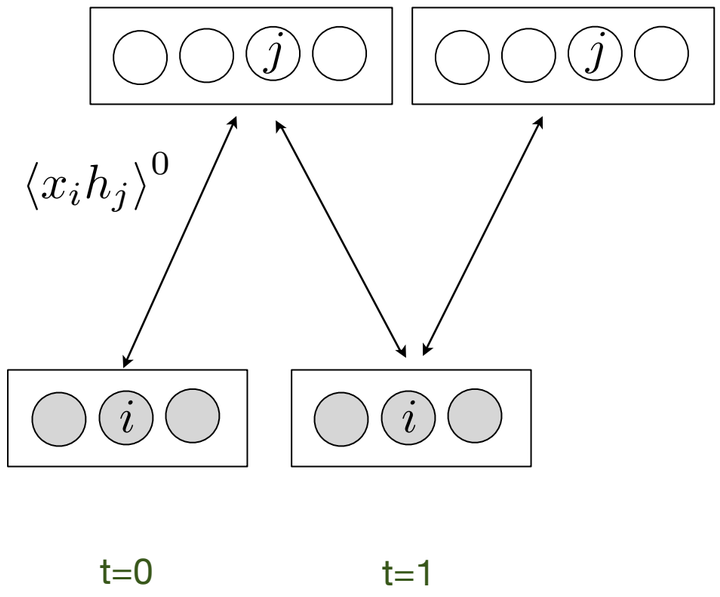
Credit: Geoff Hinton

The Boltzmann Machine Learning Algorithm - RBMs



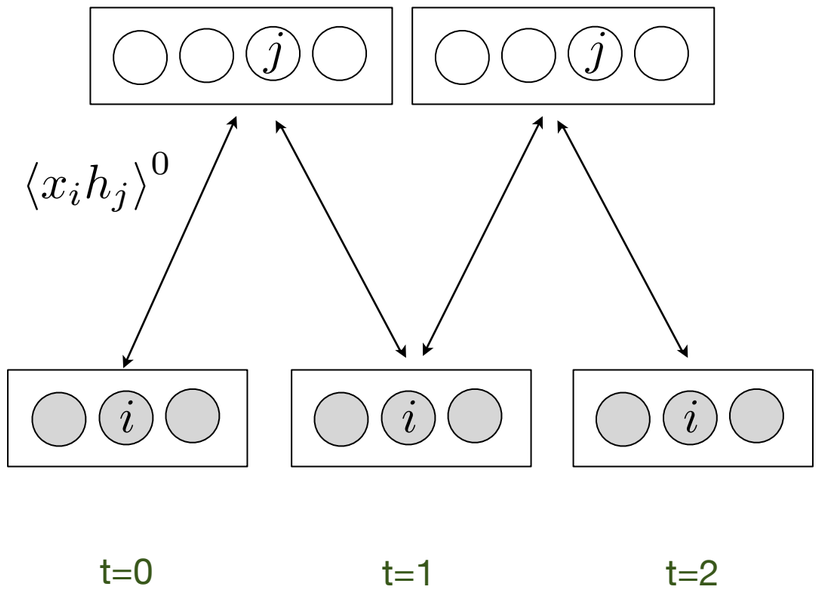
Credit: Geoff Hinton

The Boltzmann Machine Learning Algorithm - RBMs



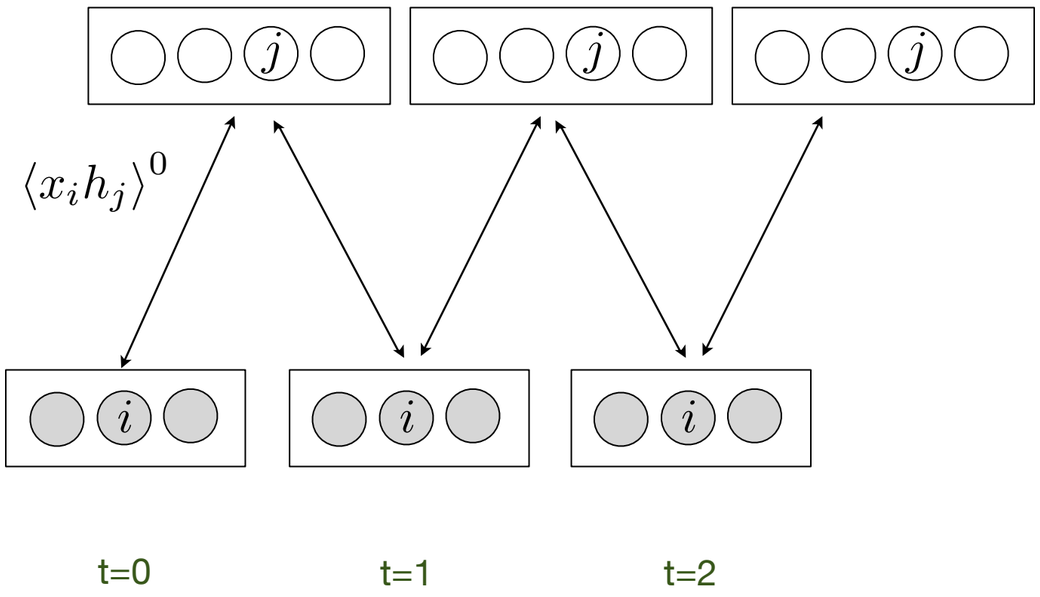
Credit: Geoff Hinton

The Boltzmann Machine Learning Algorithm - RBMs



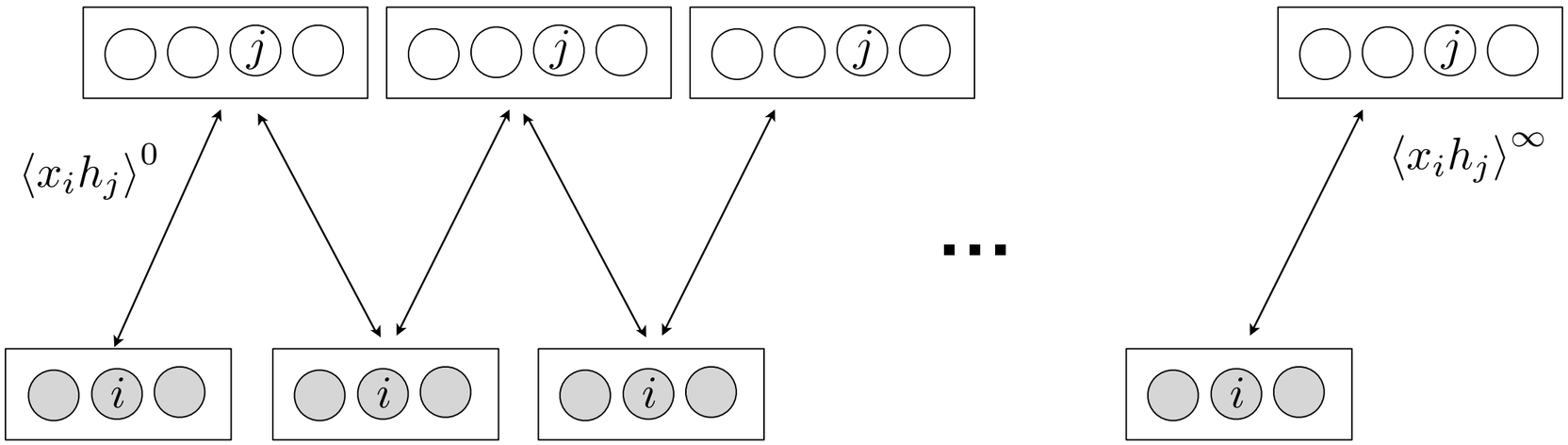
Credit: Geoff Hinton

The Boltzmann Machine Learning Algorithm - RBMs



Credit: Geoff Hinton

The Boltzmann Machine Learning Algorithm - RBMs



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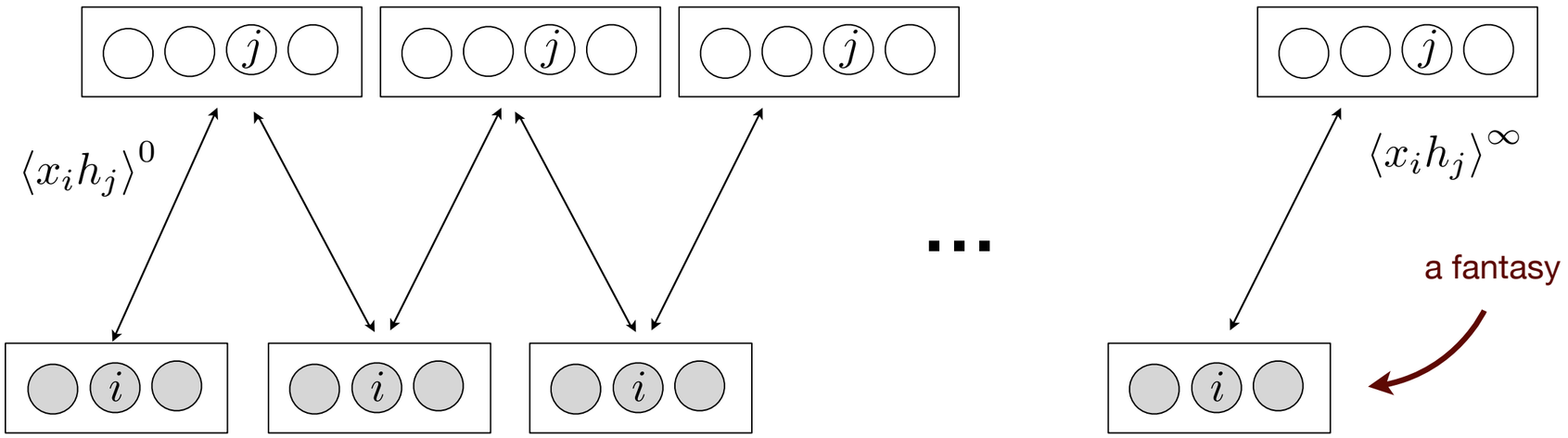
The Boltzmann Machine Learning Algorithm - RBMs



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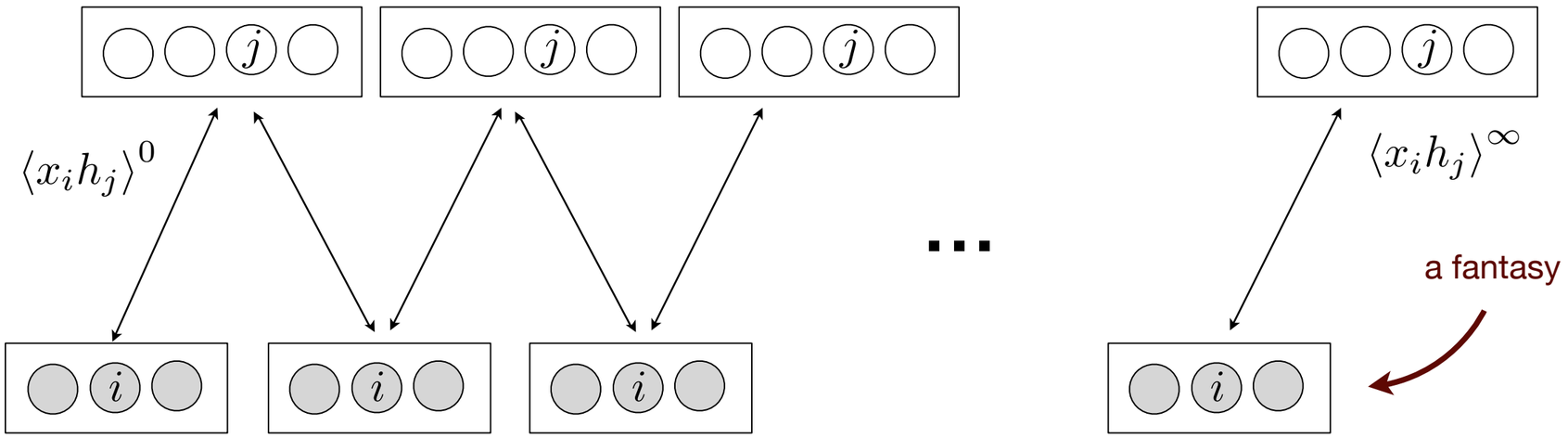
The Boltzmann Machine Learning Algorithm - RBMs



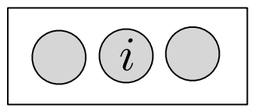
$$\Delta w_{ij} = \epsilon \left(\langle x_i h_j \rangle^0 - \langle x_i h_j \rangle^\infty \right)$$

$$\langle x_i h_j \rangle^0 = \langle x_i h_j \rangle_{\mathbf{x}}$$
$$\langle x_i h_j \rangle^\infty = \langle x_i h_j \rangle_{\text{model}}$$

Credit: Geoff Hinton

Contrastive Divergence

Instead of running the Markov chain to equilibrium, run for just one (or a few) steps!



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Credit: Geoff Hinton

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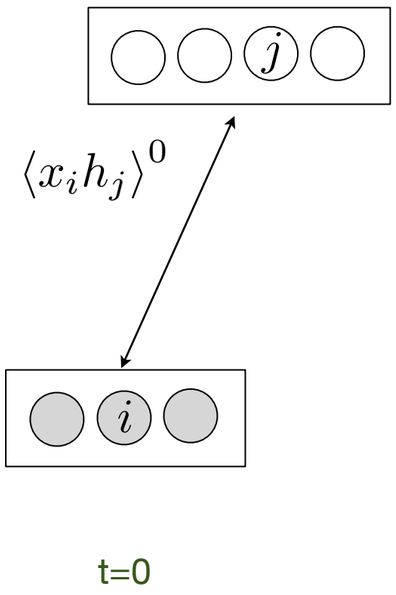

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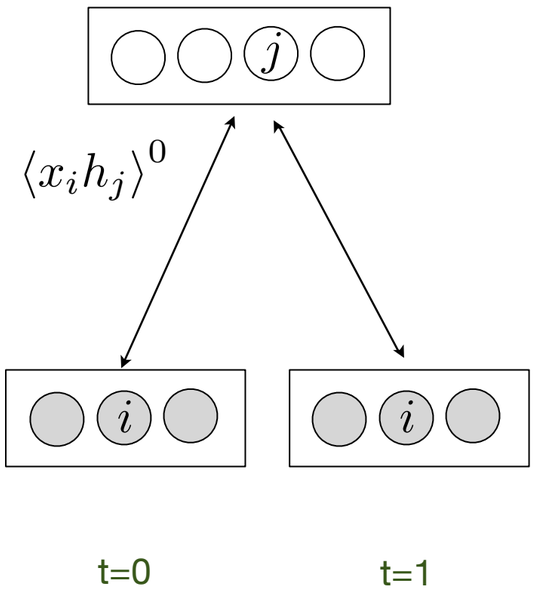

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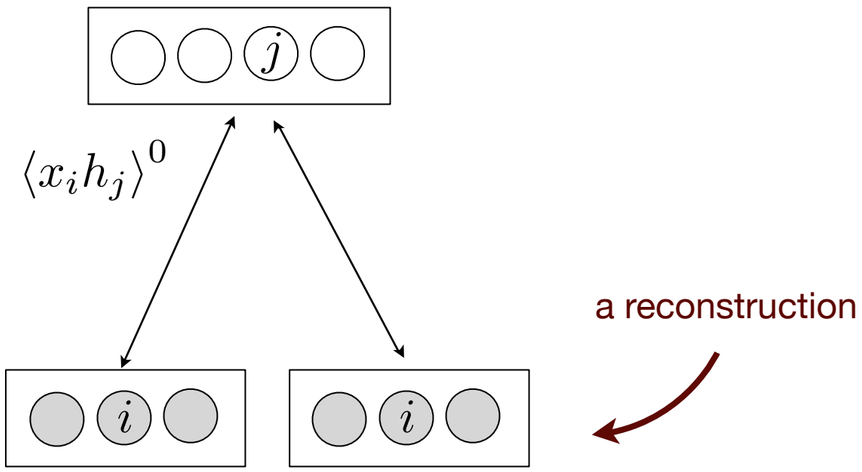

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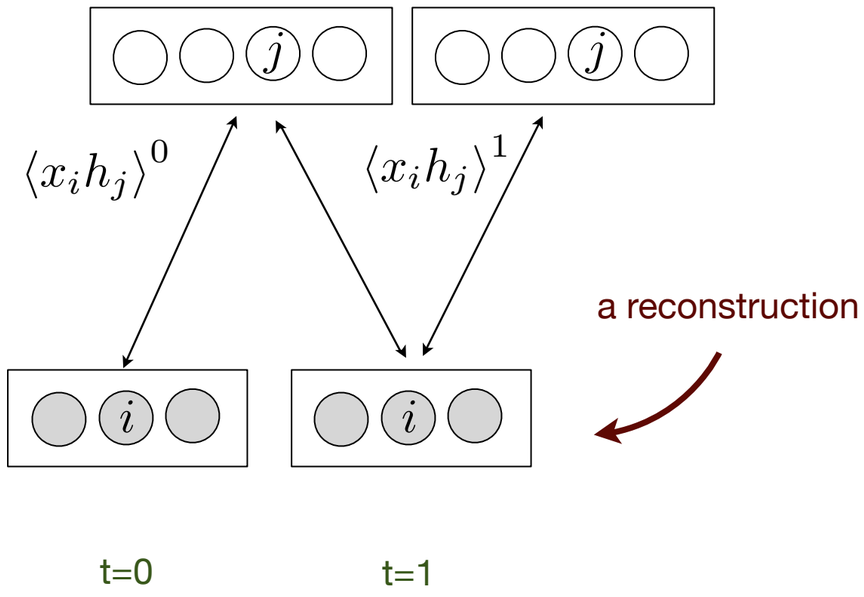

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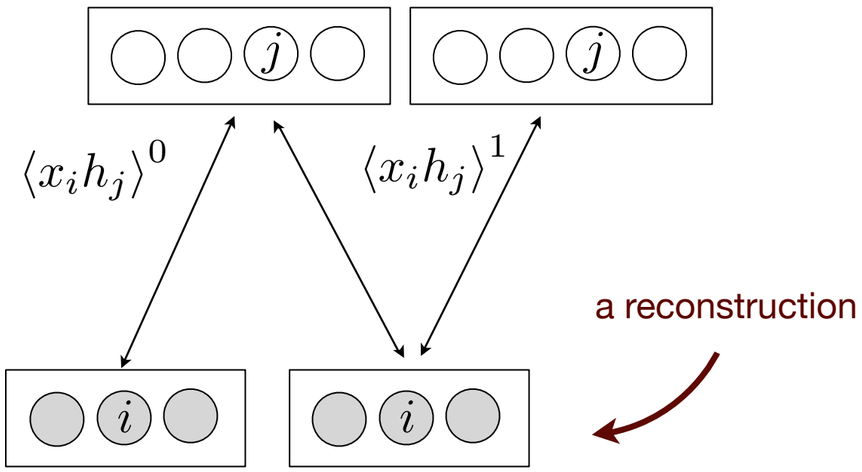

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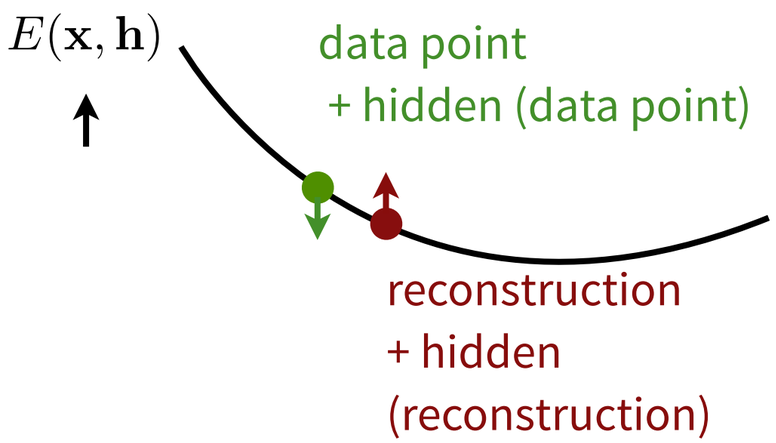
$$\Delta w_{ij} = \epsilon \left(\langle x_i h_j \rangle^0 - \langle x_i h_j \rangle^1 \right)$$

Credit: Geoff Hinton

Contrastive Divergence (A picture)

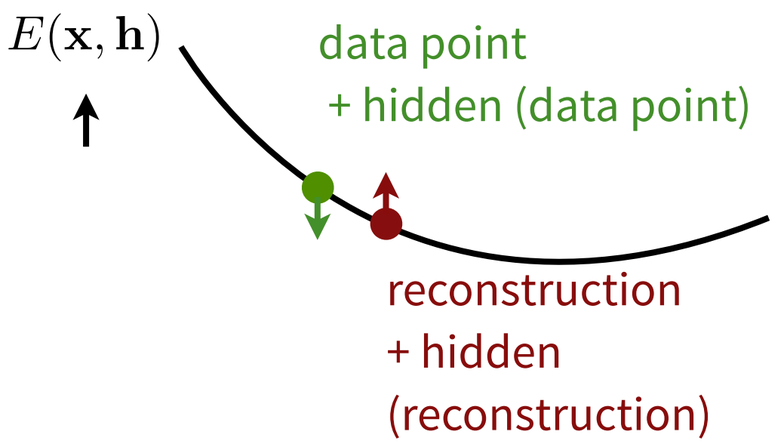


Change the weights to pull the energy down at the data point

Change the weights to pull the energy up at the reconstruction

Credit: Geoff Hinton

Contrastive Divergence (A picture)



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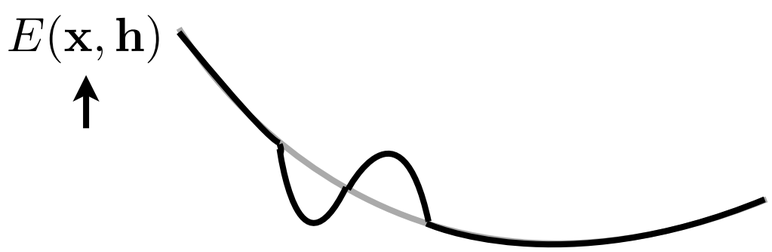


Credit: Geoff Hinton

Alternatives to CD

- Persistent CD a.k.a. Stochastic Maximum Likelihood (Tieleman 2008)
  - don’t reset the Markov chain at the data for every point
- Score Matching/Ratio Matching (Hyvarinen 2005, 2007)
  - minimize the expected distance b/w model and data “score function”
- Minimum Probability Flow (Sohl-Dickstein et al. 2011)
  - establish dynamics that would transform the observed data distribution into the model distribution
  - minimize the KL divergence b/w the data distribution and the distribution produced by running the dynamics for an infinitesimal time

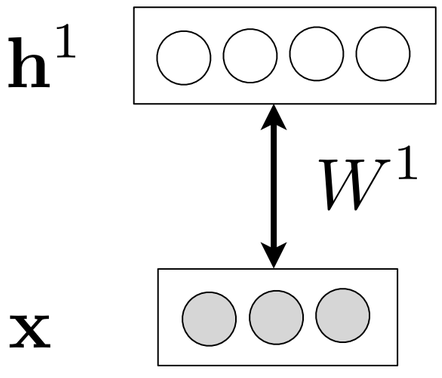
For a comparison, see *Inductive Principles for Restricted Boltzmann Machine Learning,* Marlin et al. 2010

Stacking to Build Deep Models

- Greedy layer-wise training can be used to build deep models
- It is most popular to use RBMs, but other architectures (regularized autoencoders, ICA, even k-means) can be stacked

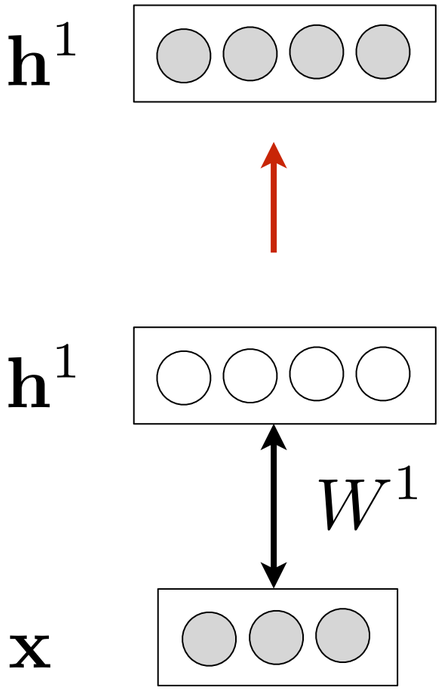
Stacking RBMs: Procedure

Stacking RBMs: Procedure



① Train an RBM

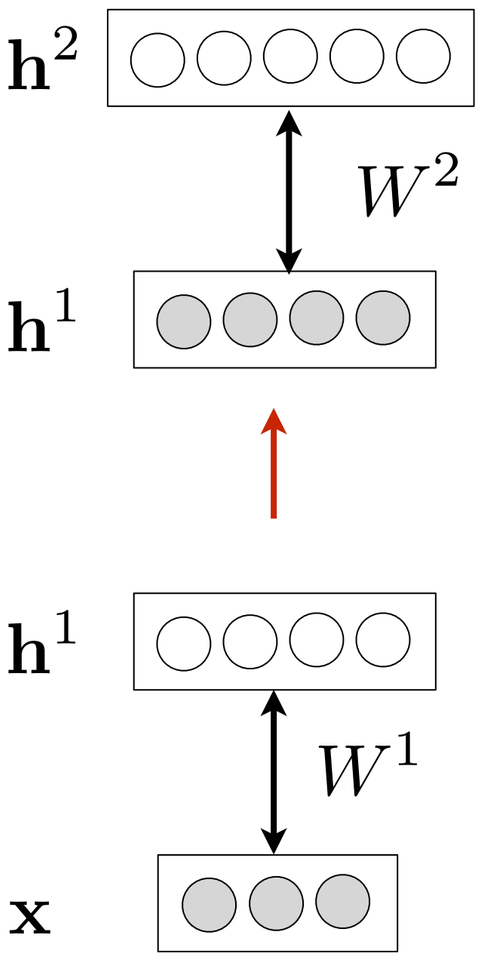
Stacking RBMs: Procedure



② Run your data through the model to generate a dataset of hidden activations

① Train an RBM

Stacking RBMs: Procedure



③ Treat the hiddens like data, train another RBM

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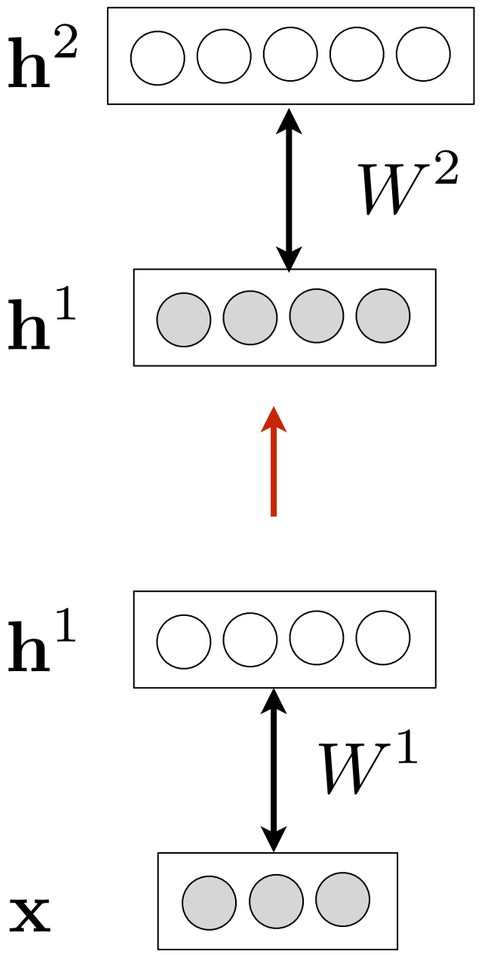
① Train an RBM

Stacking RBMs: Procedure

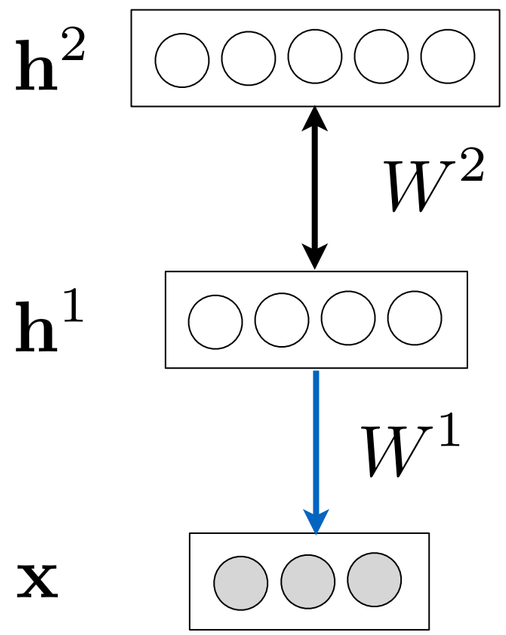


③ Treat the hiddens like data, train another RBM

② Run your data through the model to generate a dataset of hidden activations

① Train an RBM

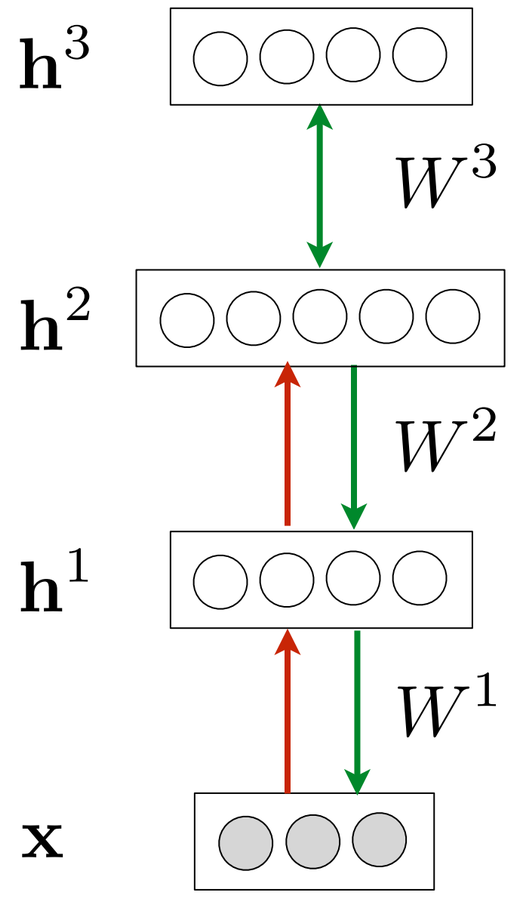
④ Compose the two models



(Hinton et al. 2006)

Deep Belief Networks

- The resulting model is called a Deep Belief Network
- Generate by alternating Gibbs sampling between the top two layers followed by a down-pass
- The lower level bottom-up connections are not part of the generative model, they are used only for inference



Stacking RBMs: Intuition

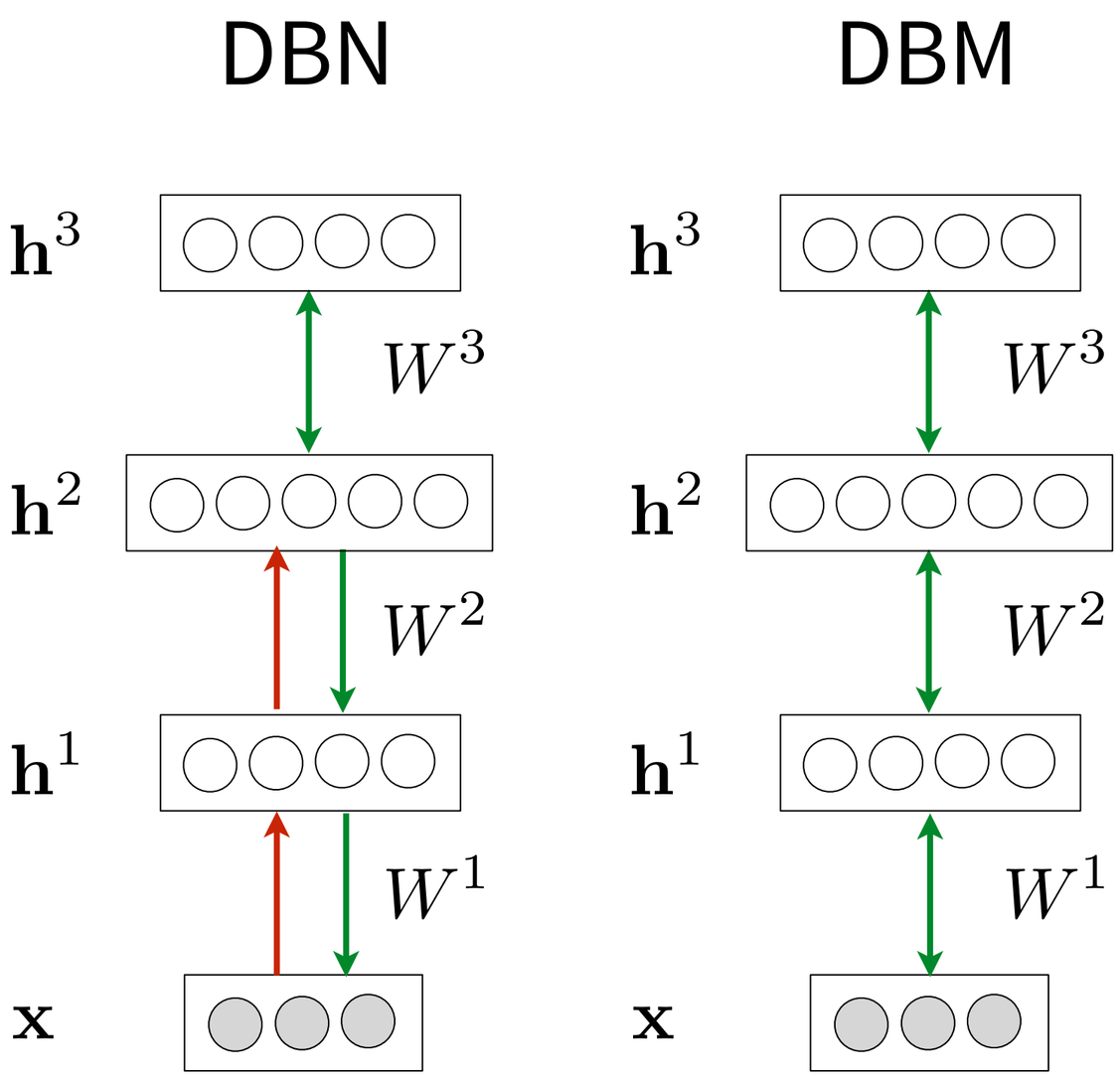
- The weights in the bottom-most RBM define many different distributions: $p(\mathbf{x}, \mathbf{h}), p(\mathbf{x}|\mathbf{h}), p(\mathbf{h}|\mathbf{x}), p(\mathbf{x}), p(\mathbf{h})$
- We can express the RBM as: $p(\mathbf{x}) = \sum_h p(\mathbf{h}) p(\mathbf{x}|\mathbf{h})$
- If we leave $p(\mathbf{x}|\mathbf{h})$ as-is and improve $p(\mathbf{h})$, we improve $p(\mathbf{x})$
- To improve $p(\mathbf{h})$ we need it to be better than $p(\mathbf{h}; W^1)$ at modeling the aggregated posterior over hidden vectors produced by applying the RBM to the data

Credit: Geoff Hinton

(Salakhutdinov and Hinton 2009)

Deep Boltzmann Machines

- DBN is a hybrid directed graphical model
  - maintains a set of “feed-forward” connections for inference
- DBN is an undirected graphical model
  - feedback is important
- Both take different approaches to dealing with intractable p(h|x)



Training DBMs

Training DBMs

- Standard DBM training procedure:

Training DBMs

- Standard DBM training procedure:
  - Greedy-wise pre-training of RBMs

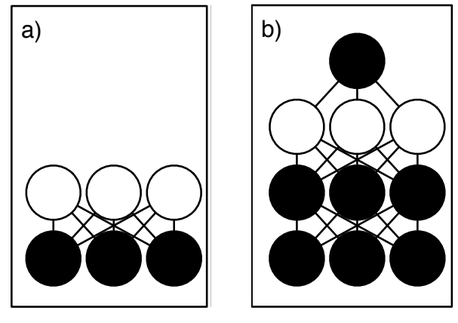


Image: (Goodfellow et al. 2013)

Training DBMs

- Standard DBM training procedure:
  - Greedy-wise pre-training of RBMs
  - Stitch the RBMs into a DBM and train with variational approximation to log-likelihood

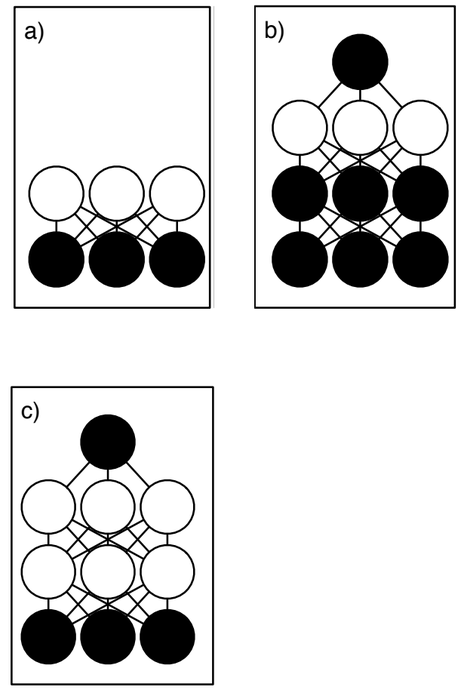


Image: (Goodfellow et al. 2013)

Training DBMs

- Standard DBM training procedure:
  - Greedy-wise pre-training of RBMs
  - Stitch the RBMs into a DBM and train with variational approximation to log-likelihood
  - Discriminative fine-tuning (DBM used as feature learner)

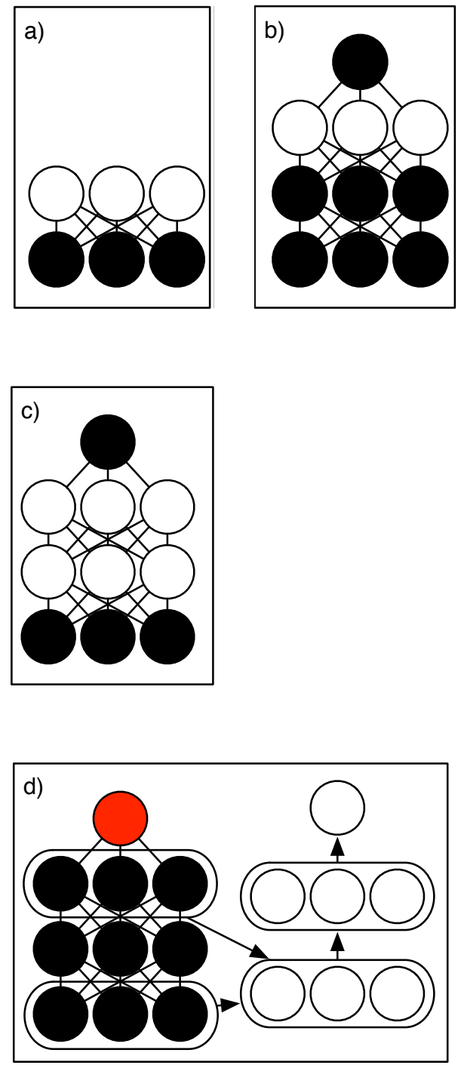


Image: (Goodfellow et al. 2013)

(Goodfellow et al. 2013)

Multi-prediction DBMs

(Goodfellow et al. 2013)

Multi-prediction DBMs

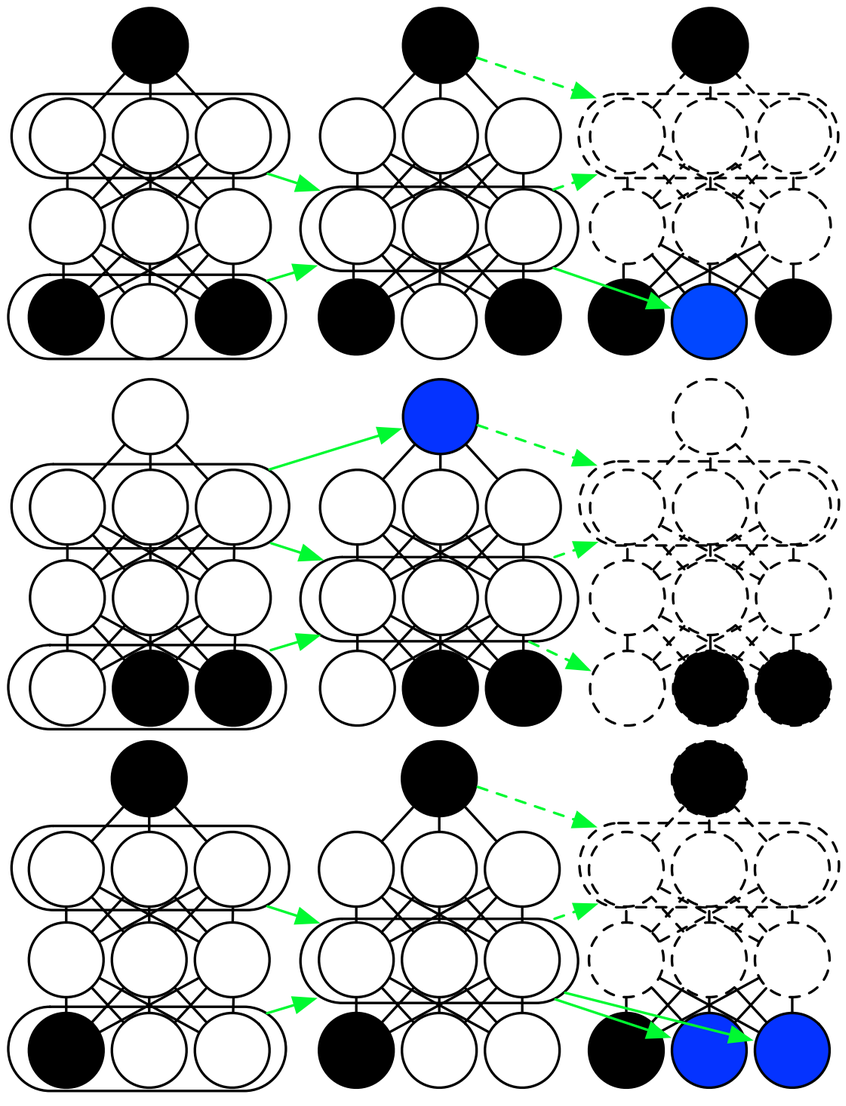
- Greedy pre-training is suboptimal
  - training procedure for each layer should account for the influence of deeper layers
  - one model for all tasks can use inference for arbitrary queries
  - needing to implement multiple models and stages makes DBMs cumbersome

(Goodfellow et al. 2013)

Multi-prediction DBMs

- Greedy pre-training is suboptimal
  - training procedure for each layer should account for the influence of deeper layers
  - one model for all tasks can use inference for arbitrary queries
  - needing to implement multiple models and stages makes DBMs cumbersome
- Joint “multi-prediction” training (Goodfellow et al. 2013)
  - Train DBM to predict any subset of vars given the complement of that subset

Multi-prediction training for classification



Black - variables net is allowed to observe
Blue - prediction targets

Conclusions and Challenges

- Most of the vision community's attention has gone towards supervised deep learning, however unsupervised learning will be key to future success
- Single-layer unsupervised learners well developed but joint unsupervised training of deep models remains difficult
- Can we train deep structured output models?

Resources

- Online courses
  - Andrew Ng's Machine Learning (Coursera)
  - Geoff Hinton's Neural Networks (Coursera)
- Websites
  - deeplearning.net
  - http://deeplearning.stanford.edu/wiki/index.php/UFLDL_Tutorial

Surveys and Reviews

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