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FIELDS

Deep Learning Summer School 2015

On manifolds and autoencoders

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PLAN

Part I: Leveraging the manifold hypothesis

Part II: Regularizing Auto-Encoders

Will be largely about
unsupervised learning

An unsupervised learning task: **dimensionality reduction**

$\mathbf{h} \in \mathbb{R}^M \quad M < D$

(0.32, -1.3, 1.2)

f_θ

(3.5, -1.7, 2.8, -3, 5, -1.4, 2.4, 2.7, 7.5)

$\mathbf{x} \in \mathbb{R}^D$

What is it useful for?

An unsupervised learning task: **dimensionality reduction**

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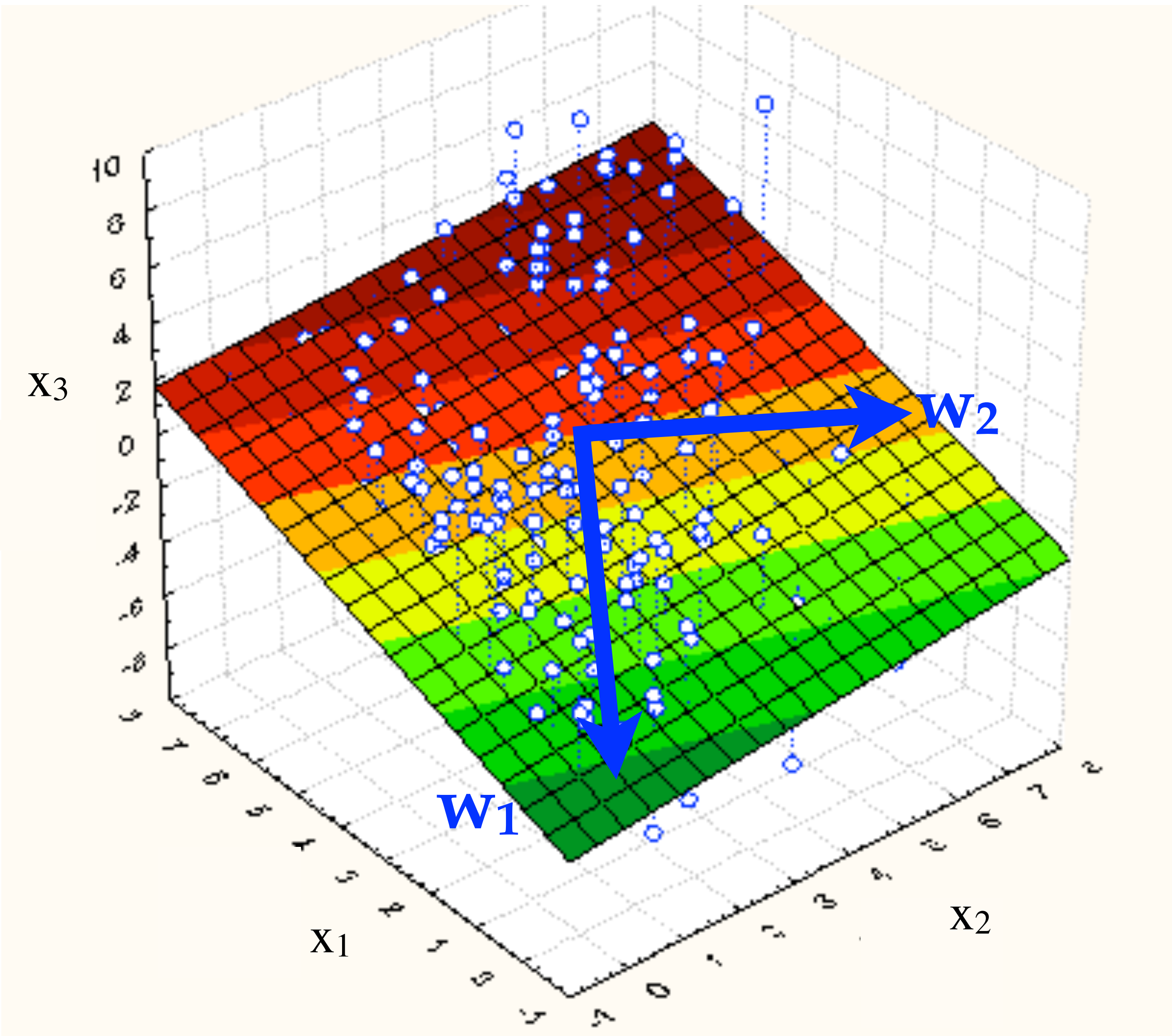
$\mathbf{x} \in \mathbb{R}^D$

What is it useful for?

- Data compression (lossy)
- Dataset visualisation (in 2D or 3D)
- Discovering «most important» features.

A classic algorithm [Pearson 1901] [Hotelling 1933]
Principal Component Analysis



- Finds (learns) k directions (a subspace) in which data has highest variance
  => *principal directions* (eigenvetors) W
- Projecting inputs x on these vetors yields reduced dimension ***representation*** (&decorrelated)
  => *principal components*
  $h = f_\theta(x) = W(x-\mu)$ with $\theta=\{W,\mu\}$

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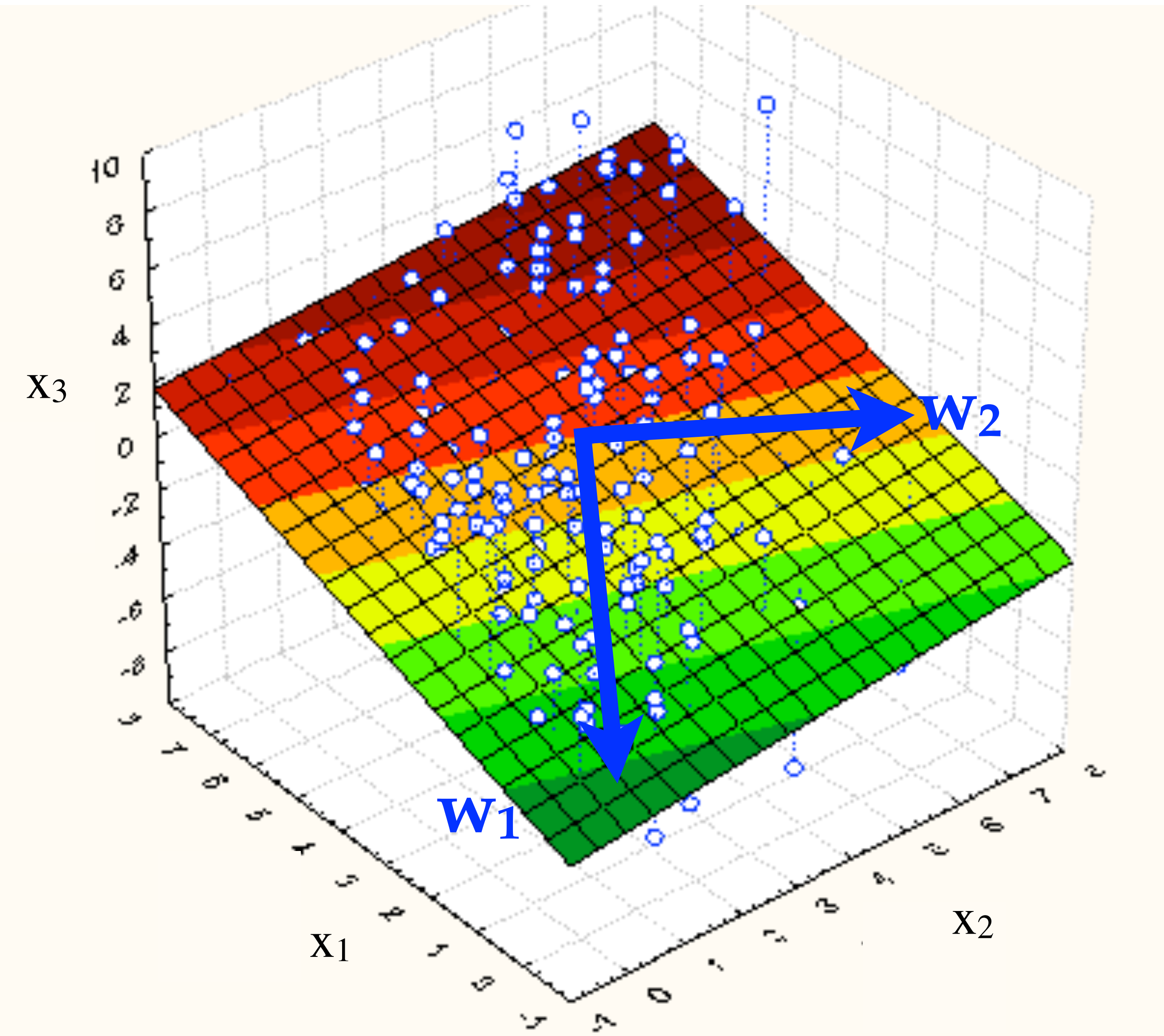
Principal Component Analysis



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Why mention PCA?

➡ Prototypical unsupervised representation learning algorithm.

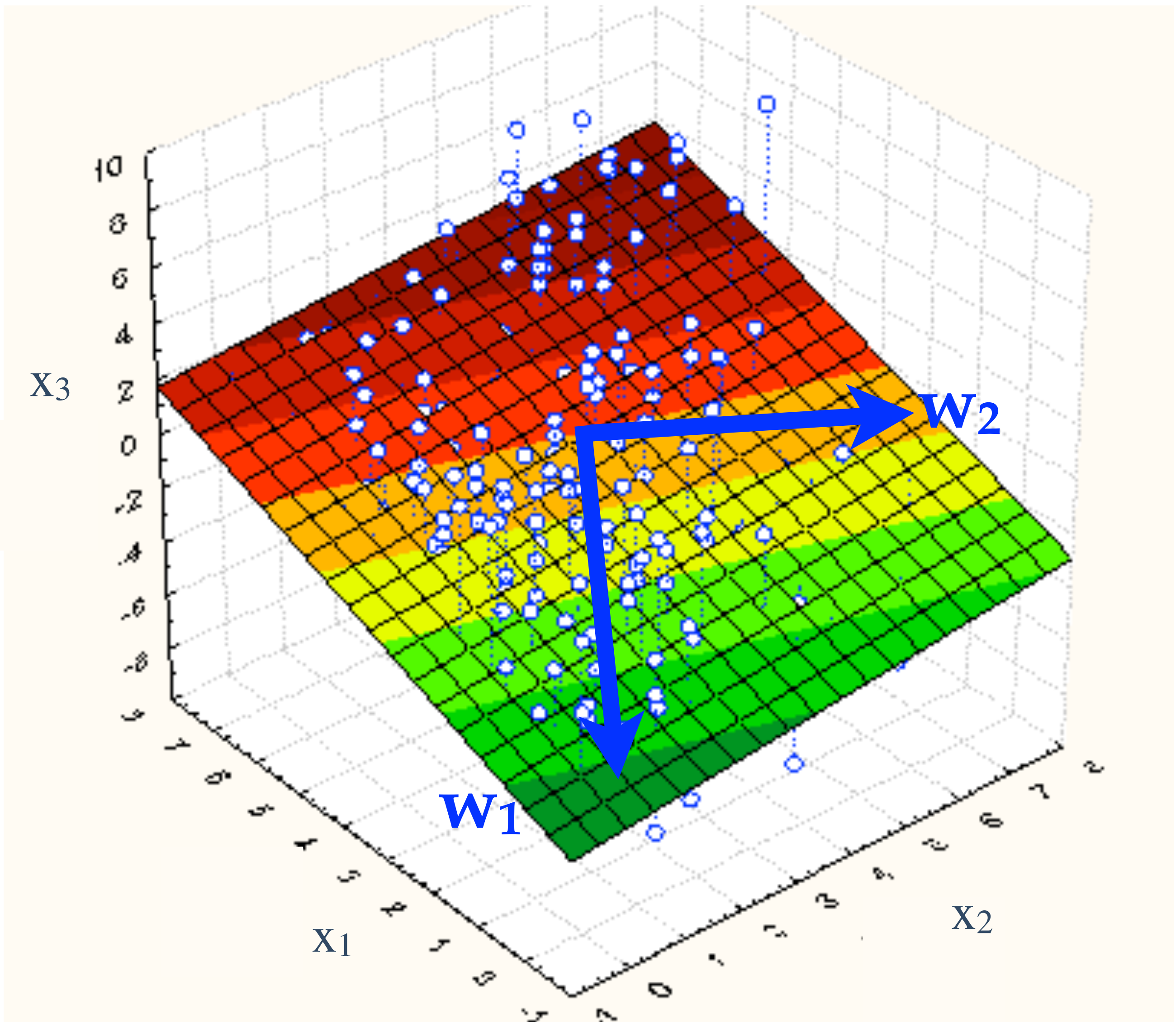
➡ Related to autoencoders

➡ Prototypical manifold modeling algorithm

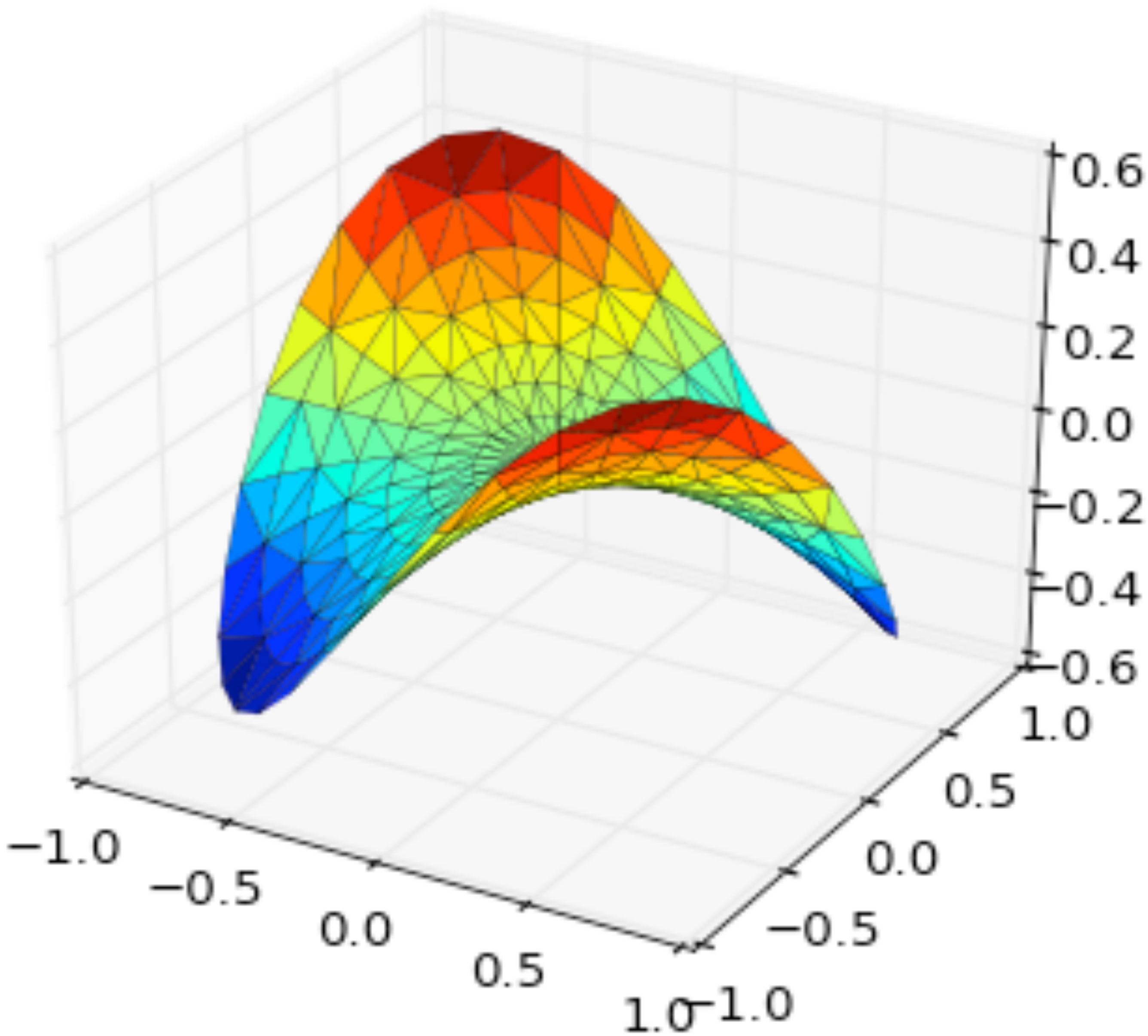
Lower-dimensional manifolds embedded in high dimensional space

Linear 2D manidold in 3D space

(ex: subspace found by PCA)



Non-linear 2D manidold in 3D input space



Principal components are coordinates in a coordinate-system on the manifold

The manifold hypothesis

(assumption)

Natural data in high dimensional spaces concentrates close to lower dimensional manifolds.

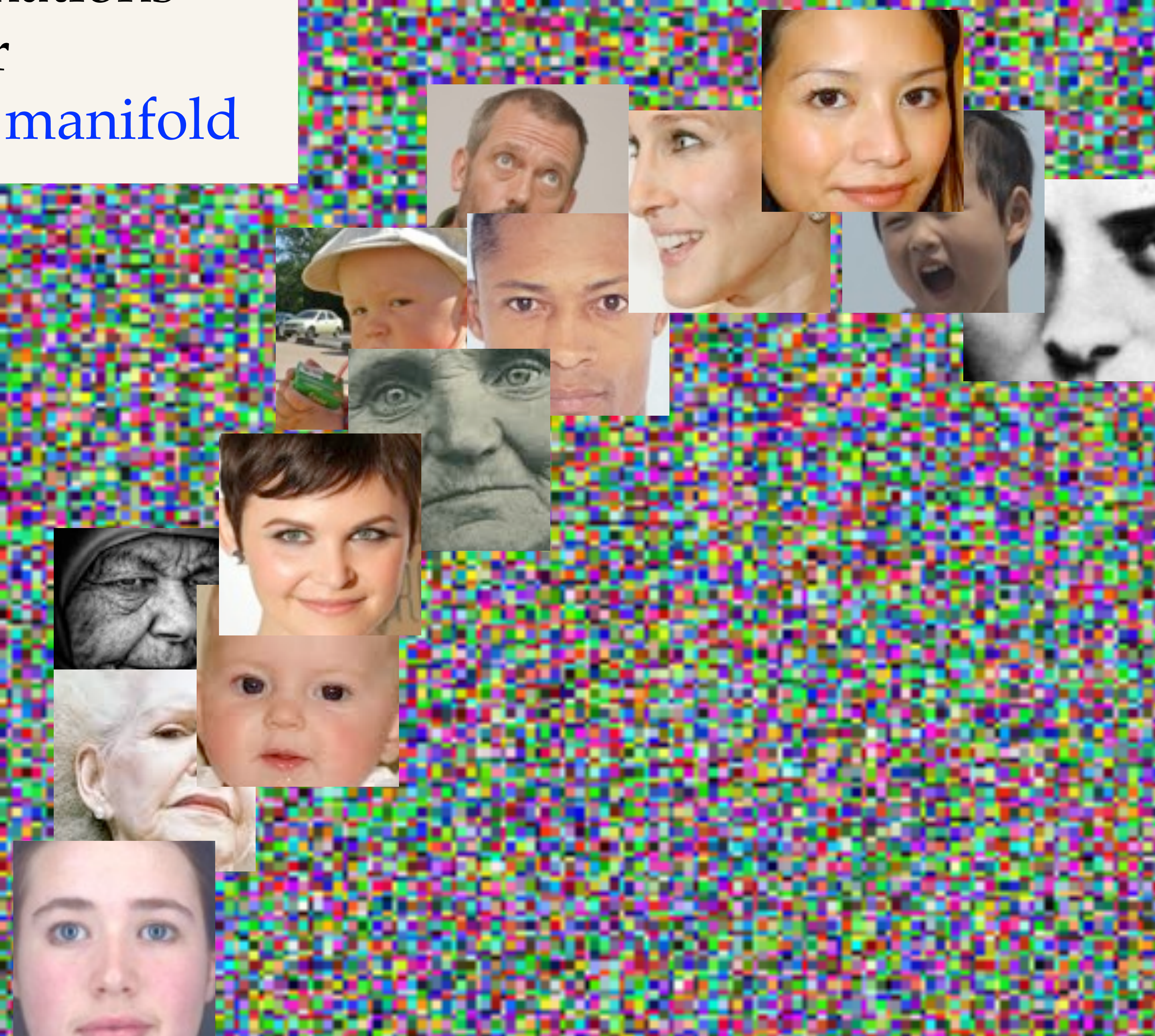
Probability density decreases very rapidly when moving away from the supporting manifold.

The curse of dimensionality

There are 10^{96329} possible 200x200 RGB images.

- Natural images occupy a tiny fraction of that space
  => suggests peaked density

- Realistic smooth transformations from one image to another
  => continuous path along manifold



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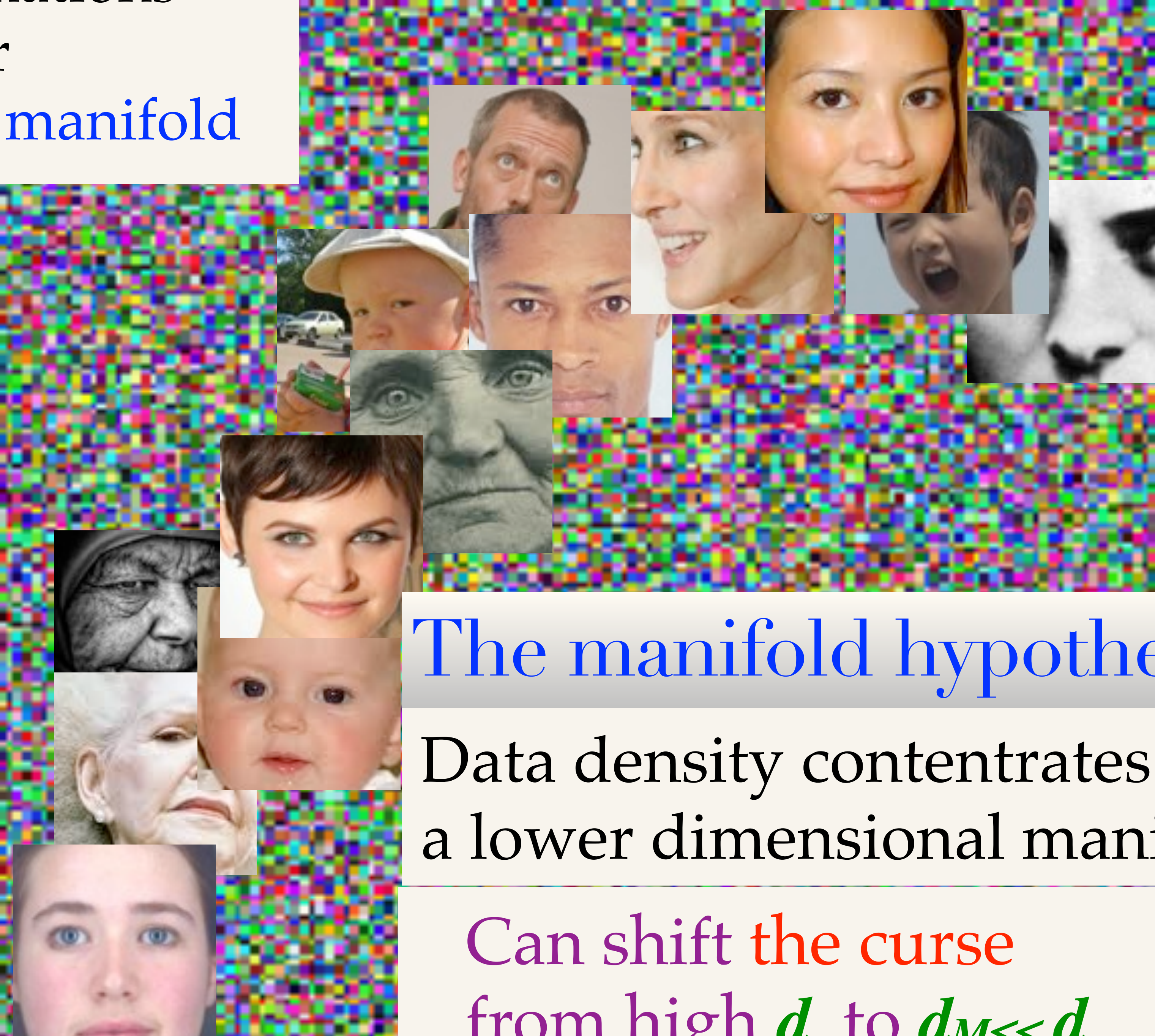


The manifold hypothesis

Data density contentrates near a lower dimensional manifold

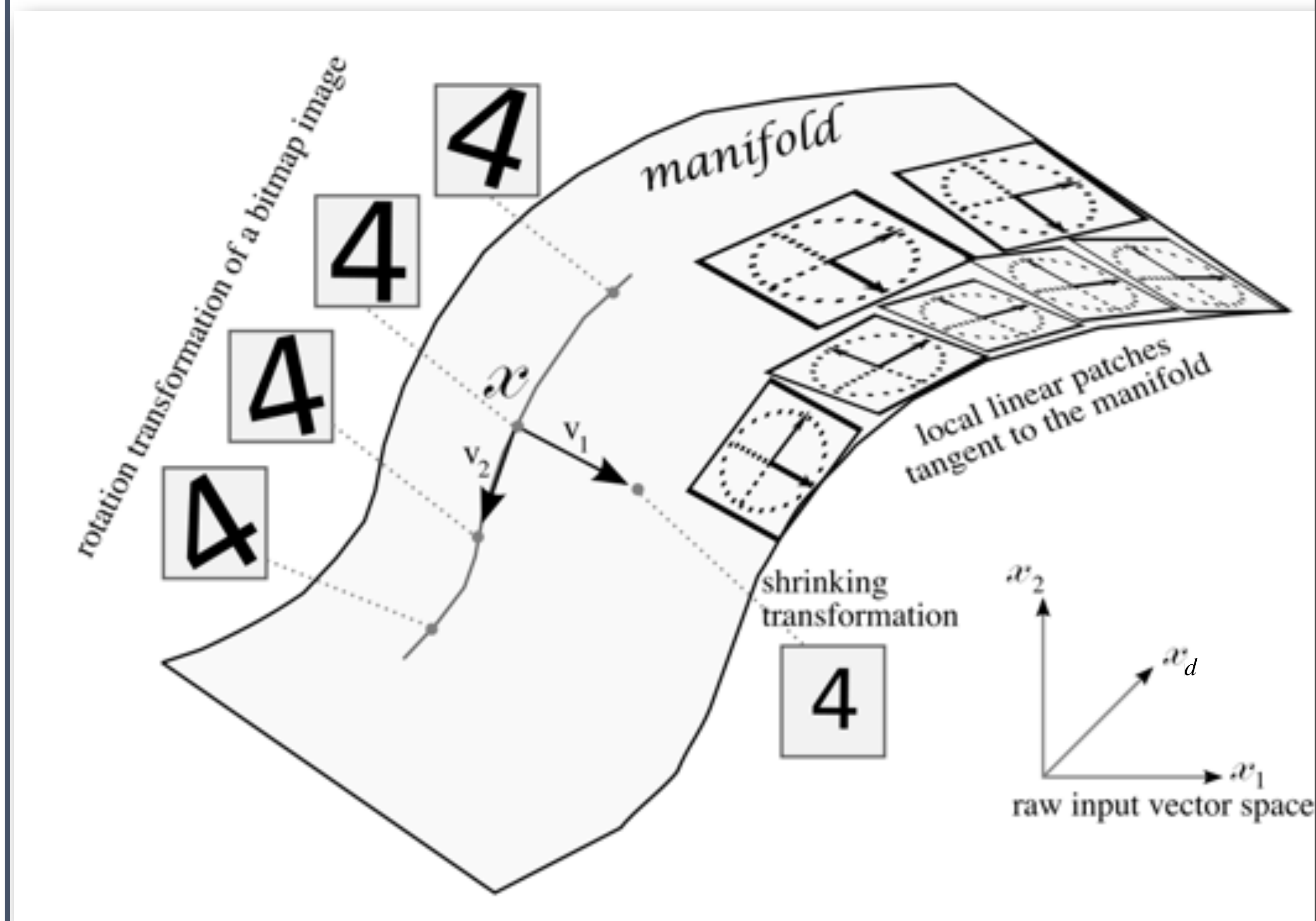
Can shift the curse from high $\boldsymbol{d}$ to $\boldsymbol{d_{M} \ll d}$

Manifold follows naturally from continuous underlying factors
(≈ intrinsic manifold coordinates)

Ex: pose parameters of a face

Image borrowed from University of Dayton Vision Lab website.

Ex: rotation, size of digits (+ line thickness, ...)

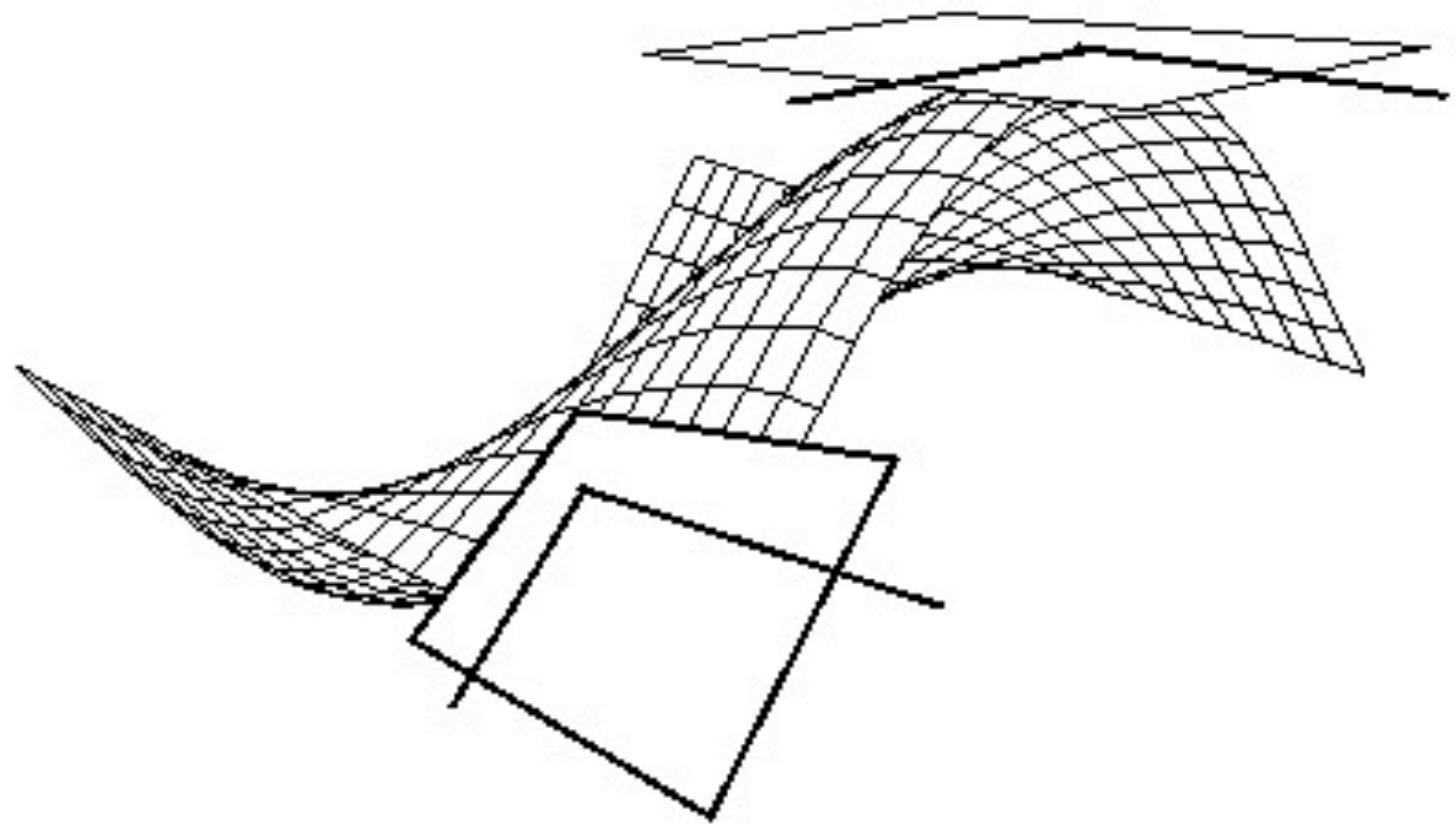


Such continuous factors are
(part of) a meaningful represetation!

Modeling local tangent spaces

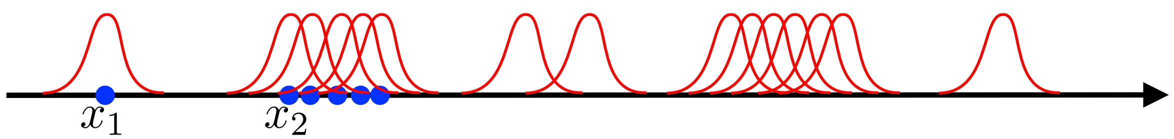
A non-linear manifold

- Can be represented by **patchwork** of **tangent spaces**
- Yields *local* linear coordinate systems (chart -> atlas)



Non-parametric density estimation

Non-parametric density estimation

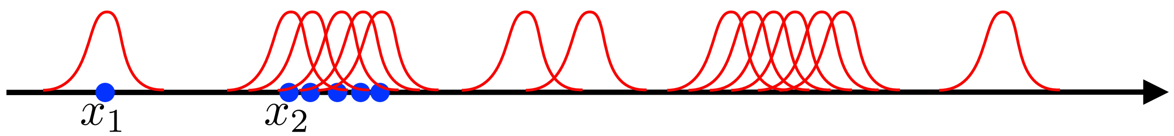


$$\hat{p}(x) = \frac{1}{n} \sum_{i=1}^{n} \mathcal{N}(x; x_i, C_i)$$

Classical Parzen Windows

density estimator

Non-parametric density estimation



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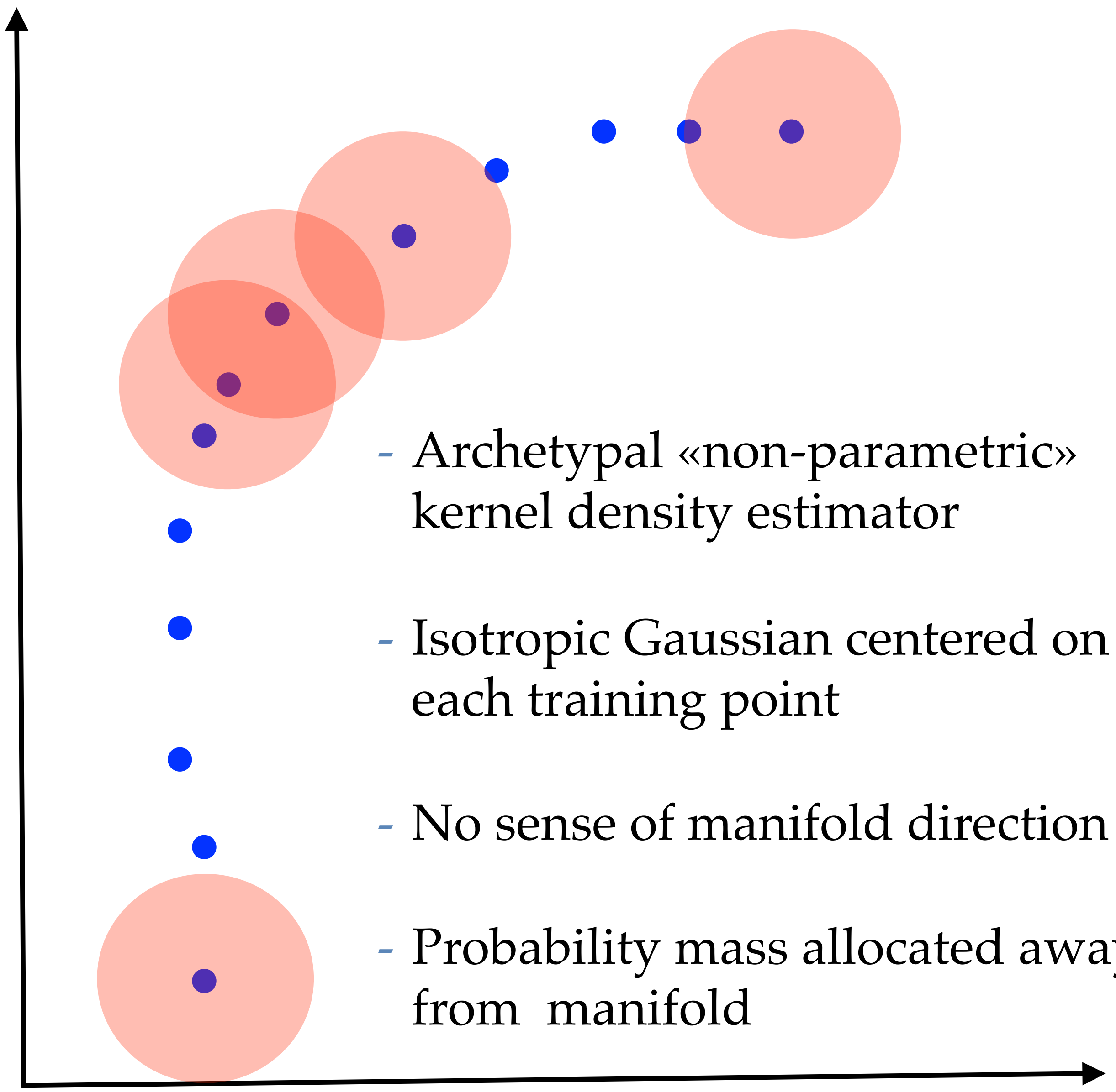
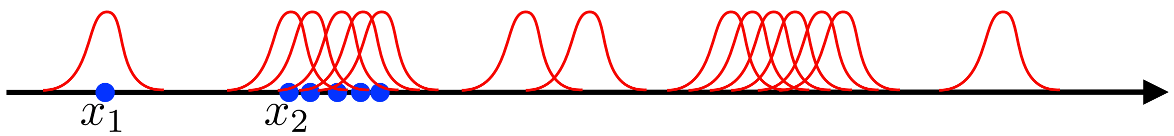


- Archetypal «non-parametric» kernel density estimator
- Isotropic Gaussian centered on each training point
- No sense of manifold direction
- Probability mass allocated away from manifold

Non-parametric density estimation



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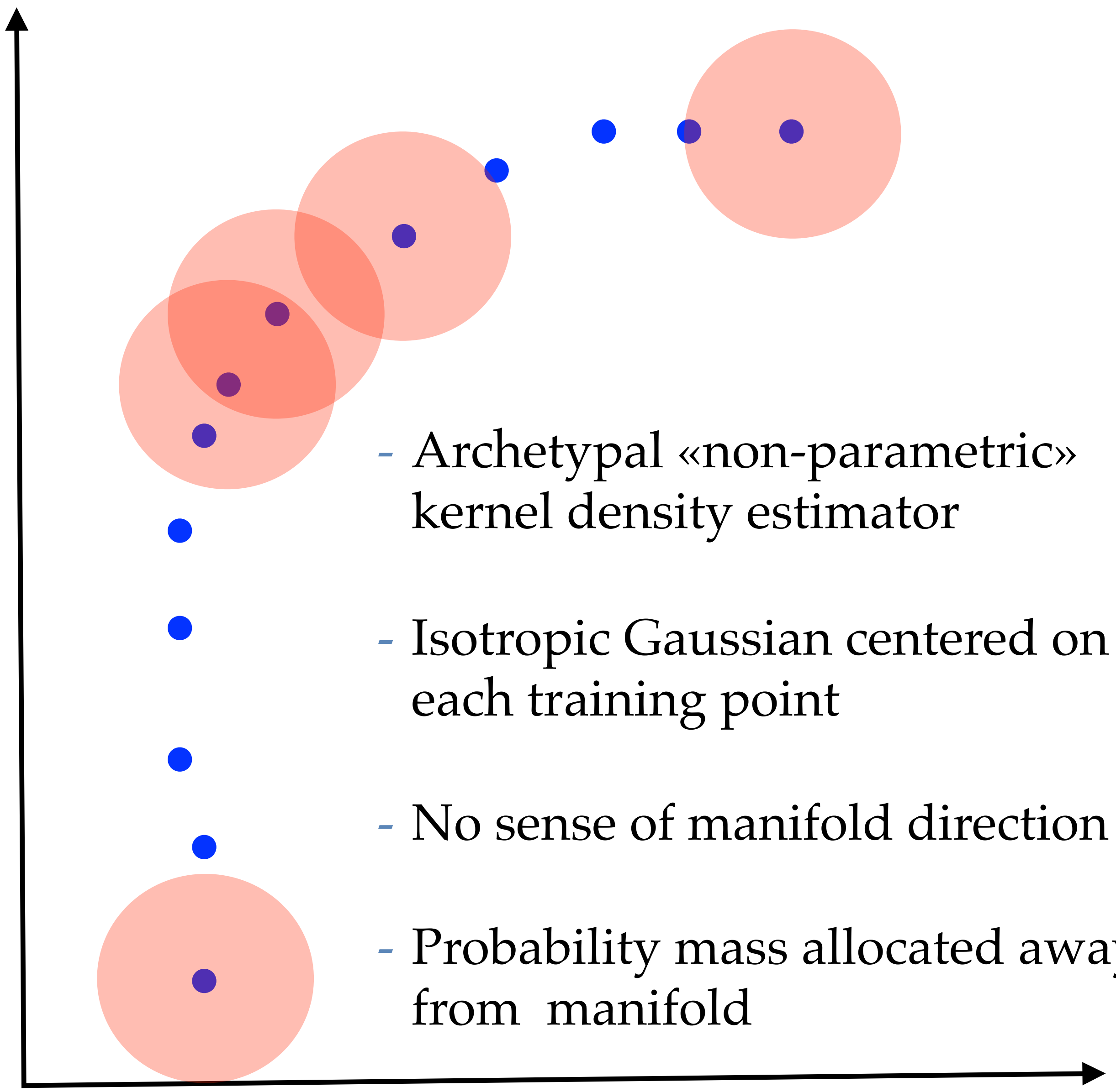

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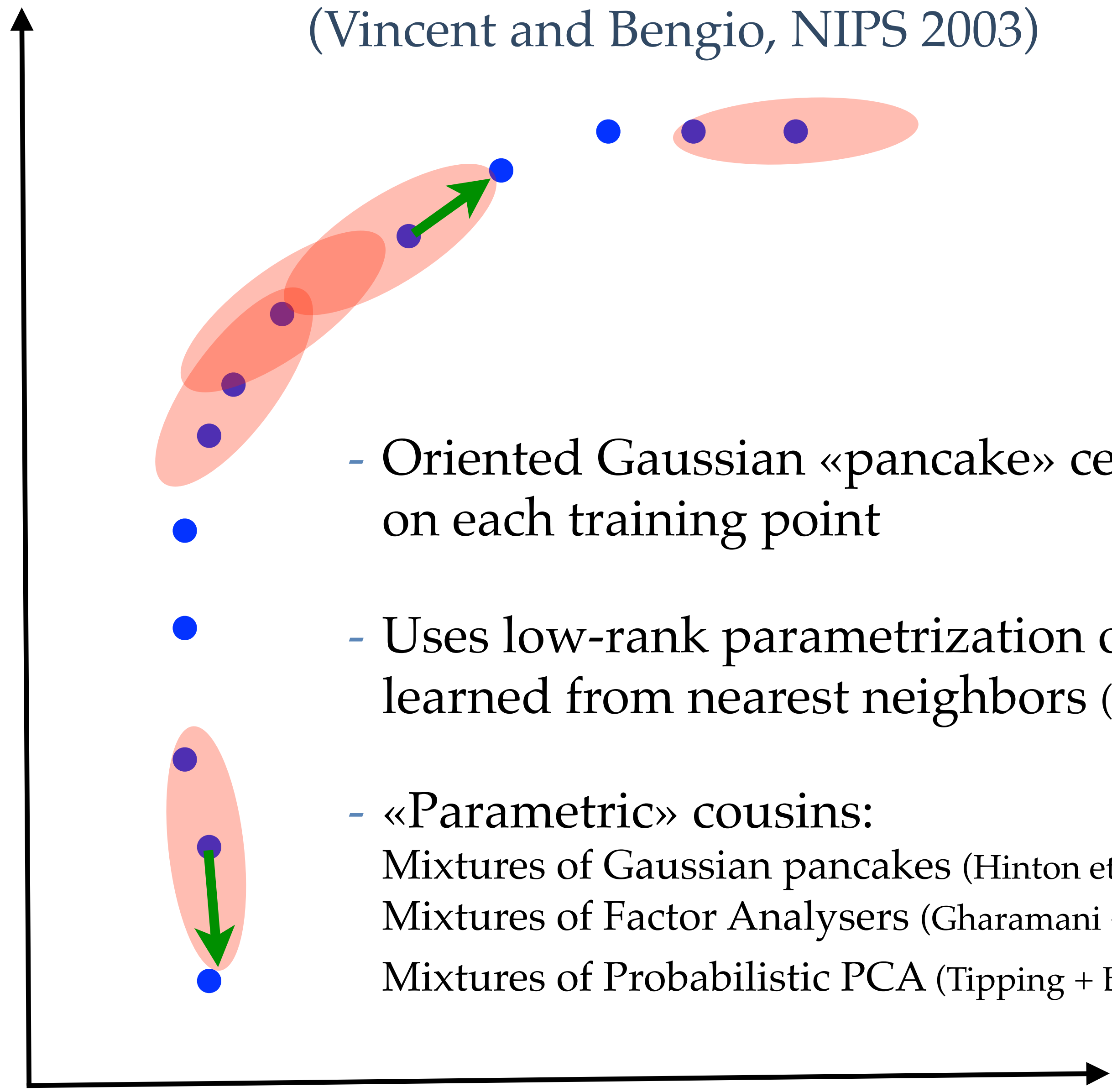
Manifold Parzen Windows

density estimator

(Vincent and Bengio, NIPS 2003)



- Oriented Gaussian «pancake» centered on each training point
- Uses low-rank parametrization of C_i, learned from nearest neighbors (local PCA)
- «Parametric» cousins:
  Mixtures of Gaussian pancakes (Hinton et al. 95)
  Mixtures of Factor Analysers (Gharamani + Hinton 96)
  Mixtures of Probabilistic PCA (Tipping + Bishop 99)

Non-local manifold Parzen windows

(Bengio, Larochelle, Vincent, NIPS 2006)

Isotropic Parzen:

$$\hat{p}(x) = \frac{1}{n} \sum_{i=1}^{n} \mathcal{N}(x; x_i, \underbrace{\sigma^2 I}_{\text{isotropic}})$$

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d_M high variance directions from PCA on k nearest neighbors

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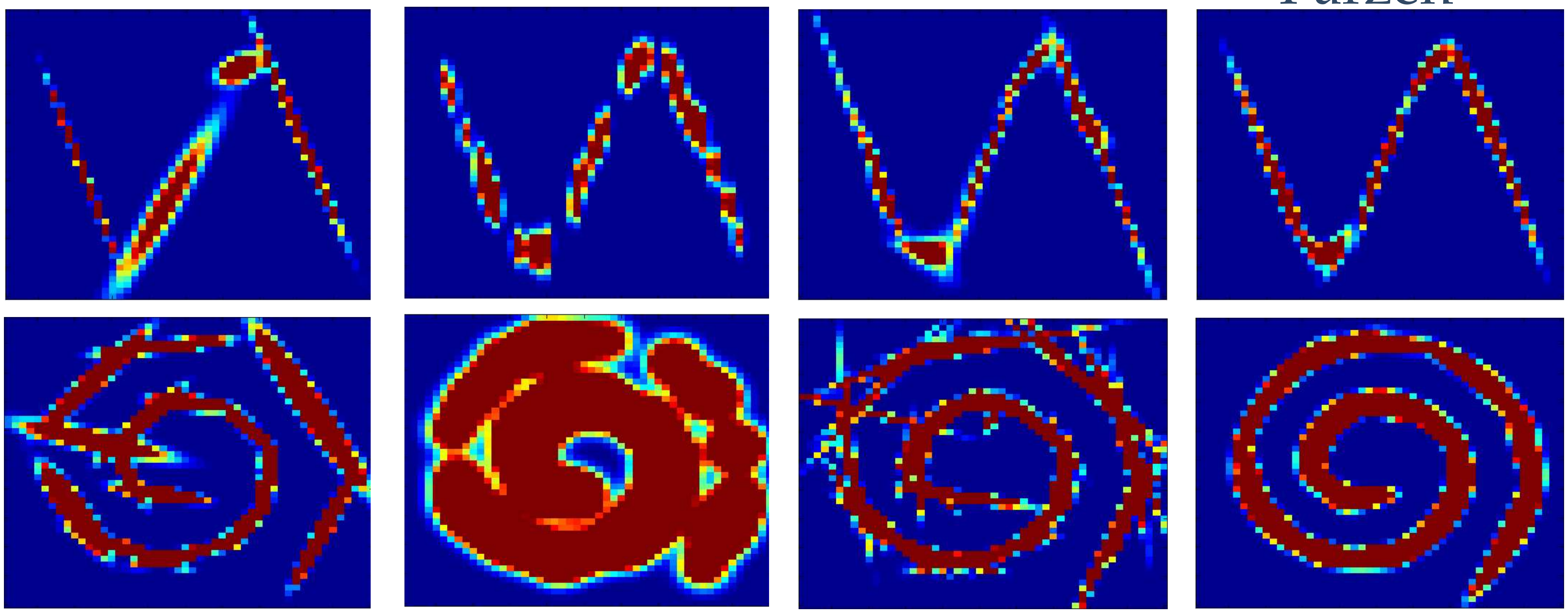
(Bengio, Larochelle, Vincent, NIPS 2006)

$$\hat{p}(x) = \frac{1}{n}\sum_{i=1}^{n}\mathcal{N}(x; \underbrace{\mu(x_i), C(x_i)}_{})$$

d_M high variance directions output by **neural network** trained to maximize likelihood of k nearest neighbors

Mixture of k Gaussians	Parzen Windows	Manifold Parzen	Non-local Manifold Parzen



Use in Bayes classifier on USPS

Algorithm	Valid.	Test	Hyper-Parameters
SVM	1.2%	4.68%	$C = 100, \sigma = 8$
Parzen Windows	1.8%	5.08%	$\sigma = 0.8$
Manifold Parzen	0.9%	4.08%	$d = 11, k = 11, \sigma_0^2 = 0.1$
Non-local MP	**0.6%**	**3.64% (-1.5218)**	$d = 7, k = 10, k_\mu = 10,$ $\sigma_0^2 = 0.05, n_{hid} = 70$
Non-local MP*	**0.6%**	**3.54% (-1.9771)**	$d = 7, k = 10, k_\mu = 4,$ $\sigma_0^2 = 0.05, n_{hid} = 30$

Manifold learning is a rich subfield

Purely non-parametric:

- Manifold Parzen, LLE, Isomap, Laplacian eigenmaps, t-SNE, ...

Learned parametrized function:

- Parametric t-SNE, semi-supervised embedding, **non-local** manifold Parzen, ...

What do all these approaches have in common ?

Neighborhood-based training!

- They explicitly use distance-based neighborhoods.
- Training with k-nearest neighbors, or pairs of points.
- Typically Euclidean neighbors
- But in **high** ***d***, your nearest Euclidean neighbor can be **very** different from you...

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Neighborhood-based training!

Unreliable!

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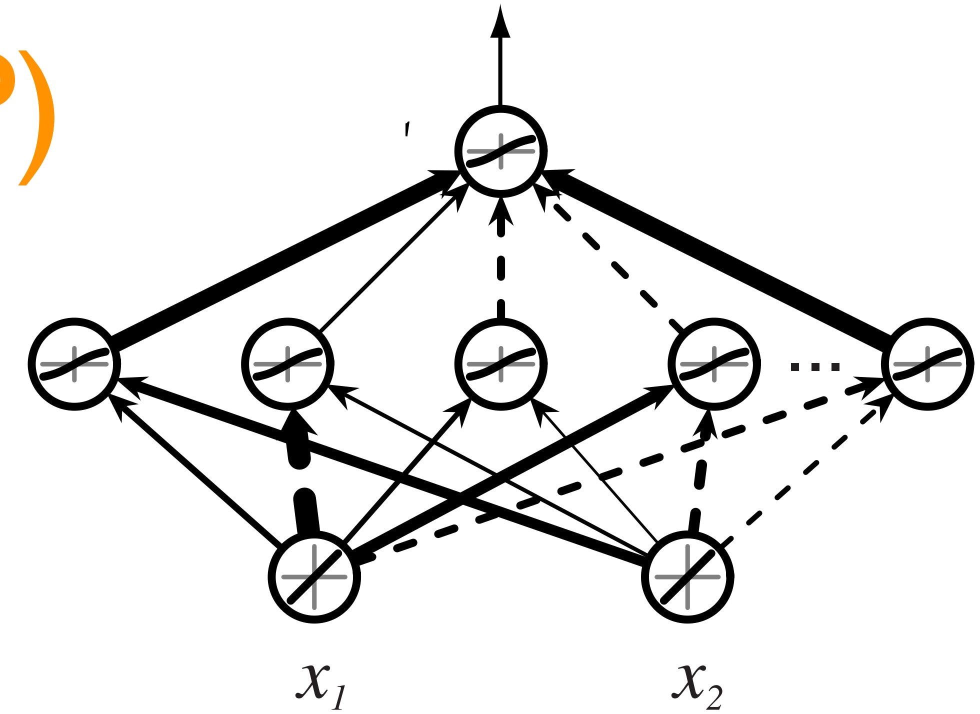
PART II

On Auto-Encoders
and
their regularization,

Multi-Layer Perceptron (MLP)

with **one** hidden layer of size *d'* neurons



Functional form (parametric):

$$y = f_\theta(\mathbf{x}) = \mathrm{sigmoid}\left(\langle \mathbf{w}, \underbrace{\mathbf{h}} \rangle + b\right)$$

$$\mathbf{h} = \mathrm{sigmoid}(\underbrace{\mathbf{W}}_{d' \times d}{}^{\mathrm{hidden}}\mathbf{x} + \underbrace{\mathbf{b}}_{d' \times 1}{}^{\mathrm{hidden}})$$

Parameters:

$$\theta = \{\mathbf{W}^{\mathrm{hidden}}, \mathbf{b}^{\mathrm{hidden}}, \mathbf{w}, b\}$$

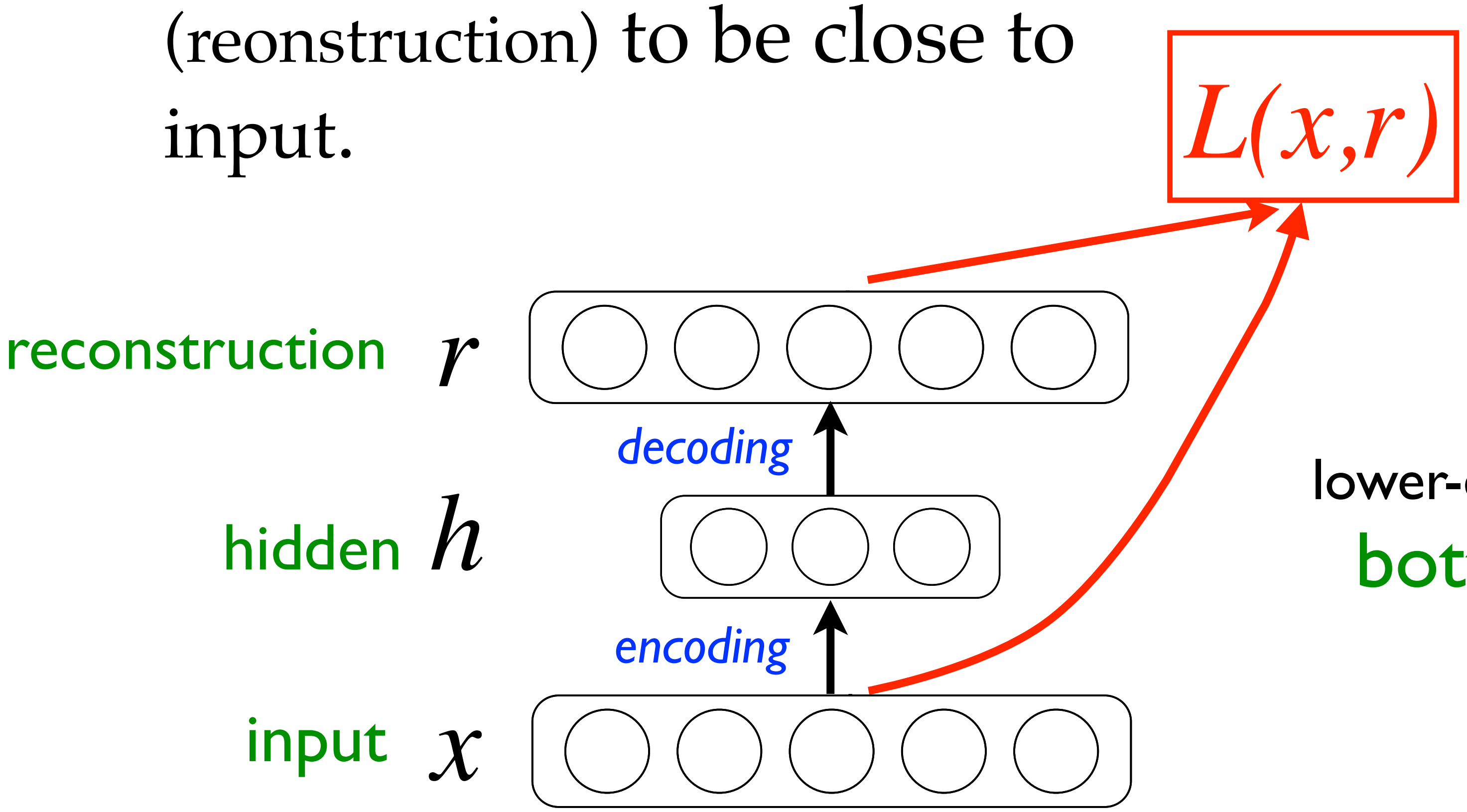
Optimizing parameters on training set *(training the network)*:

$$\theta^\star = \arg\min_\theta \underbrace{\hat{R}_\lambda(f_\theta, D_n)}$$

$$\mathcal{J}_{\mathrm{MLP}}(\theta) = \Bigg(\underbrace{\sum_{(x,t)\in D} L(t, f_\theta(x))}_{\text{empirical risk}}\Bigg) + \underbrace{\lambda\Omega(\theta)}_{\substack{\text{regularization term} \\ \text{(weight decay)}}}$$

Autoencoders: MLPs used for «unsupervised» representation learning

- Make output layer same size as input layer
- Have target = input
- Loss encourages output (reonstruction) to be close to input.



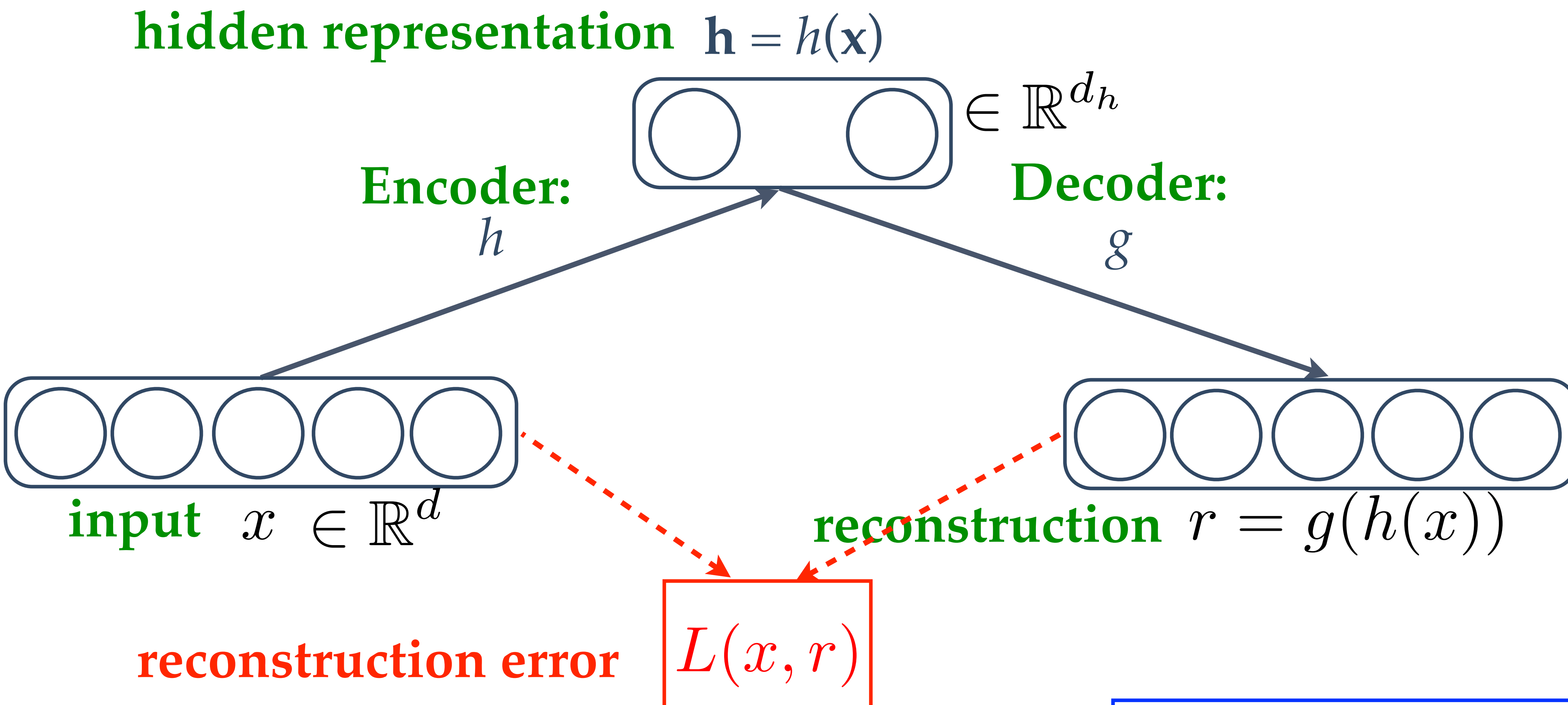
Autoencoders are also called

- Autoencoders
- Auto-associators
- Diabolo networks
- Sandglass-shaped net

lower-dimensional
bottleneck

The Diabolo

Auto-Encoders (AE)
for learning representations

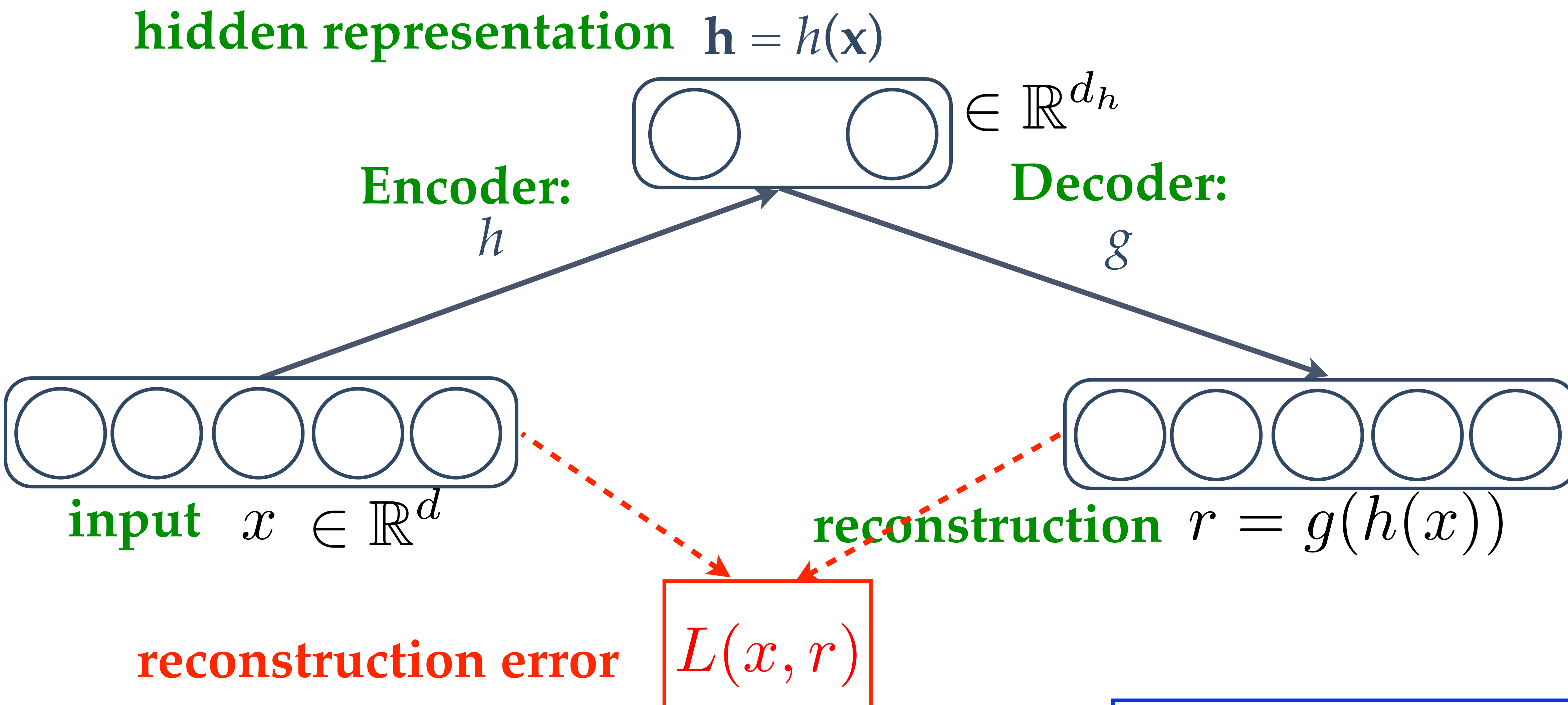


Minimize

$$\mathcal{J}_{\text{AE}} = \sum_{x \in D} L(x, g(h(x)))$$

Auto-Encoders (AE)
for learning representations

Typical form



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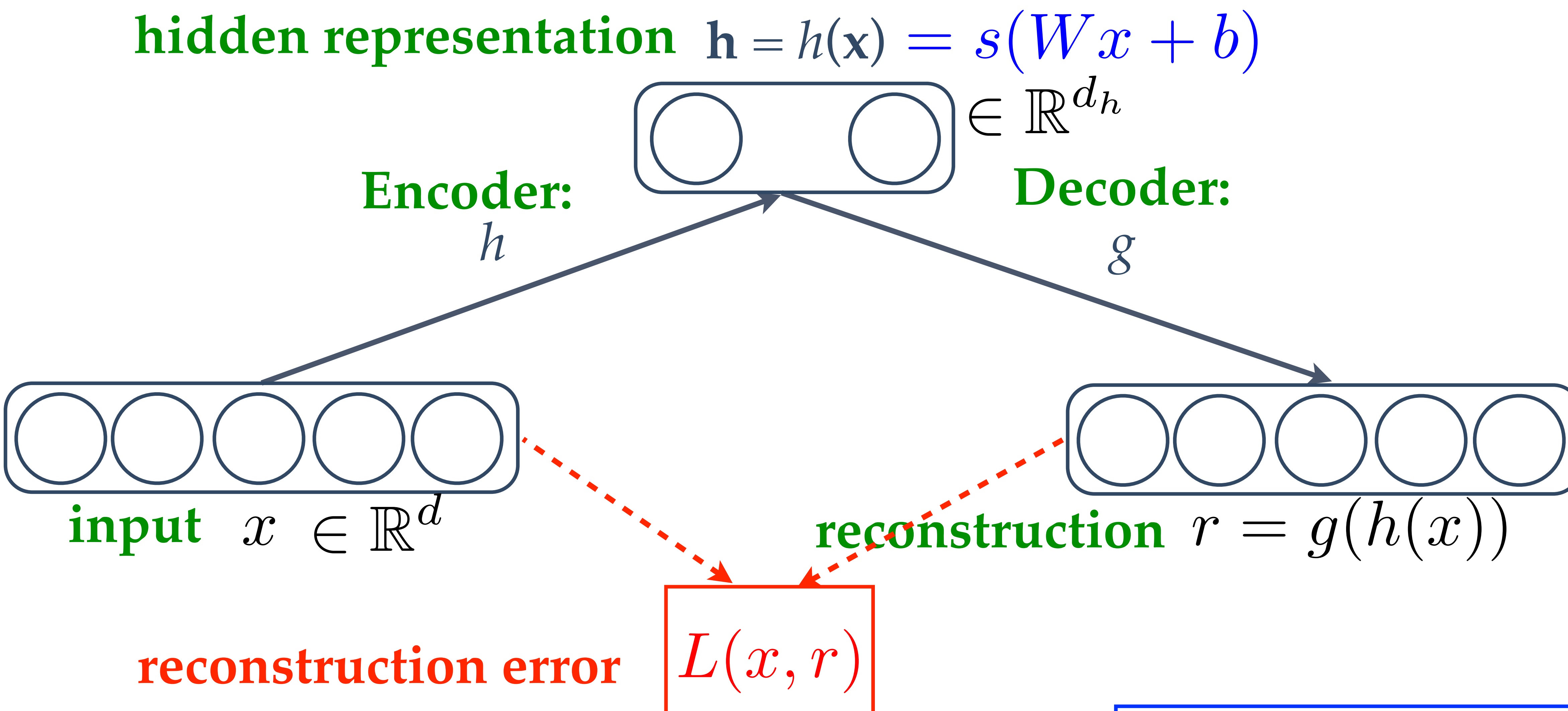

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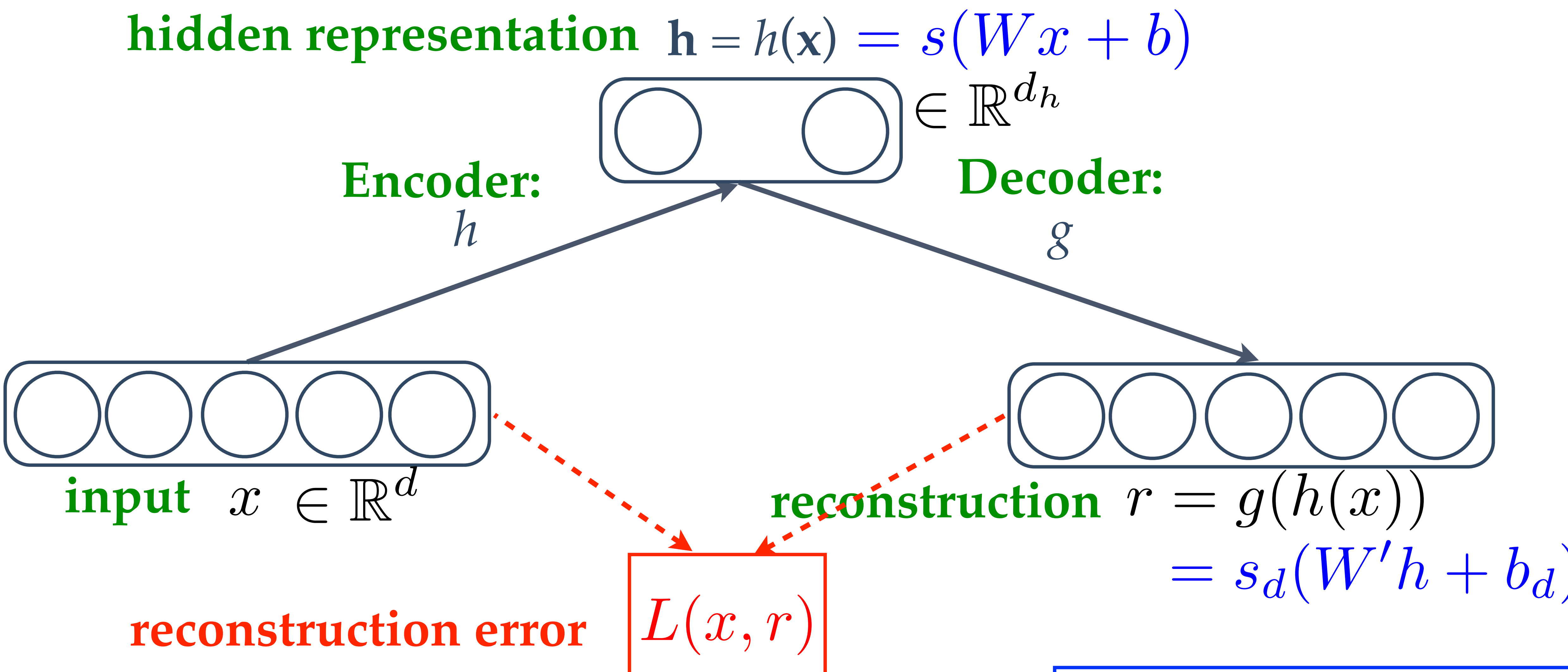

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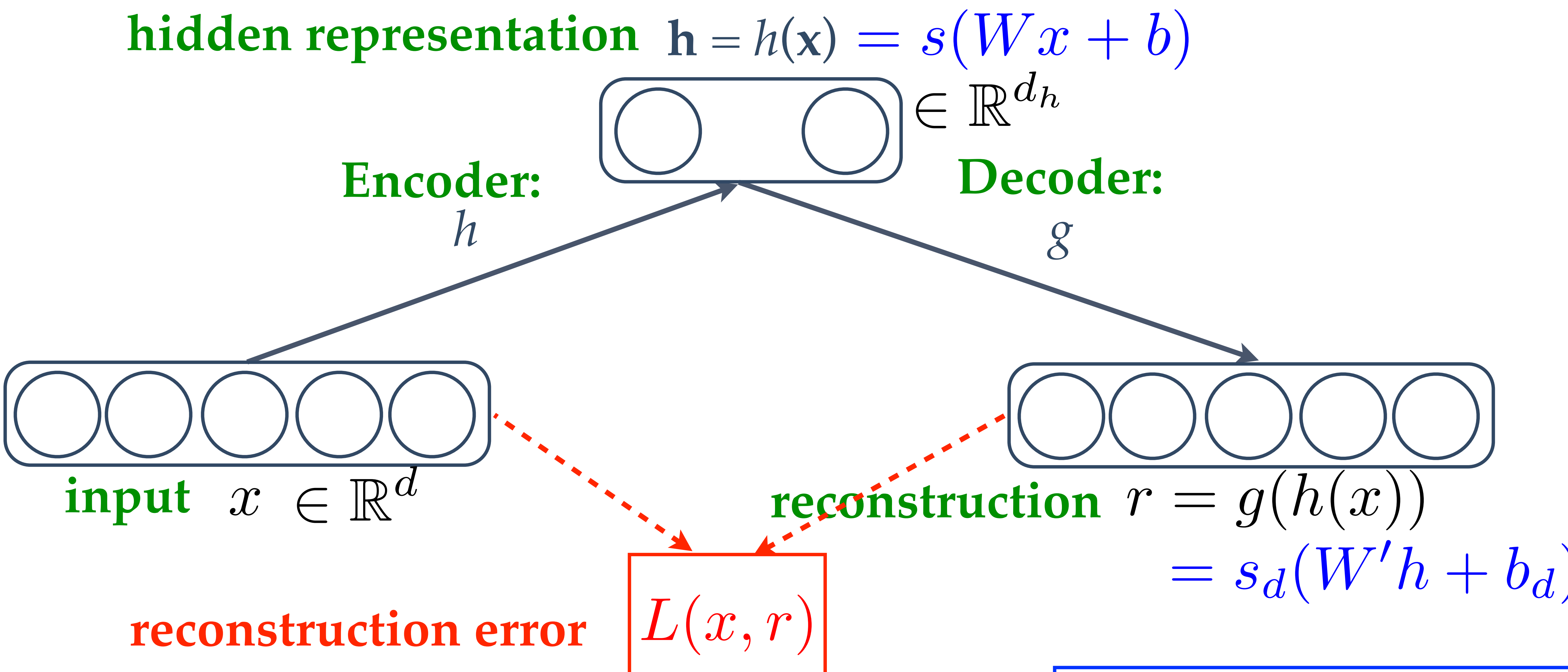


squared error: $\|x - r\|^2$

or Bernoulli cross-entropy

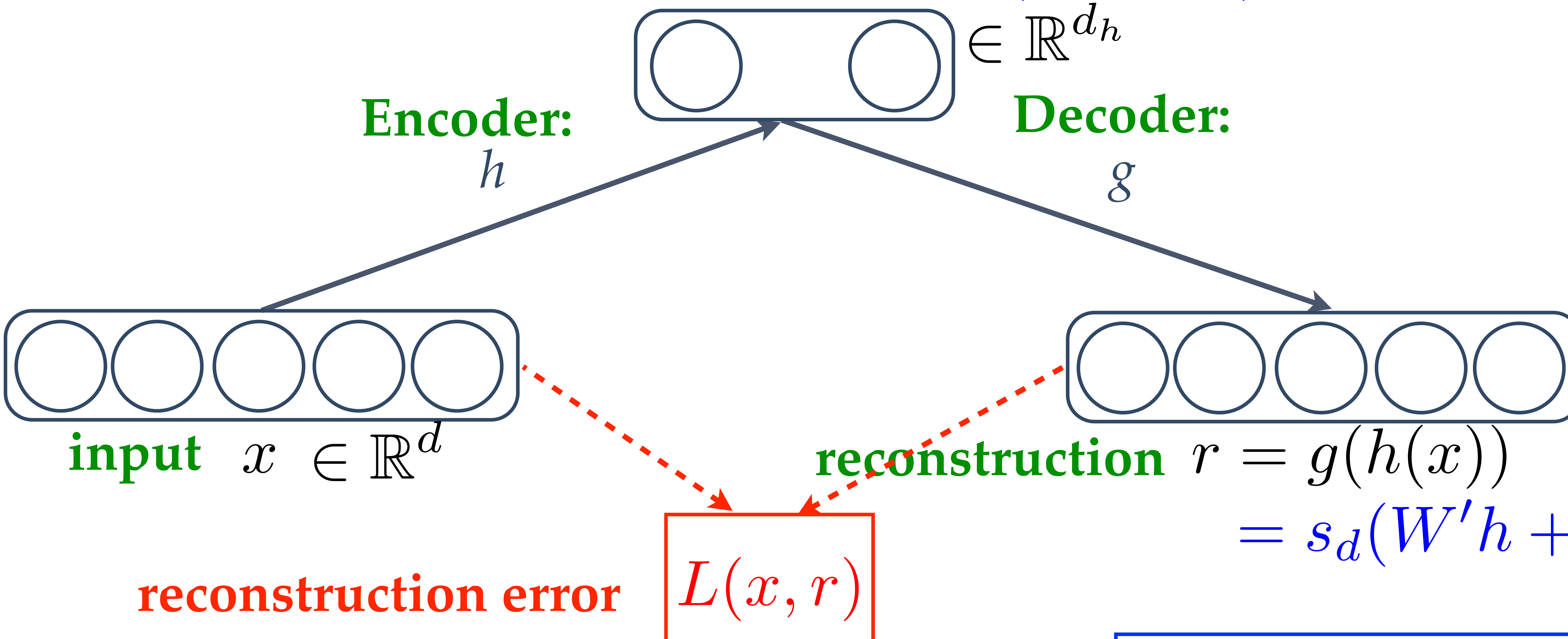
Minimize

$$\mathcal{J}_{\text{AE}} = \sum_{x \in D} L(x, g(h(x)))$$

Auto-Encoders (AE)
for learning representations

Typical form

hidden representation $\mathbf{h} = h(\mathbf{x}) = s(Wx + b)$ s is typically sigmoid



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$$\mathcal{J}_{\mathrm{AE}} = \sum_{x \in D} L(x, g(h(x)))$$

conection between

Linear auto-encoders and PCA

d_h<d (bottleneck, undercomplete representation)**:**

- With linear neurons and squared loss
  ➠ autoencoder learns same **suspace** as PCA
- Also true with a single sigmoidal hidden layer, if using linear output neurons with squared loss [Baldi& Hornik 89] and untied weights.
- Won't learn the exact same **basis** as PCA, but W will span the same **subspace**.

similarity between

Auto-encoders and RBM

Consider an auto-encoder MLP

- with a single hidden layer with sigmoid non-linearity
- and sigmoid output non-linerity.
- Tie encoder and decoder weights: $W' = W^T$.

Autoencoder:

$$h_i = \mathrm{s}(W_i x + b_i)$$
$$r_j = \mathrm{s}(W_j^T h + b_{dj})$$

RBM:

$$P(h_i = 1 \mid v) = \mathrm{s}(W_i v + c_i)$$
$$P(v_j = 1 \mid h) = \mathrm{s}(W_j^T h + b_j)$$

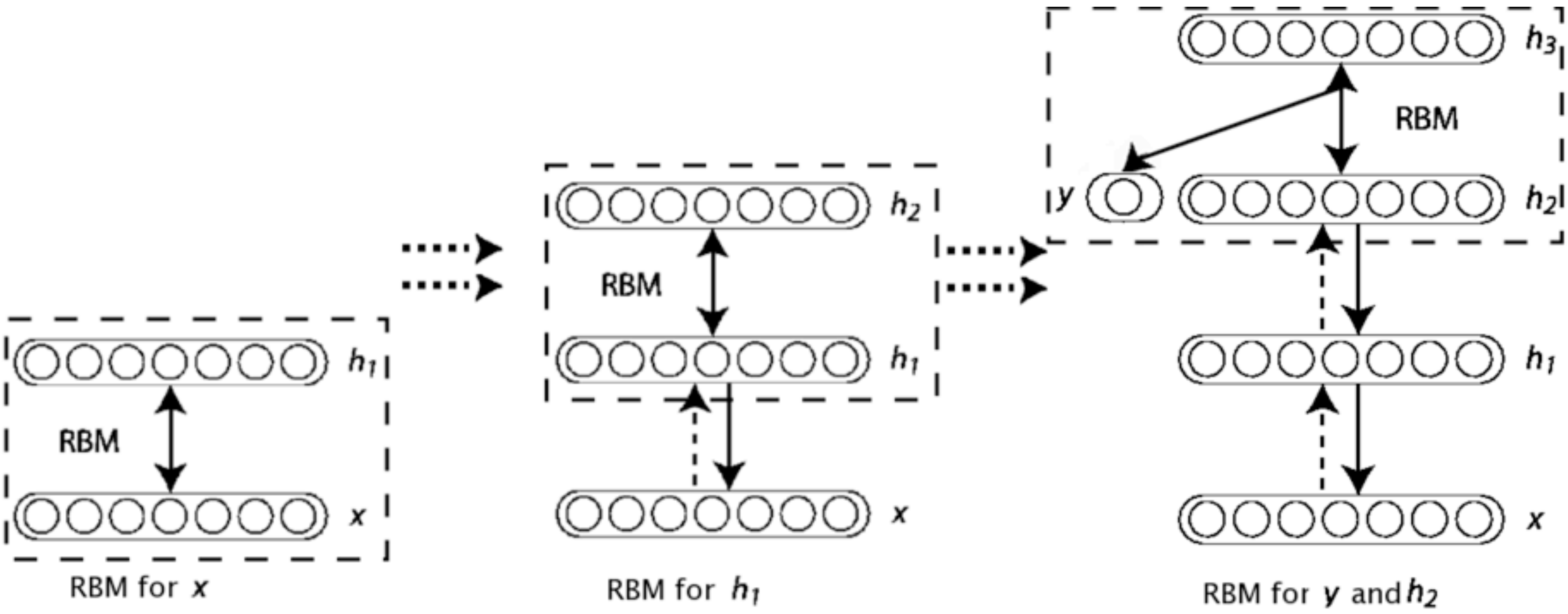
Differences: deterministic mapping
h is a function of x.

stochastic mapping
h is a random variable

Greedy Layer-Wise Pre-training with RBMs

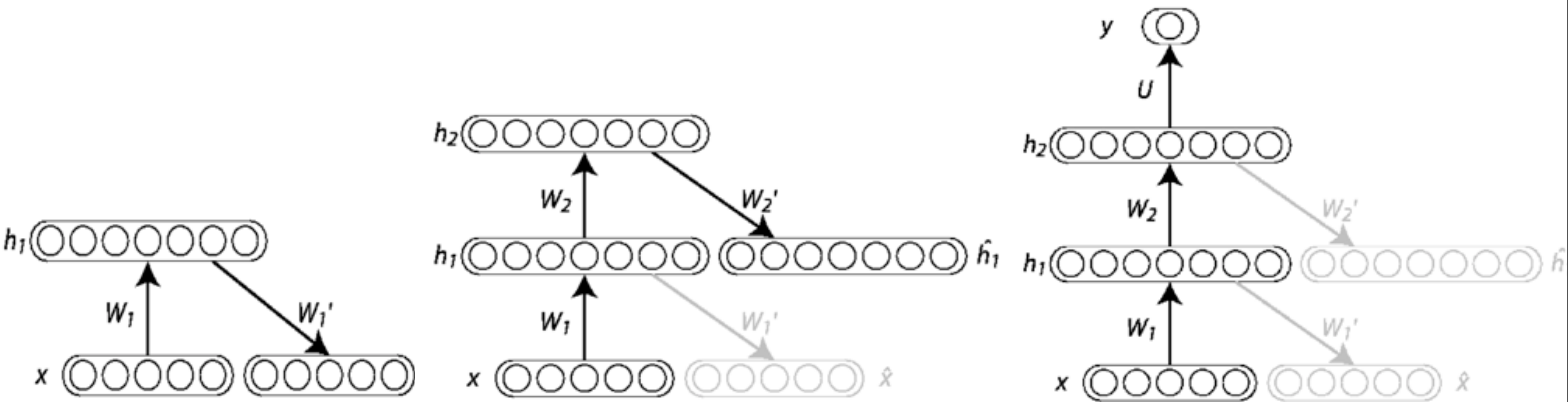
Stacking Restricted Boltzmann Machines (RBM)

➪ Deep Belief Network (DBN) [Hinton et al. 2006]



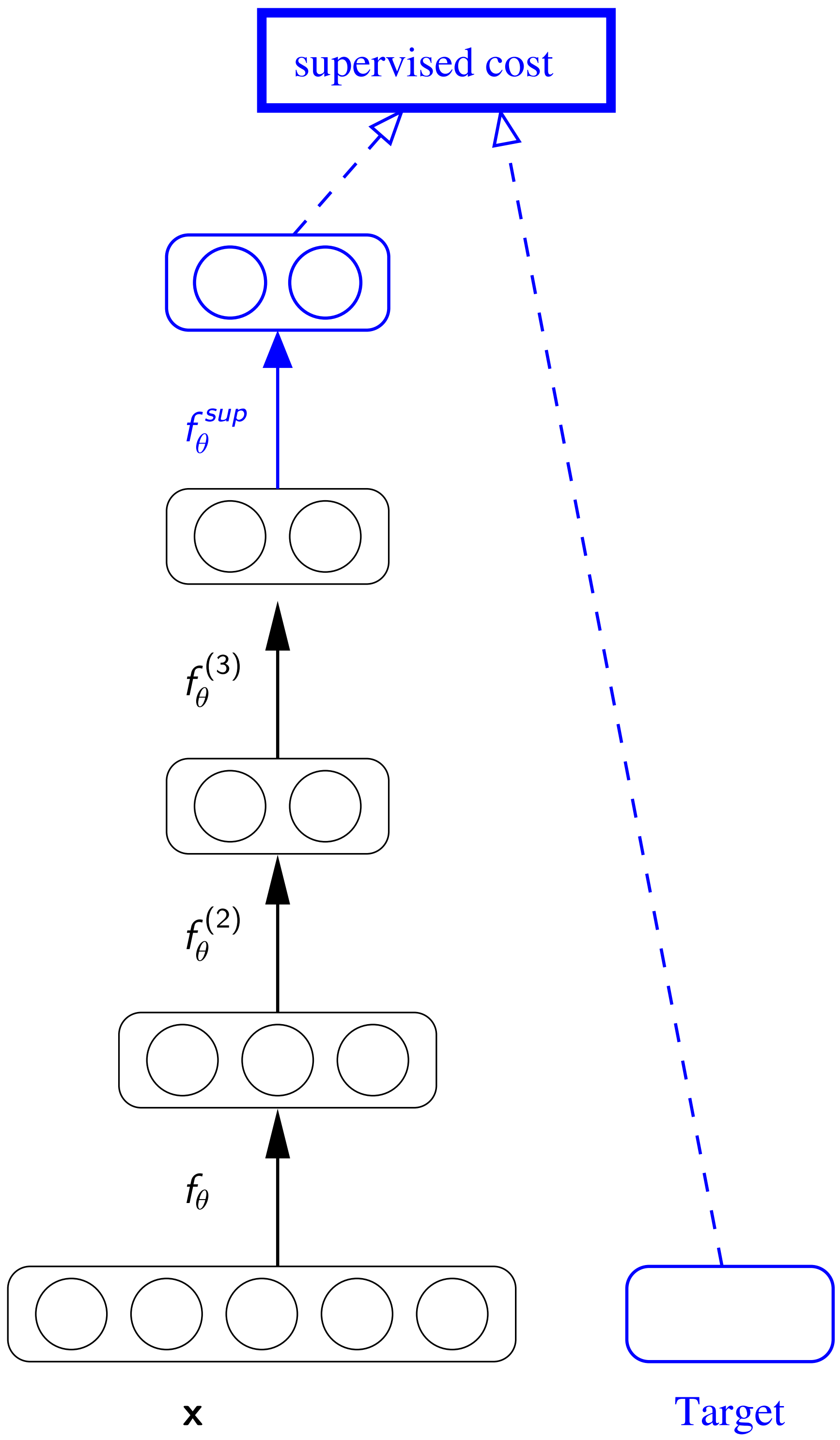
Greedy Layer-Wise Pre-training with Auto-Encoders

Stacking basic Auto-Encoders [Bengio et al. 2007]



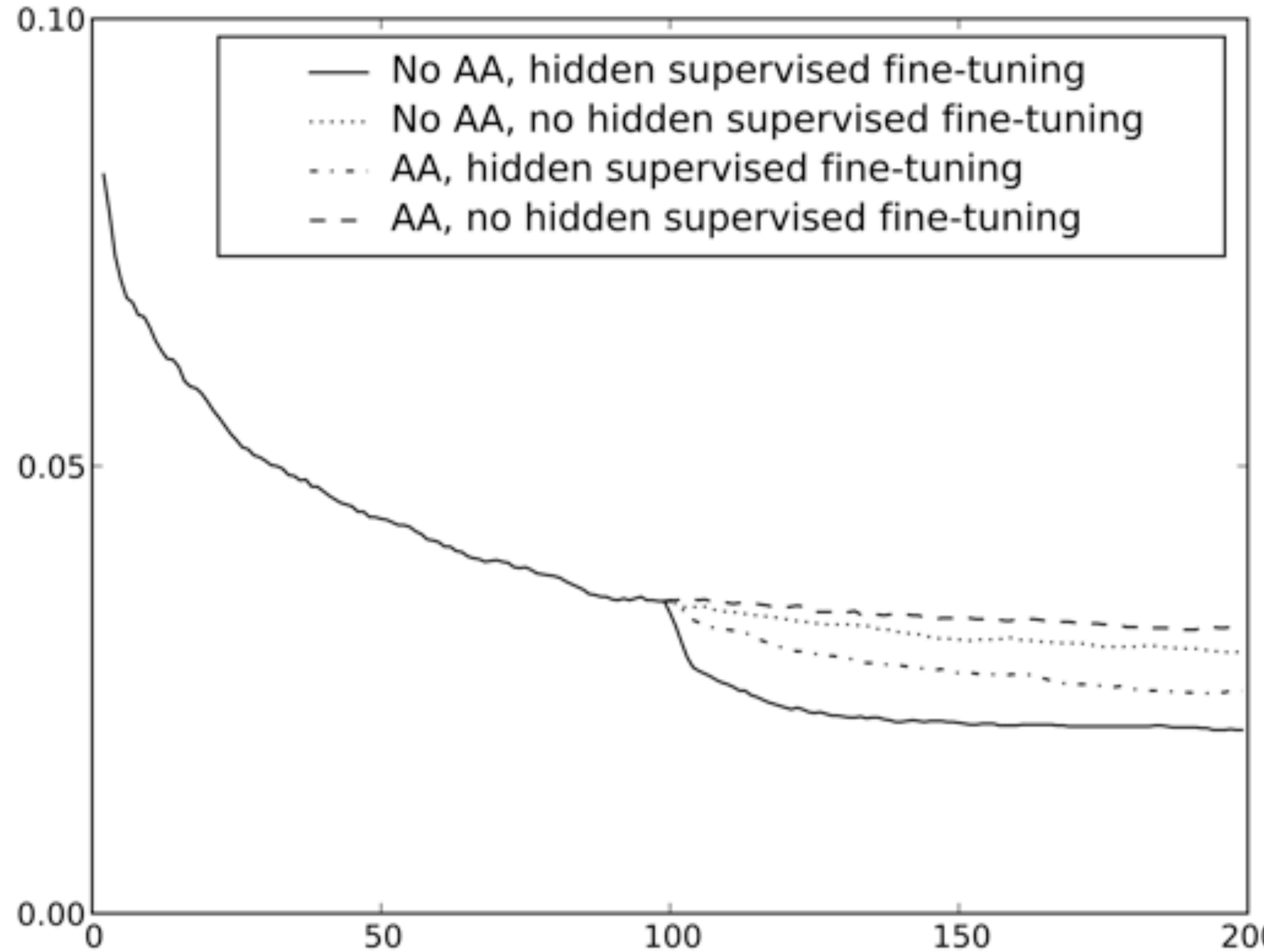
Supervised fine-tuning

- Initial deep mapping was learnt in an unsupervised way.
- $\rightarrow$ initialization for a supervised task.
- Output layer gets added.
- Global fine tuning by gradient descent on supervised criterion.



Supervised Fine-Tuning is Important

- Greedy layer-wise unsupervised pre-training phase with RBMs or auto-encoders on MNIST
- Supervised phase with or without unsupervised updates, with or without fine-tuning of hidden layers



Classiffication performance on benchmarks:

- Pre-training basic auto-encoder stack better than no pre-training
- Basic auto-encoder stack **almost** matched RBM stack...

Basic auto-encoders not as good feature learners as RBMs...

What's the problem?

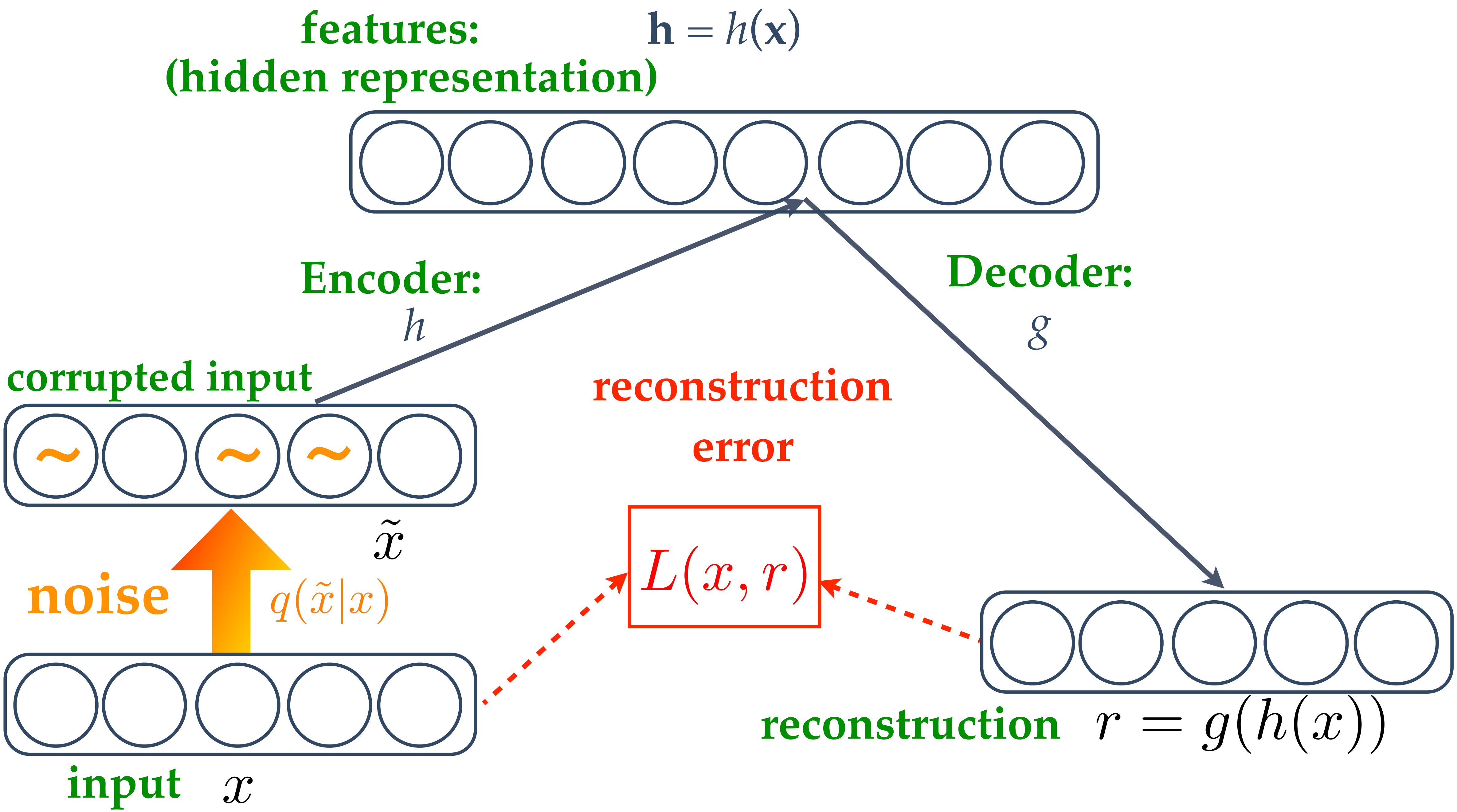
- Traditional autoencoders were for **dimensionality reduction** ($d_h < d_x$)
- Deep learning success seems to depend on ability to learn **overcomplete representations** ($d_h > d_x$)
- Overcomplete basic autoencoder yields trivial *useless* solutions: identity mapping!
- Need for alternative **regularization/ constraining**

Denoising auto-encoders: motivation

(Vincent, Larochelle, Bengio, Manzagol, ICML 2008)

- Simple idea «destroying information» of randomly selected input features; train to restore it.
  => 0-masking noise (now called «dropout» noise)
- Denoising corrupted input is a vastly **more challenging** task than mere reconcstruction.
- Even in widely **over-complete case**...
  it **must** learn intelligent encoding/decoding.
- Will encourage **representation that is robust** to small perturbations of the input.

Denoising auto-encoder (DAE)



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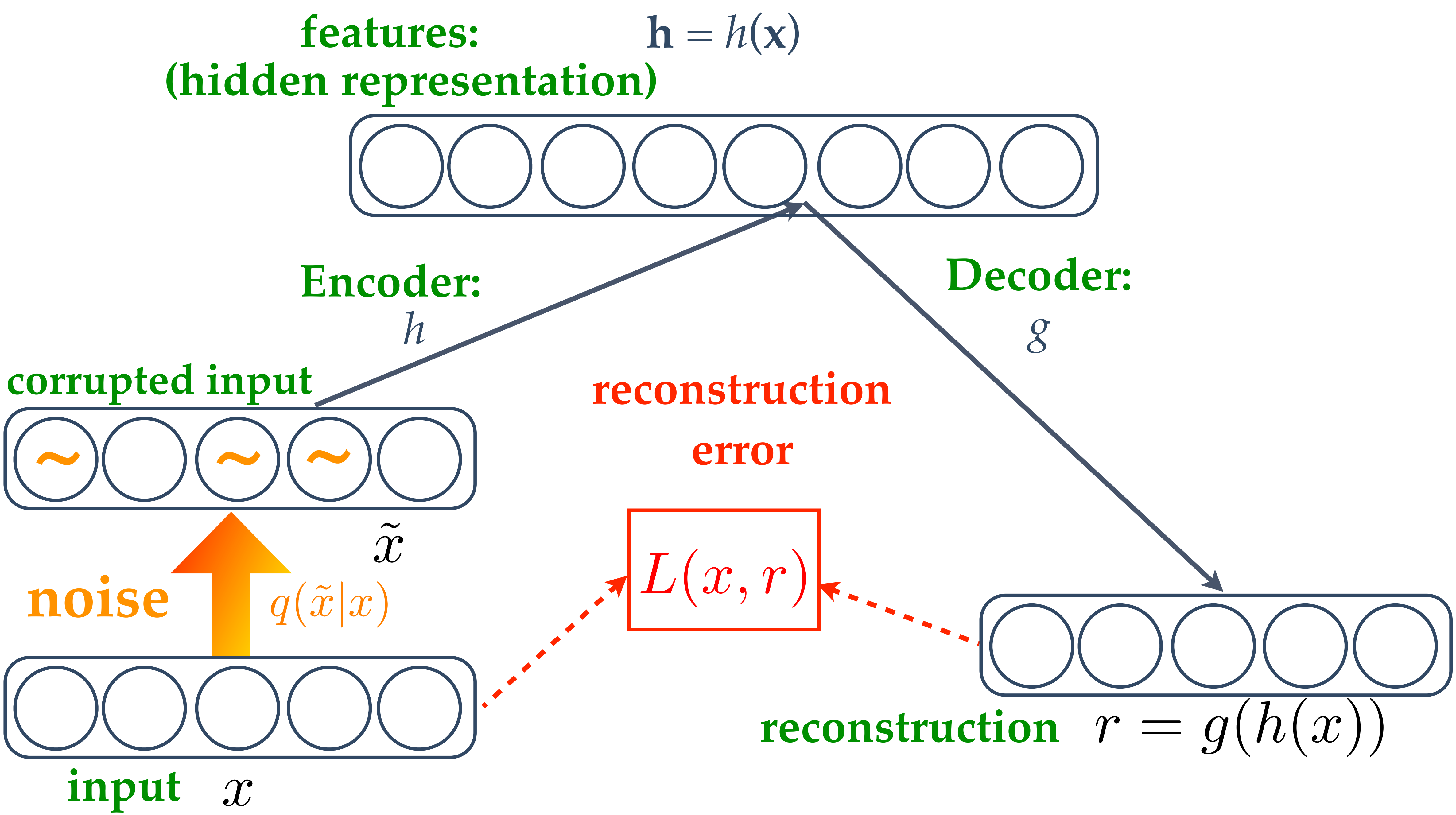

Minimize:

$$\mathcal{J}_{\mathrm{DAE}}(\theta) = \sum_{x \in D} \mathbb{E}_{q(\tilde{x}|x)} \left[L(x, g(h(\tilde{x}))) \right]$$

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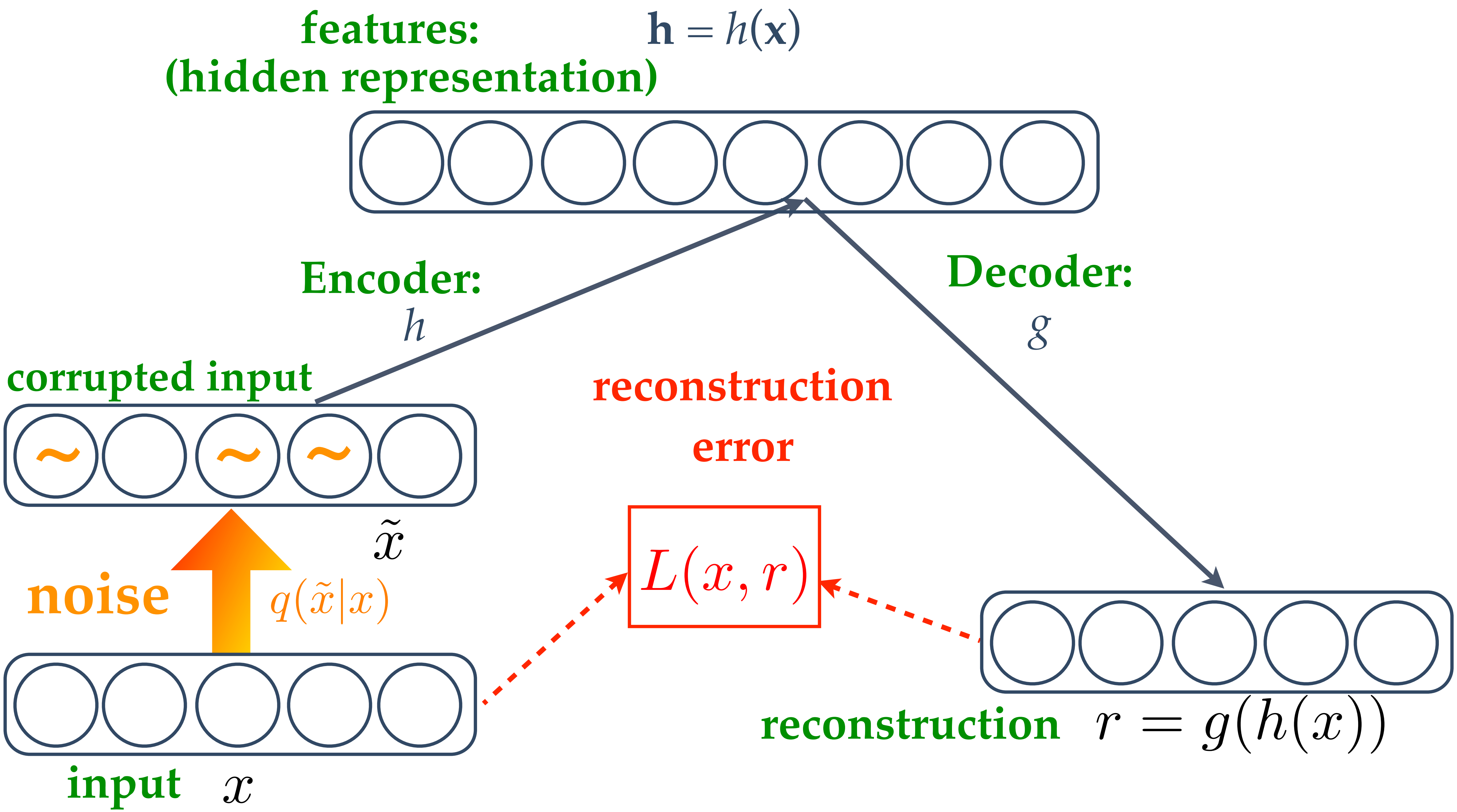

- ➡ learns robust & useful features
- ➡ easier to train than RBM features
- ➡ yield similar or better classification performance (as deep net pre-training)

Minimize:

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Denoising auto-encoder (DAE)

- Autoencoder training minimizes:

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- Denoising autoencoder training minimizes

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Cannot compute expectation exactly
➪ use stochastic gradient descent,
sampling corrupted inputs $\tilde{x}|x$

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Possible corruptions q:

- zeroing pixels at random (now called «dropout» noise)
- additive Gaussian noise
- salt-and-pepper noise
- ...

Denoising auto-encoder (DAE)

Stochastic perturbation

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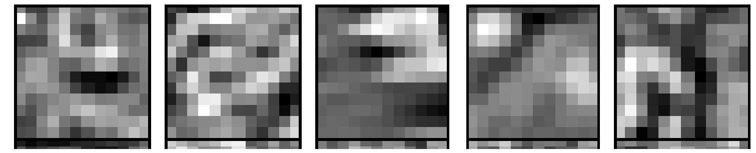
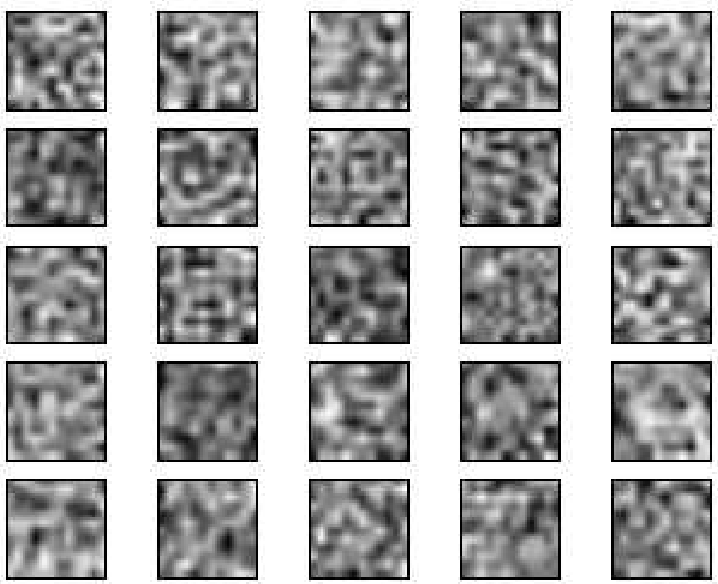
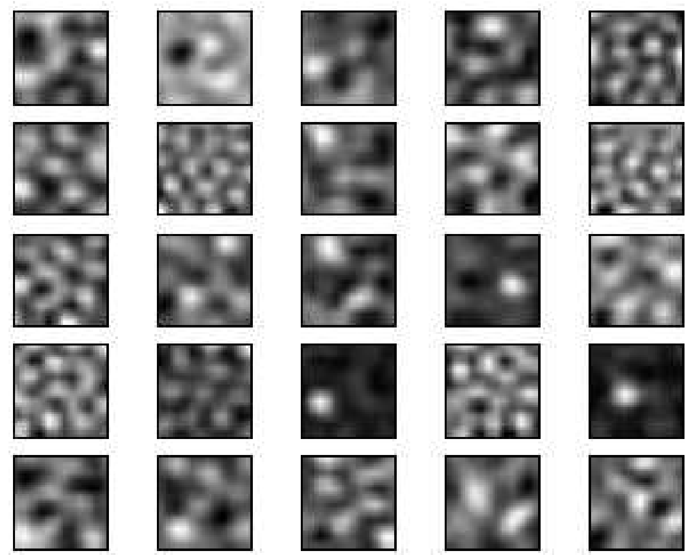
Learned filters

a) Natural image patches e.g.: 

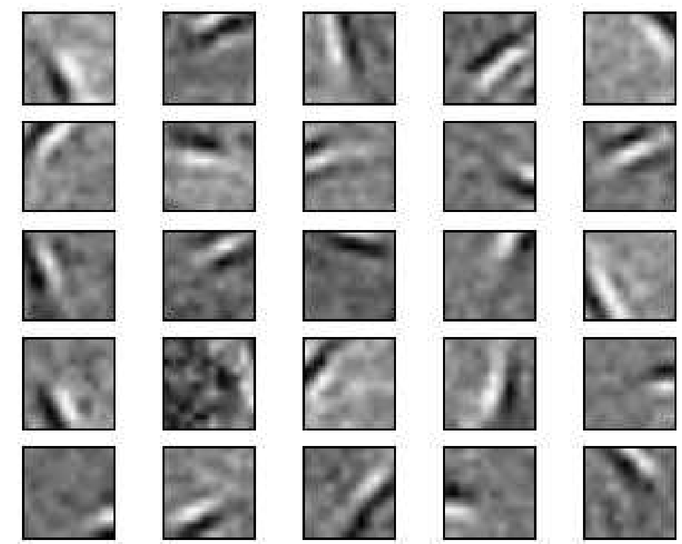
AE



AE with weight decay

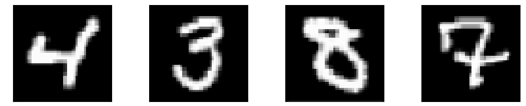


DAE

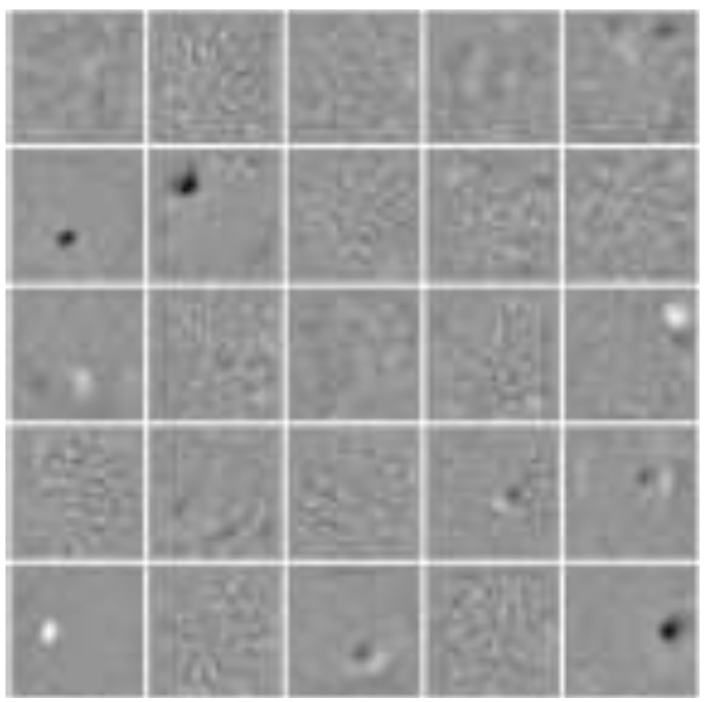


Learned filters

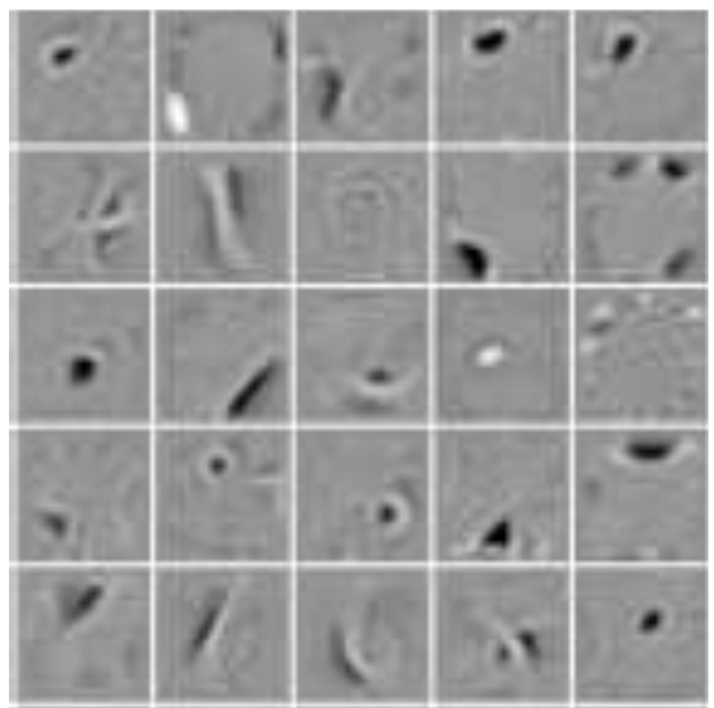
b) MNIST digits

e.g.: 

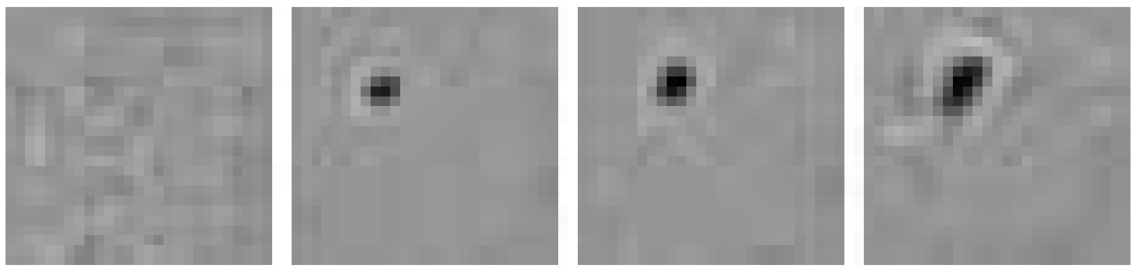
AE



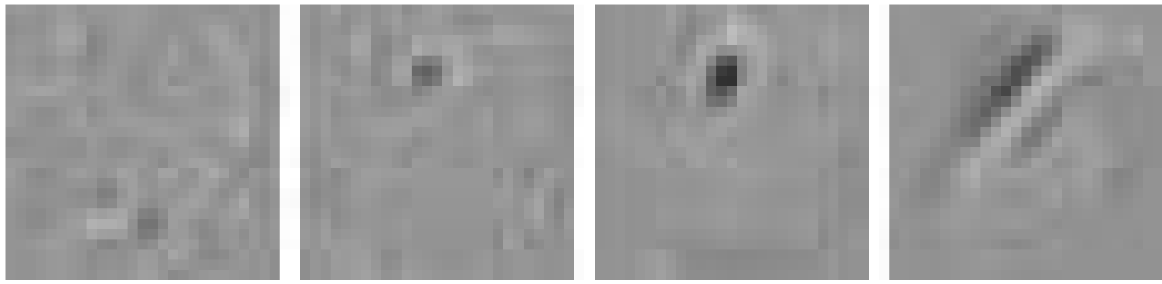
DAE



Increasing noise



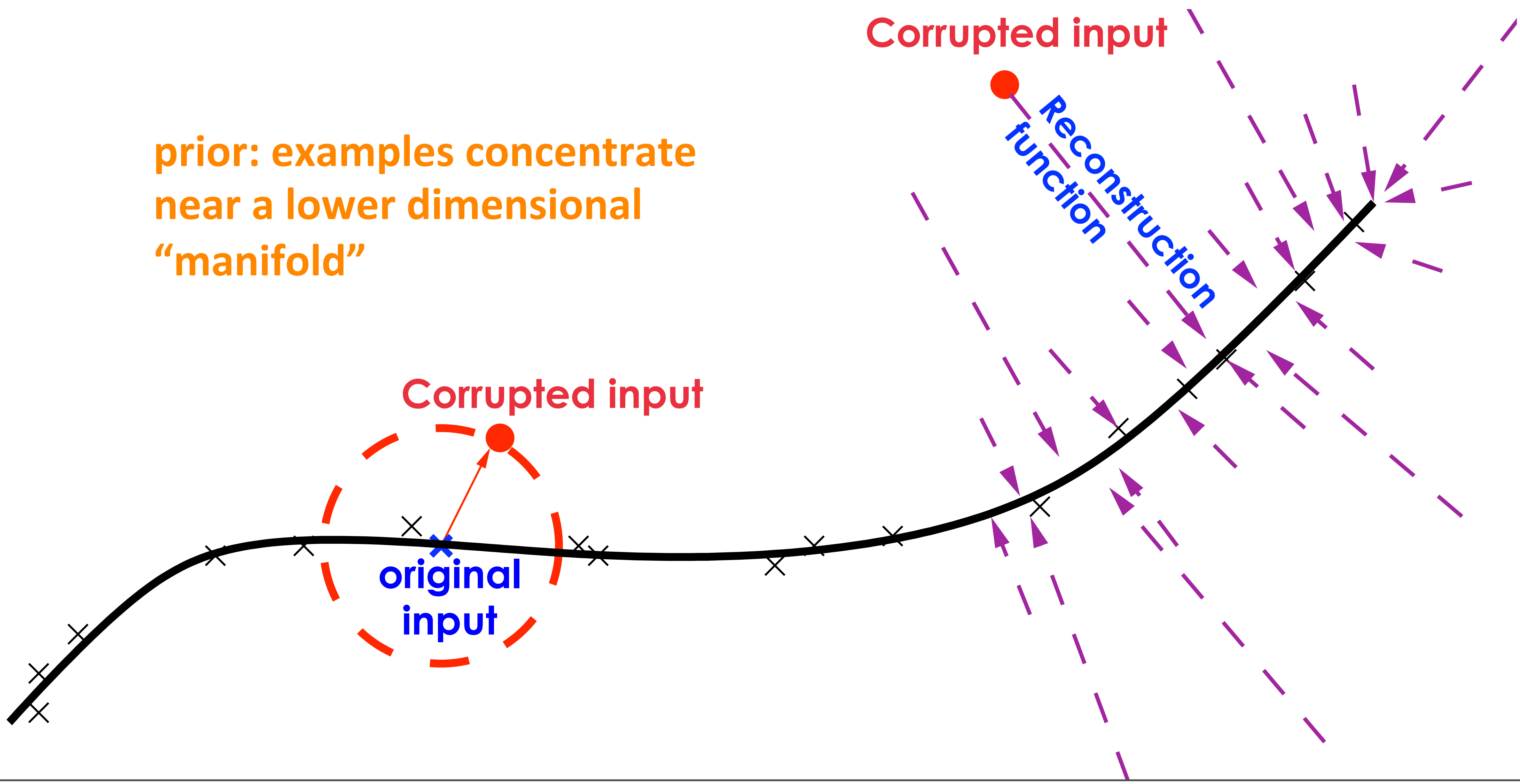
(d) Neuron A (0%, 10%, 20%, 50% corruption)



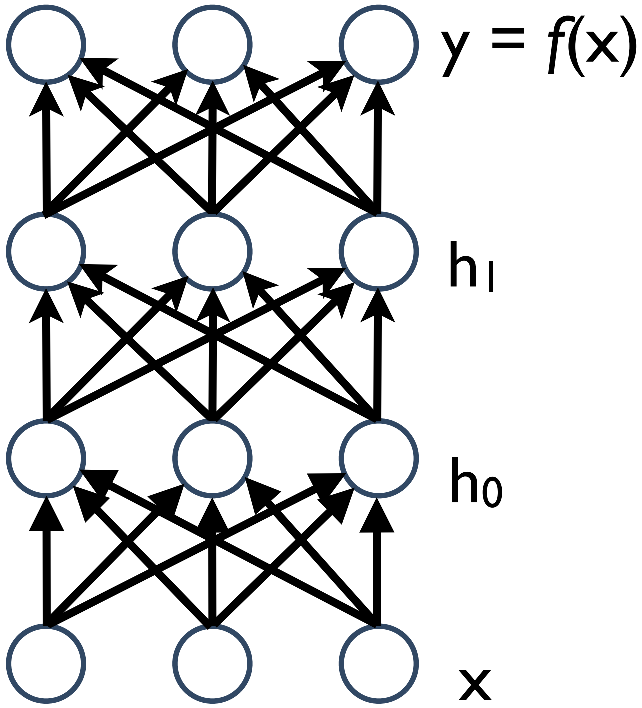
(e) Neuron B (0%, 10%, 20%, 50% corruption)

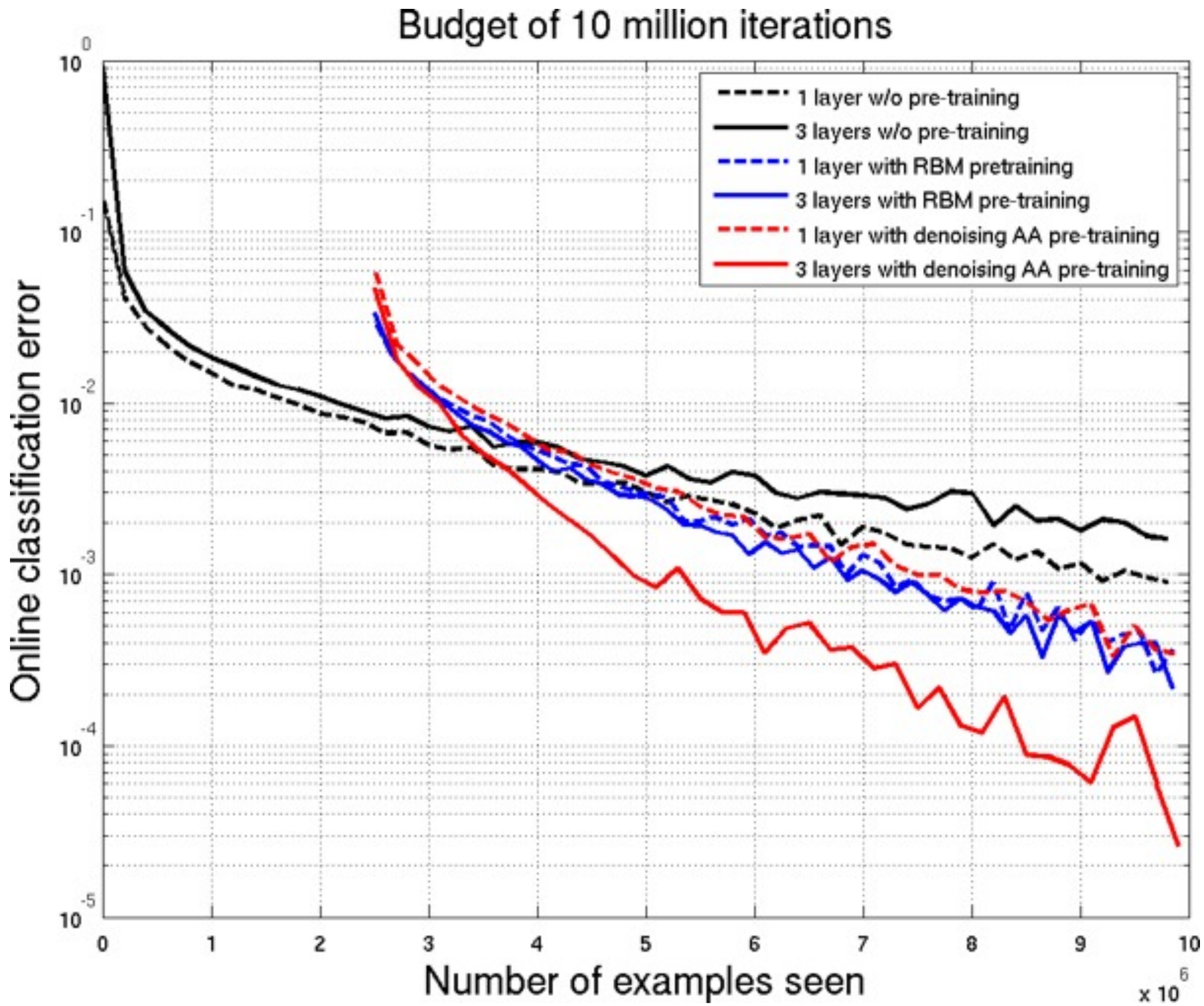
Denoising auto-encoders: manifold interpretation

- DAE learns to «project back» corrupted input onto manifold.
- Representation $h \approx$ location on the manifold



Stacked Denoising Auto-Encoders (SDAE)





Advantages over stacking RBMs

- No partition function, can measure training criterion
- Very flexible: encoder & decoder can use any parametrization (more layers...)
- Performs as well or better than stacking RBMs for usupervised pre-training

Infinite MNIST

Encouraging representation to be insensitive to corruption

- DAE encourages **reconstruction** to be insensitive to input corruption
- Alternative: encourage **representation** to be **insensitive**

$$\mathcal{J}_{\mathrm{SCAE}}(\theta) = \sum_{x \in D} \underbrace{L(x, g(h(x)))}_{\text{Reconstruction error}} + \underbrace{\lambda \mathbb{E}_{q(\tilde{x}|x)} \left[\| h(x) - h(\tilde{x}) \|^2 \right]}_{\text{stochastic regularization term}}$$

- Tied weights i.e. $W' = W^T$ prevent W from collapsing h to 0.

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Reconstruction error

stochastic regularization term

- Tied weights i.e. $W' = W^T$ prevent W from collapsing h to 0.

Stochastic regularization

From stochastic to analytic penalty

- SCAE stochastic regularization term: $\mathbb{E}_{q(\tilde{x}|x)}\left[\|h(x) - h(\tilde{x})\|^2\right]$
- For small additive noise $\tilde{x}|x = x + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma^2 I)$
- Taylor series expansion yields $h(x+\epsilon) = h(x) + \frac{\partial h}{\partial x}\epsilon + \ldots$
- It can be showed that

$$\underbrace{\mathbb{E}_{q(\tilde{x}|x)}\left[\|h(x) - h(\tilde{x})\|^2\right]}_{\substack{\text{stochastic} \\ \text{(SCAE)}}} \approx \underbrace{\sigma^2 \left\|\frac{\partial h}{\partial x}(x)\right\|_F^2}_{\substack{\text{analytic} \\ \text{(CAE)}}}$$

Contractive Auto-Encoder (CAE)

(Rifai, Vincent, Muller, Glorot, Bengio, ICML 2011)

- Minimize $$\mathcal{J}_{\mathrm{CAE}} = \sum_{x \in D}^{n} L(x, g(h(x))) + \lambda \left\| \frac{\partial h(x)}{\partial x} \right\|^2$$

Reconstruction error

analytic contractive term

- For training examples, encourages both:
  - ➡small reconstruction error
  - ➡representation insensitive to small variations around example

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Analytic regularization

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Computational considerations
CAE for a simple encoder layer

We defined $\mathbf{h} = h(\mathbf{x}) = s(\underbrace{Wx + b}_{a})$

Further suppose: s is an elementwise non-linearity
s' its first derivative.

Let $J(x) = \frac{\partial h}{\partial x}(x)$

$J_j = s'(b + x^T W_j) W_j$ where J_j and W_j represent j^th row

CAE penalty is: $\|J\|_F^2 = \sum_{j=1}^{d_h} s'(a_j)^2 \|W_j\|^2$

Compare to L2 weight decay: $\|W\|_F^2 = \sum_{j=1}^{d_h} \|W_j\|^2$

Same complexity: *O*(d_h *d*)

Gradient backprop wrt parameters: *O*(d_h *d*)

Higher order Contractive Auto-Encoder (CAE+H)

(Rifai, Mesnil, Vincent, Muller, Bengio, Dauphin, Glorot; ECML 2011)

- CAE penalizes Jacobian norm
- We could also penalize higher order derivatives
- Computationally too expensive: second derivative is a 3-tensor, ...
- **Stochastic approach for efficiency:**
  Encourage Jacobian at x and at $x+\varepsilon$ to be the same.

$$\mathcal{J}_{\mathrm{CAE+H}} = \sum_{x \in D}^{n} L(x, g(h(x))) + \lambda \left\| \frac{\partial h}{\partial x}(x) \right\|^2 + \gamma \mathbb{E}_{\epsilon \sim \mathcal{N}(0,\sigma^2)} \left[\left\| \frac{\partial h}{\partial x}(x) - \frac{\partial h}{\partial x}(x+\epsilon) \right\|^2 \right]$$

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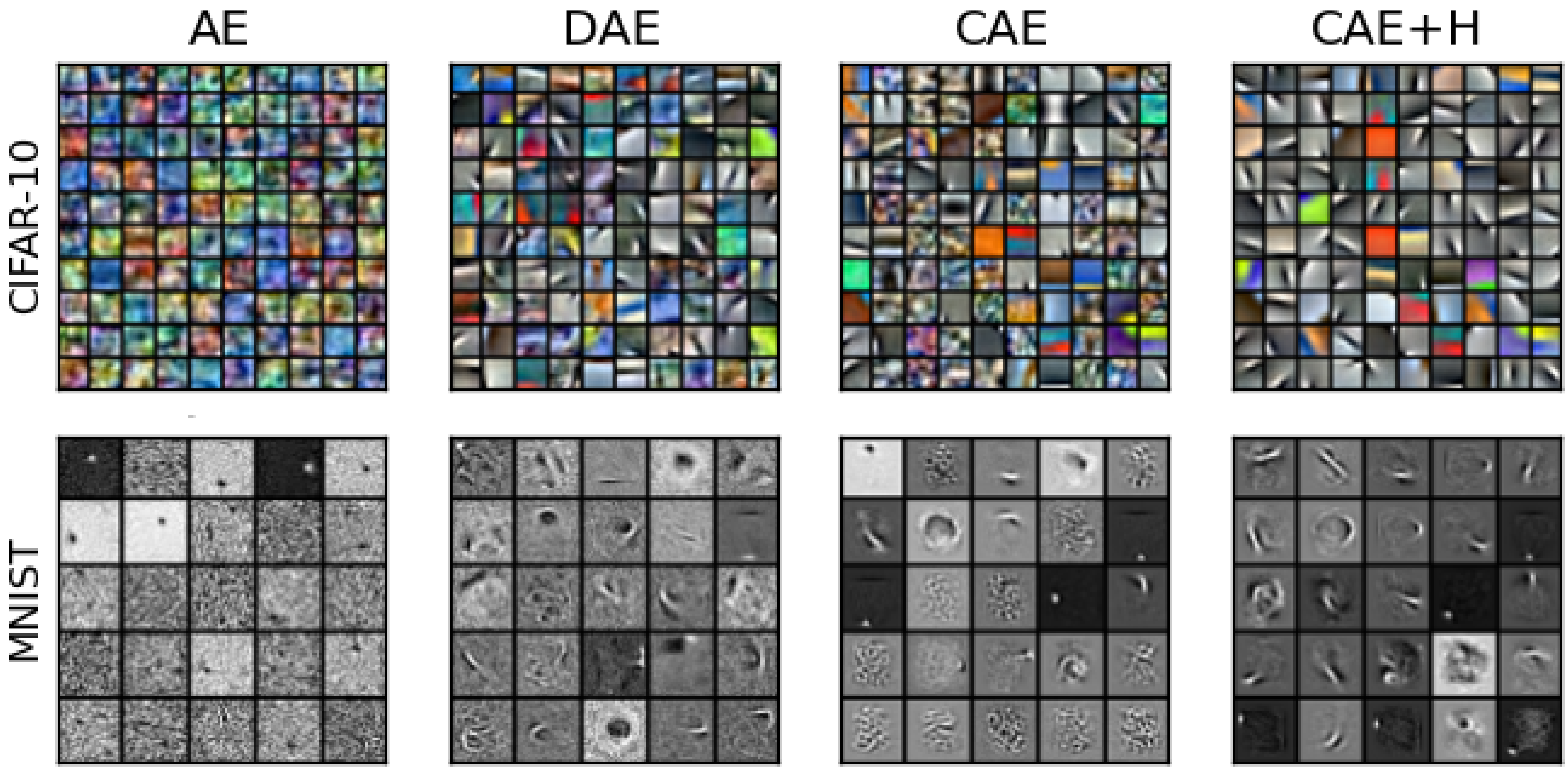
Stochastic
& analytic
regularization

Learned filters



CAE must capture manifold directions

$$\mathcal{J}_{\text{CAE}} = \sum_{x\in D}^{n} L(x, g(h(x))) + \lambda \left\| \frac{\partial h(x)}{\partial x} \right\|^2$$

Reconstruction $\Leftarrow$ **tradeoff** $\Rightarrow$ **Contraction**

(warning: may require tied weights)

pressure to be insensitive to ***all*** directions

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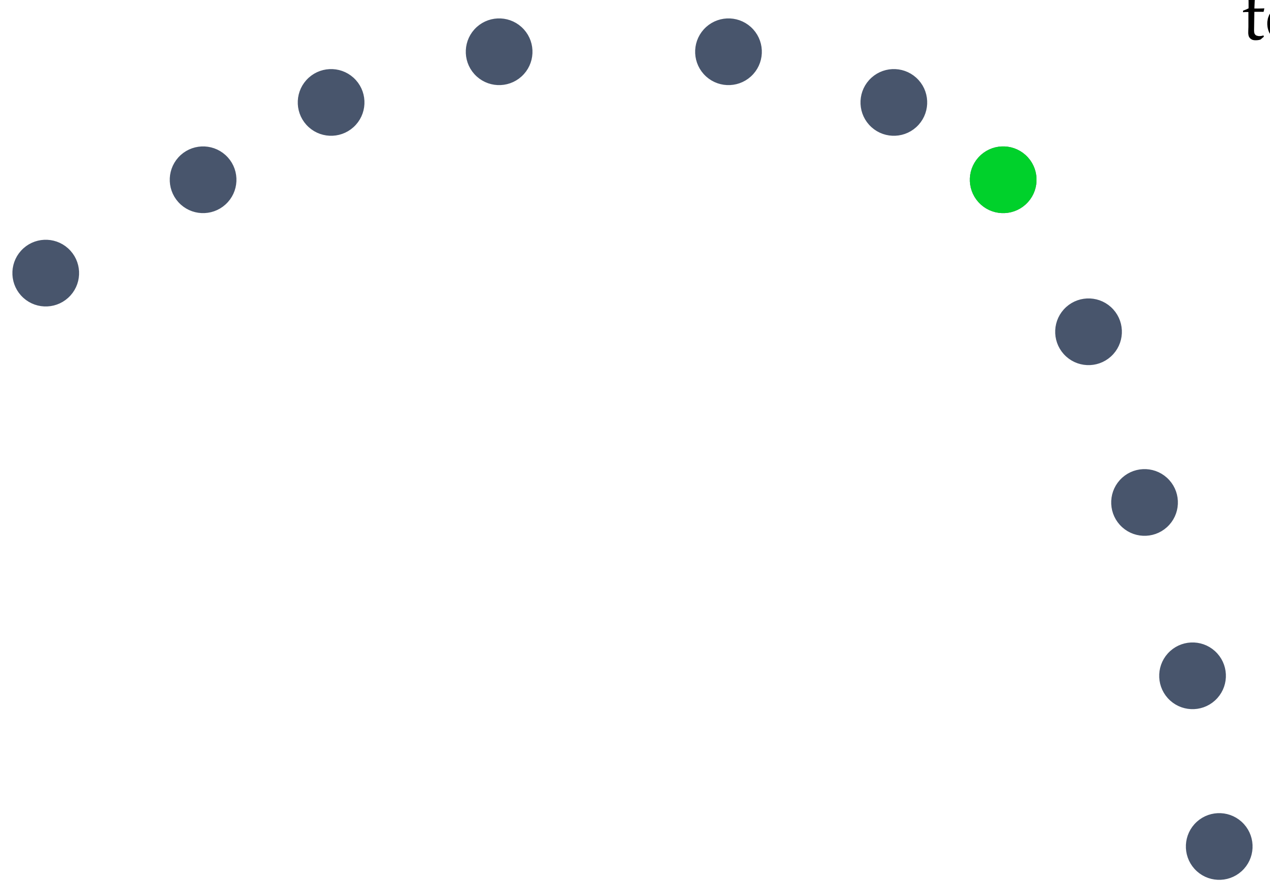

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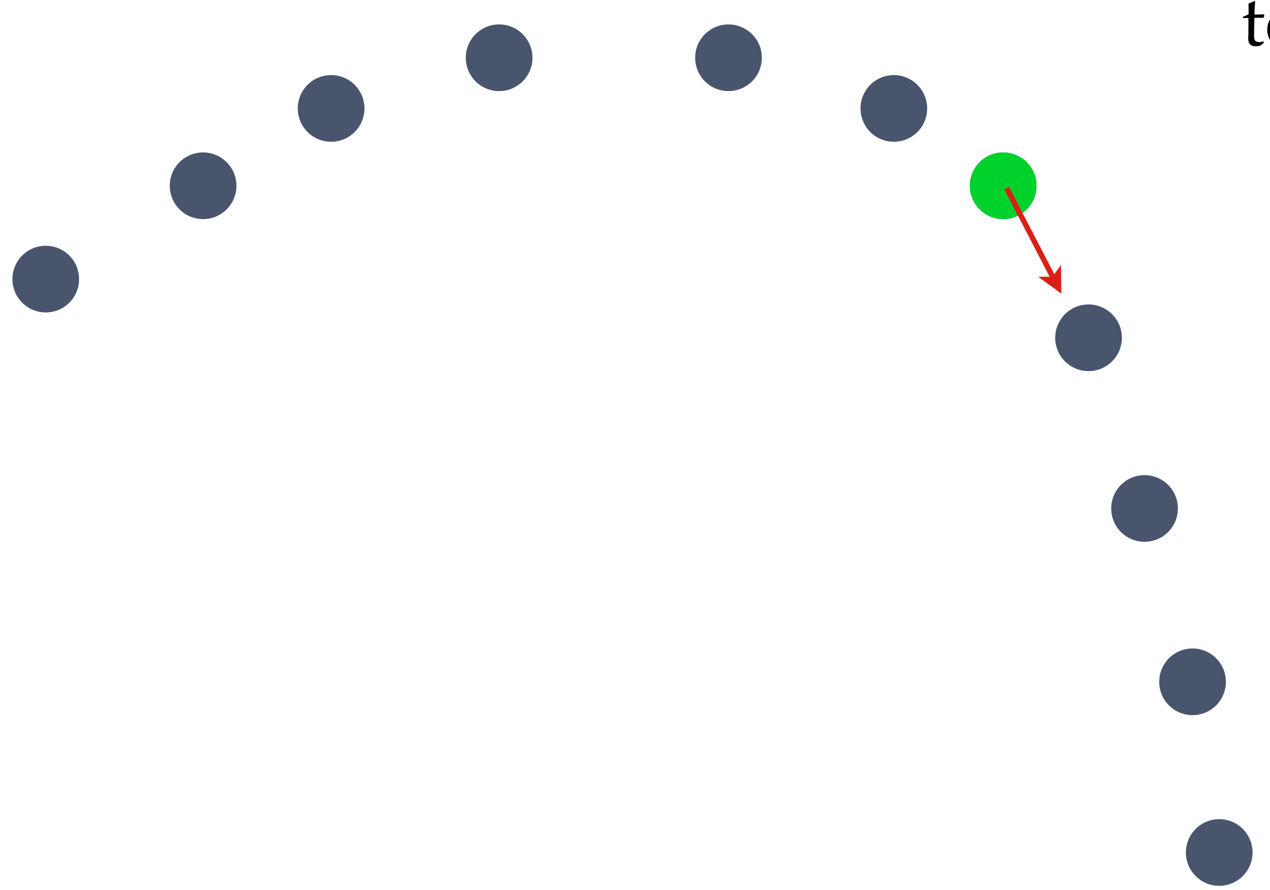

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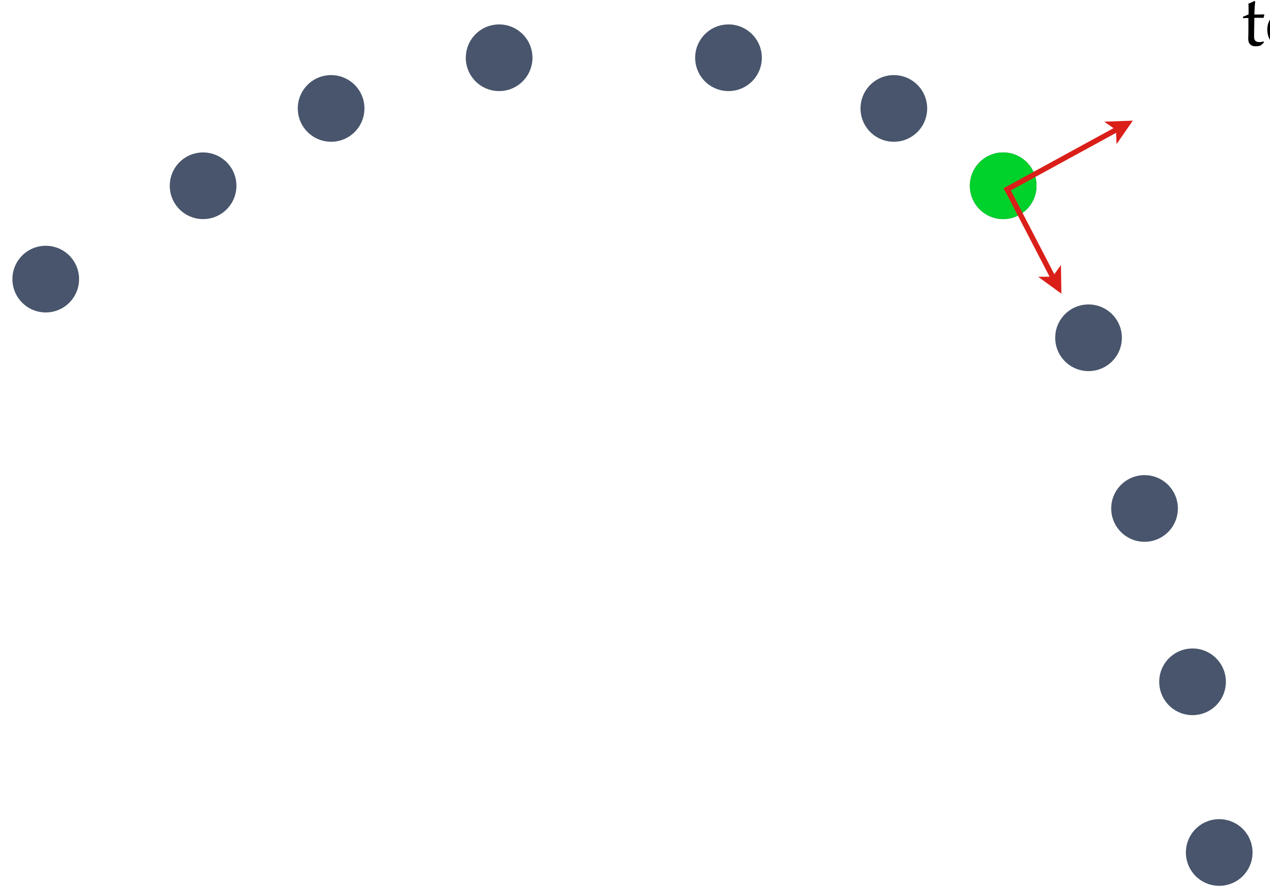

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Reconstruction

⇐ tradeoff ⇒

(warning: may require tied weights)

Contraction

pressure to be insensitive
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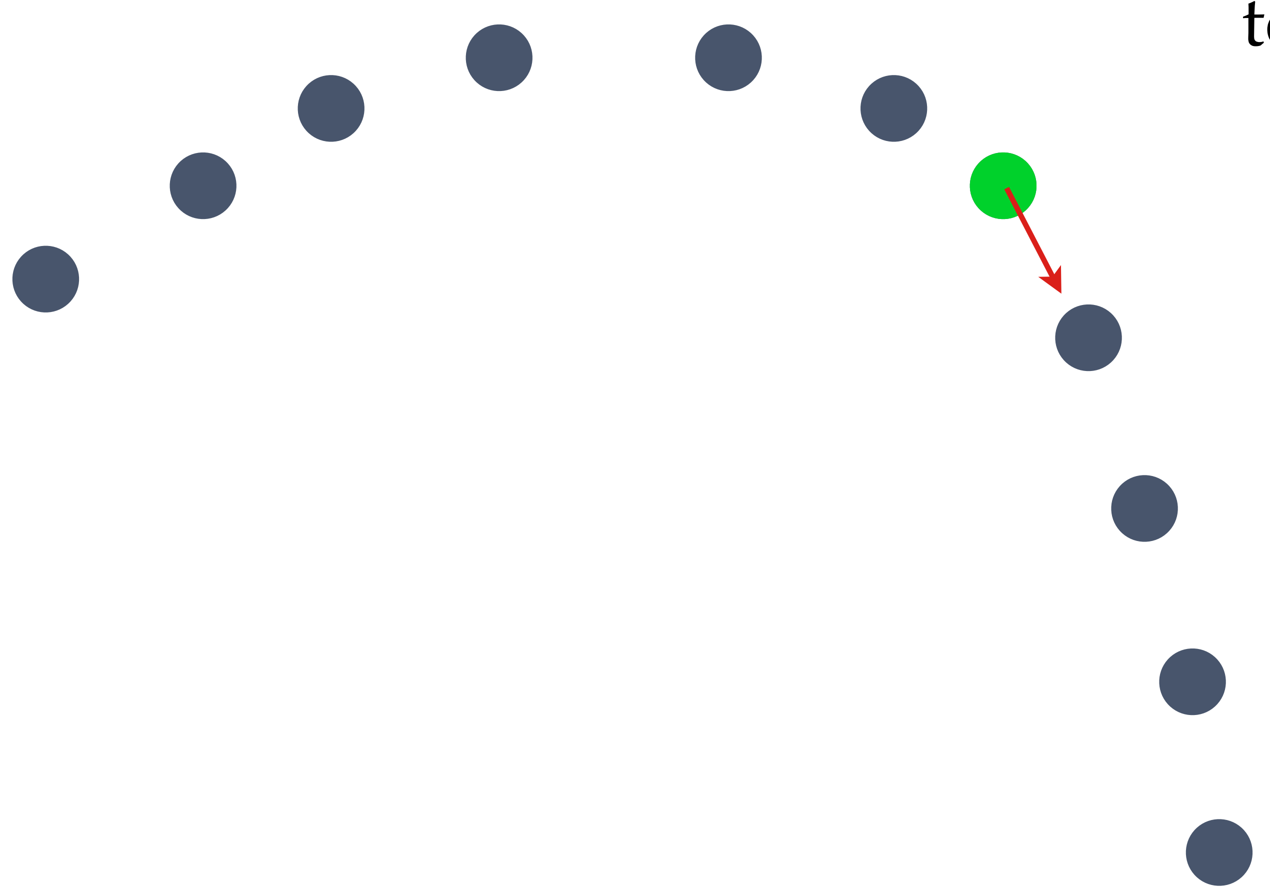

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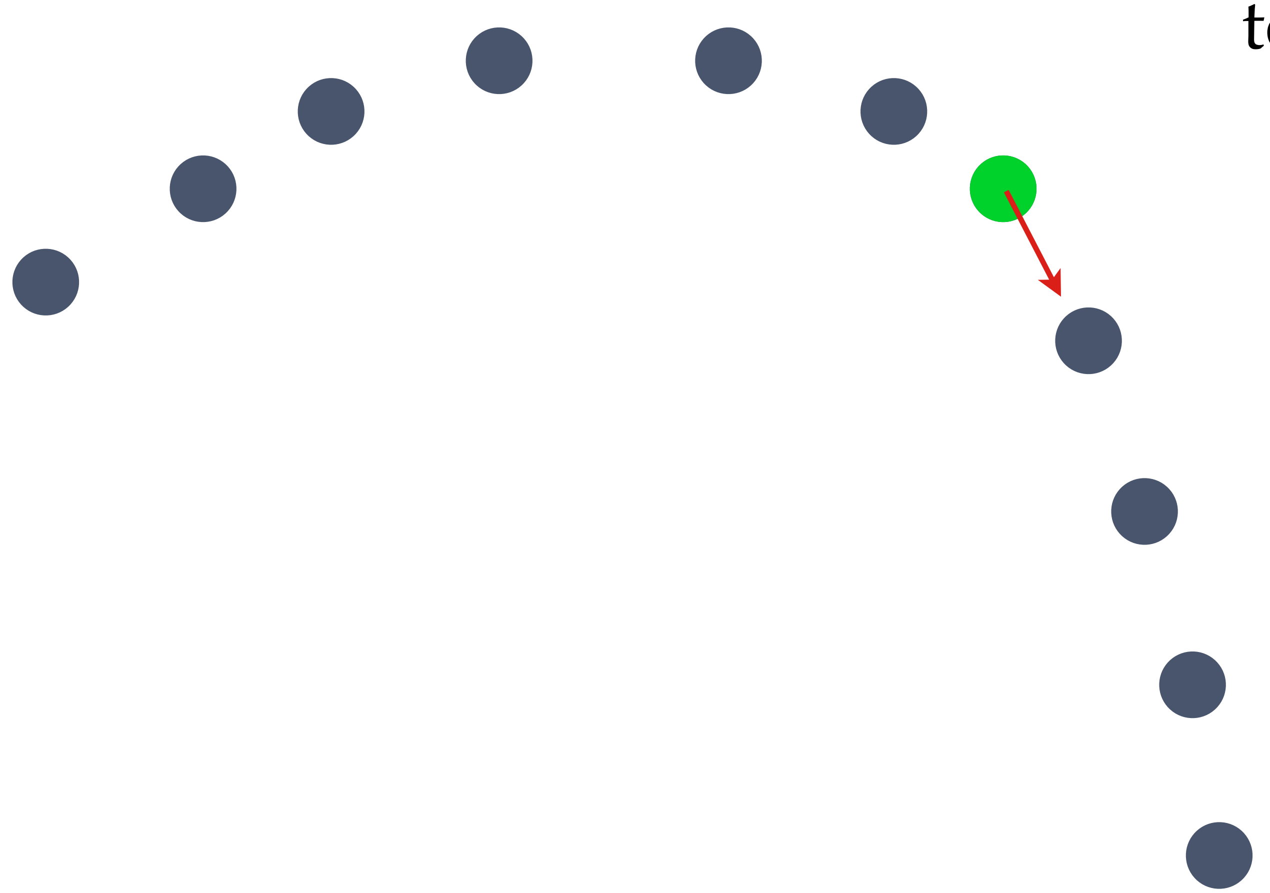


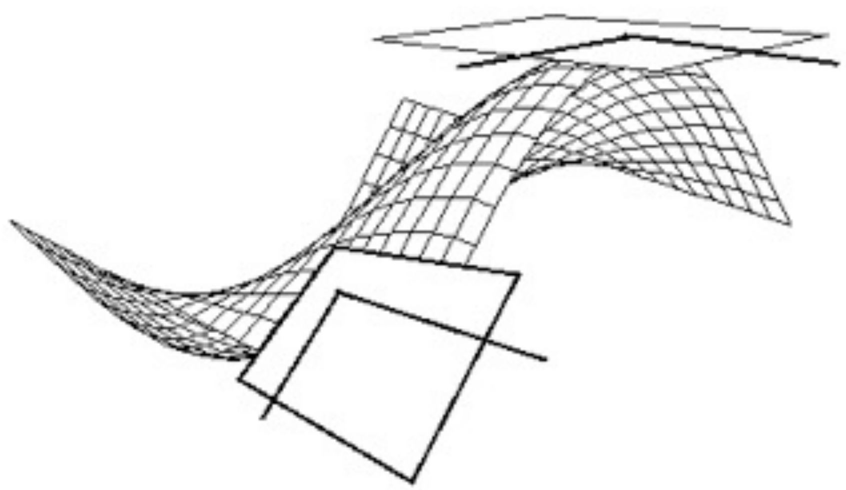
Learned tangent space

- Jacobian $J_h(x) = \frac{\partial h}{\partial x}(x)$ measures

sensitivity of h locally around x

SVD:

$$\frac{\partial h(\mathbf{x})}{\partial \mathbf{x}}^T = \mathbf{U}\mathbf{S}\mathbf{V}^T$$

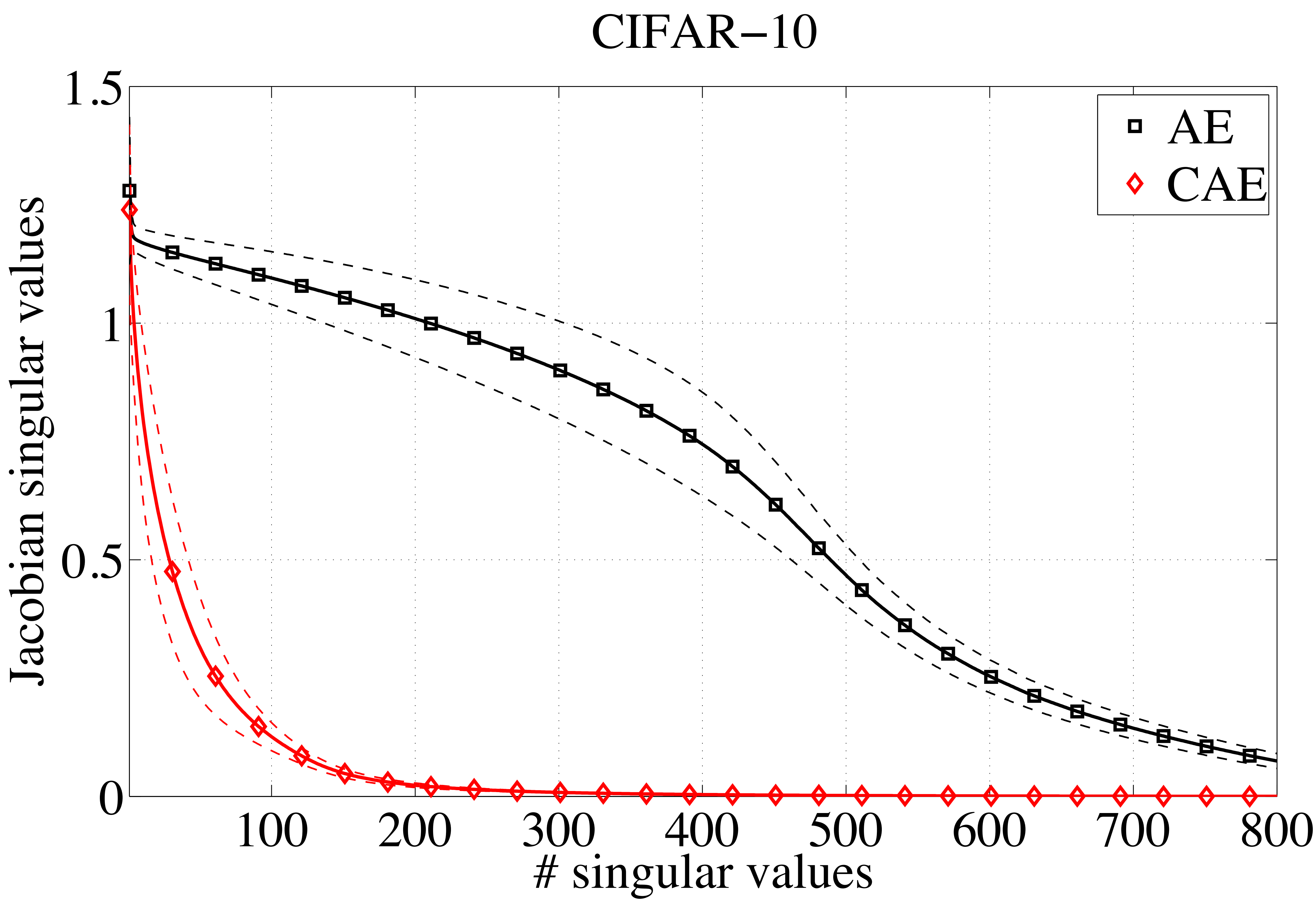


f

Top **singular vectors** are **tangent** directions to which h is most sensitive.

$$\mathbf{T}_x = \{\mathbf{U}_{\cdot k} | \mathbf{S}_{kk} > \epsilon\}$$

SVD of $J_h(x) = \frac{\partial h}{\partial x}(x)$

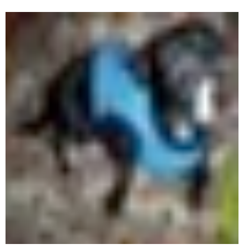


Learned tangents CIFAR-10

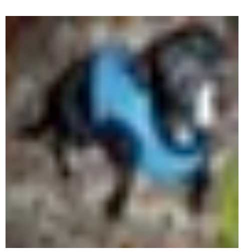
Input Point

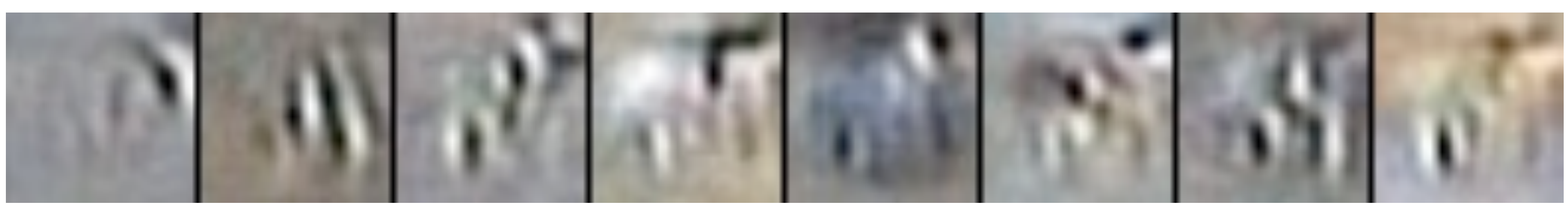
Tangents

Local PCA (as e.g. in Manifold Parzen)



Contractive Auto-Encoder (singular vectors of $J_h(x)$)





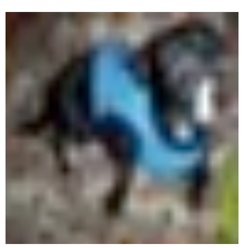
Not based on explicit neighbors or pairs of points!

Learned tange

Input Point

T

Local PCA (as e.g. in



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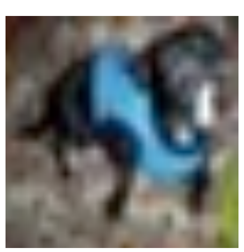
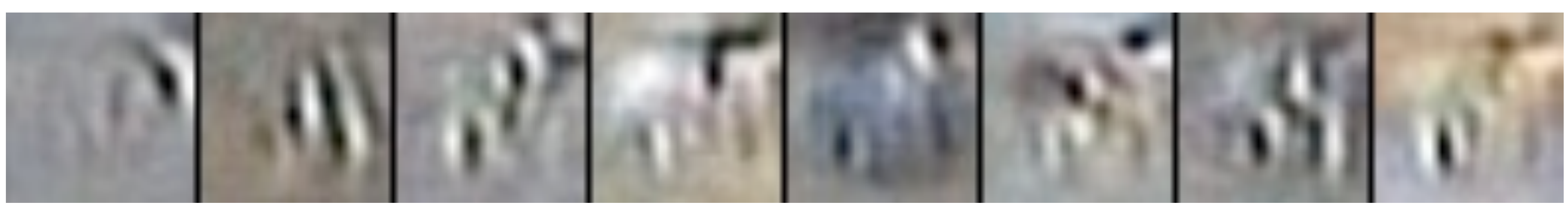
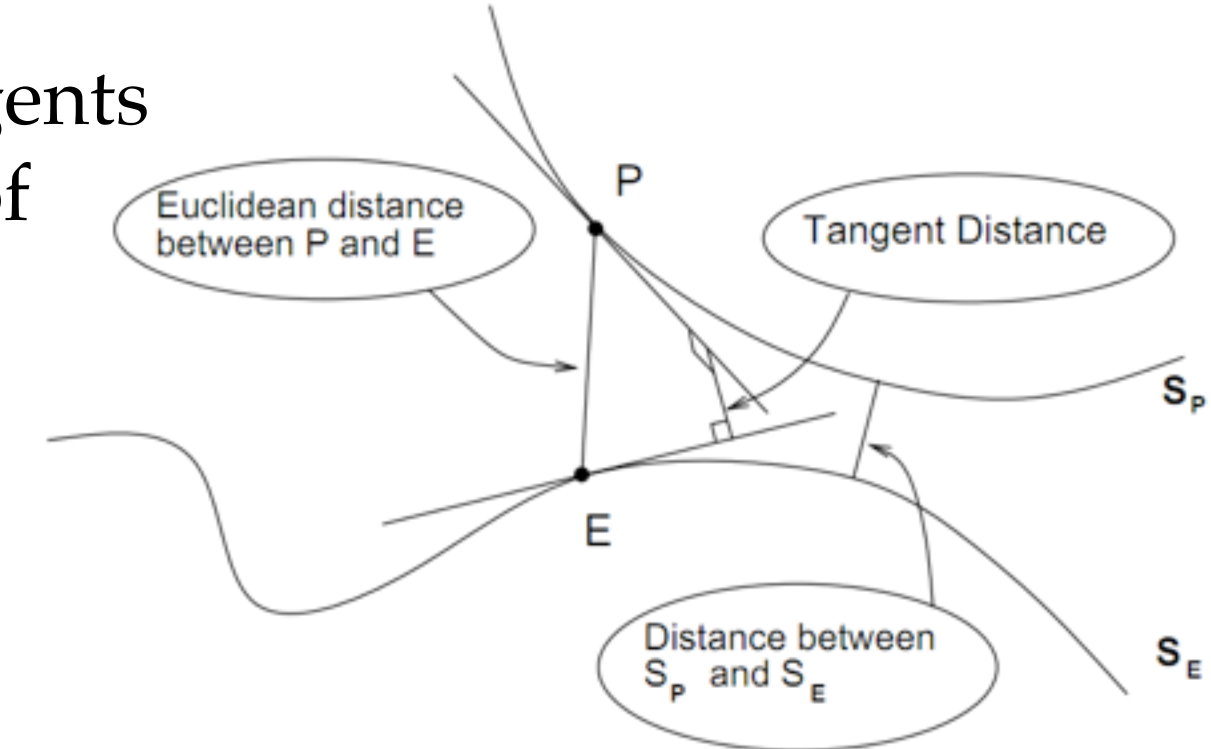




Not based on explicit neighbors or pairs of points!

How to leverage the learned tangents

- **Simard et al, 1993** exploited tangents derived from prior-knowledge of image deformations **we can use our learned tangents instead**.



- Use them to define **tangent distance** to use in your favorite distance (k-NN) or kernel-based classifier...

- Use them with **tangent propagation** when fine-tuning a deep-net classifier to make class prediction insensitive to tangent directions. (*Manifold Tangent Classifier*, Rifai et al. NIPS 2011) 0.81% on MNIST

- Moving preferably along tangents allows **efficient quality sampling**

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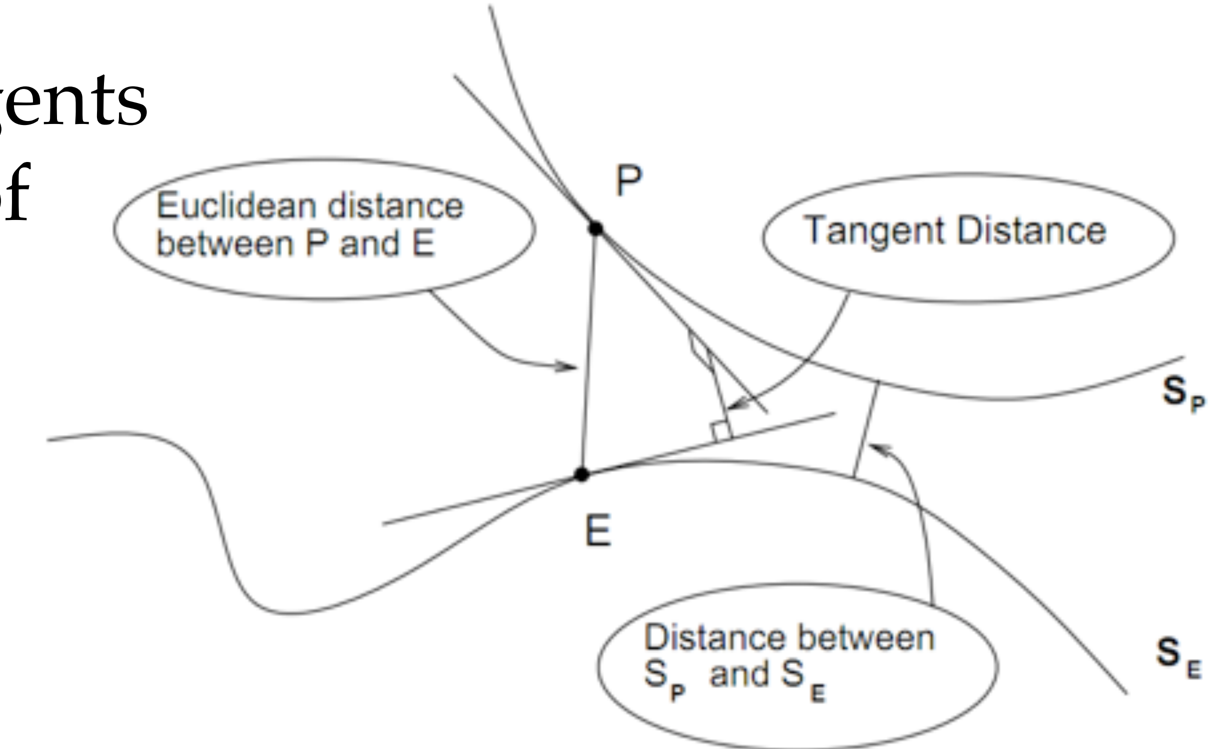

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Analytic v.s. stochastic ?

a) Analytic approximation of stochastic perturbation

- - Equiv. to tiny perturbations: does not probe far away
- + Potentially more efficient. Ex:
  CAE's Jacobian penalty probes sensitivity in all d directions in $O(d_h d)$
  With DAE or SCAE it would require encoding d corrupted inputs: $O(d_h d^2)$

b) Stochastic approximation of analytic criterion

- + can render practical otherwise computationally infeasible criteria
  Ex: CAE+H
- - less precise, more noisy

CAE+H actually leverages both

Score matching
(Hyvärinen 2005)

We want to learn a p.d.f. : $$p_\theta(x) = \frac{1}{Z(\theta)} e^{-E_\theta(x)}$$

with **intractable** partition function Z

Score matching: alternative inductive principle to max. likelihood

Find parameters that minimize objective:

$$J_{SM}(\theta) = \sum_{x \in D} \left(\left\| \frac{\partial E}{\partial x}(x) \right\|^2 - \sum_{i=1}^{d} \frac{\partial^2 E}{\partial x_i^2}(x) \right)$$

Score matching

my geometric interpretation

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$\|J_E(x)\|^2$

First derivative encouraged to be small: ensures training points stay close to local minima of E

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Laplacian

First derivative encouraged to be small: ensures training points stay close to local minima of E

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$\|J_E(x)\|^2$

Laplacian

$\mathrm{Tr}(H_E(x))$

First derivative encouraged to be small: ensures training points stay close to local minima of E

Encourage large positive curvature in all directions

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my geometric interpretation

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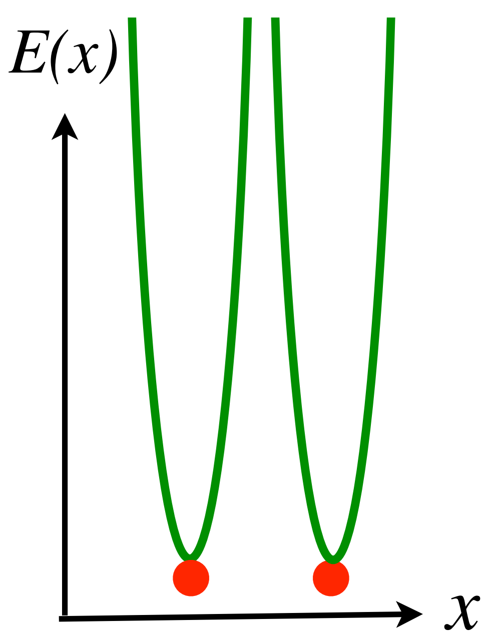
Encourage large positive curvature in all directions



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$\|J_E(x)\|^2$

Laplacian

$\mathrm{Tr}(H_E(x))$

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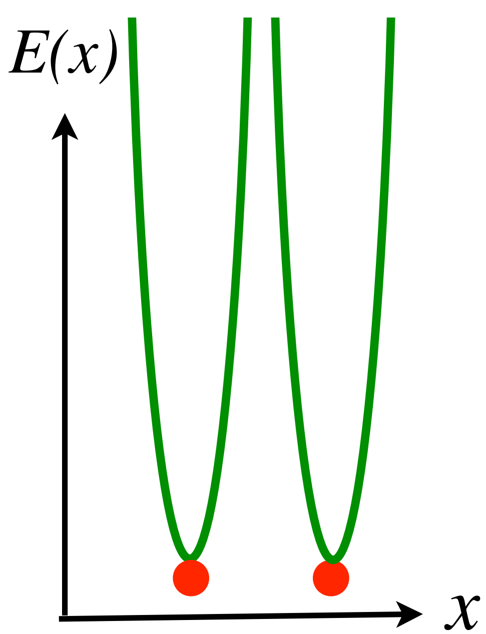
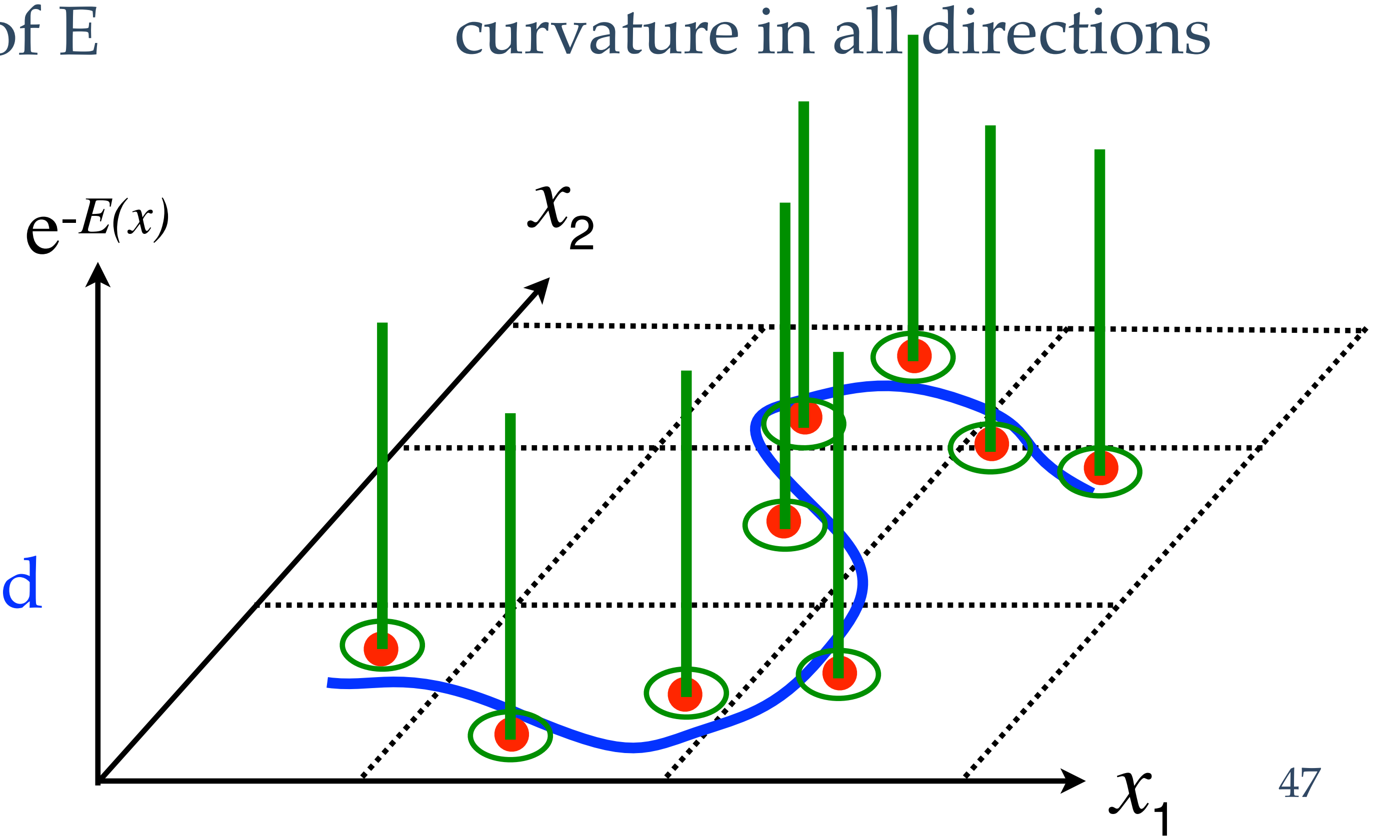


sharply peaked density



Score matching variants

Original score matching (Hyvärinen 2005):

$$J_{SM}(\theta) = \sum_{x \in D} \left(\frac{1}{2} \left\| \frac{\partial E}{\partial x}(x) \right\|^2 - \sum_{i=1}^{d} \frac{\partial^2 E}{\partial x_i^2}(x) \right)$$

Analytic

Regularized score matching (Kingma & LeCun 2010):

$$J_{SMreg,\lambda}(\theta) = J_{SM} + \sum_{x \in D} \lambda \sum_{i=1}^{d} \frac{\partial^2 E}{\partial x_i^2}(x)$$

Analytic

Denoising score matching (Vincent 2011)

$$J_{DSM,\sigma} = \sum_{x \in D} \left(\mathbf{E}_{\epsilon \sim \mathcal{N}(0,\sigma^2 I)} \left[\frac{1}{2} \left\| \frac{\partial E}{\partial x}(x+\epsilon) - \frac{1}{\sigma^2}\epsilon \right\|^2 \right] \right)$$

Stochastic

DAE training has a deeper relationsip to RBMs

- Same functional form as RBM:
  h(x) is expected hidden given visible
  g(**h**) is expected visible given hidden

- With linear reconstruction and squared error,
  DAE amounts to learning the following energy

$$E(\mathbf{x}; \underbrace{\mathbf{W}, \mathbf{b}, \mathbf{c}}_{\theta}) = -\frac{\langle \mathbf{c}, \mathbf{x} \rangle - \frac{1}{2} \|\mathbf{x}\|^2 + \sum_{j=1}^{d_h} \text{softplus}\left(\langle \mathbf{W}_j, \mathbf{x} \rangle + \mathbf{b}_j \right)}{\sigma^2}$$

  using the denoising score matching inductive principle.

- Above energy closely related to free energy of Gaussian-binary RBM (identical for σ=1)

Questions ?