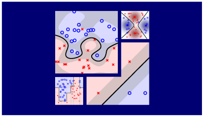
Machine Learning Techniques
(機器學習技法)



Lecture 13: Deep Learning

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Roadmap

1. Embedding Numerous Features: Kernel Models
2. Combining Predictive Features: Aggregation Models
3. Distilling Implicit Features: Extraction Models

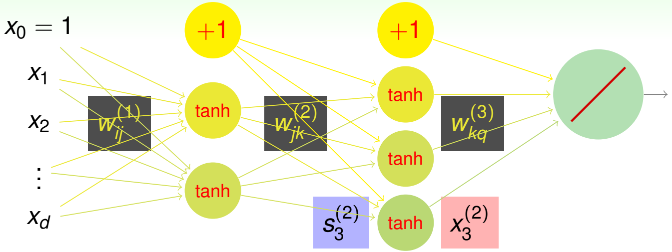
Lecture 12: Neural Network

automatic **pattern feature extraction** from **layers of neurons** with **backprop** for GD/SGD

Lecture 13: Deep Learning

- Deep Neural Network
- Autoencoder
- Denoising Autoencoder
- Principal Component Analysis

Physical Interpretation of NNet Revisited



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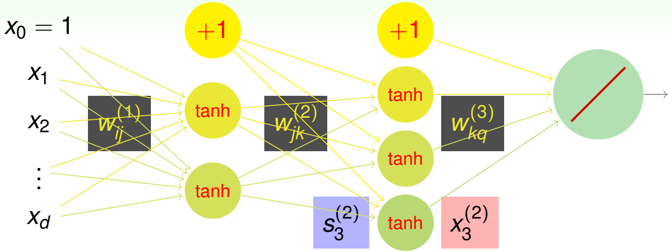

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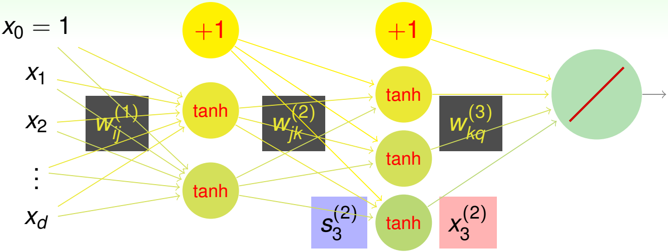

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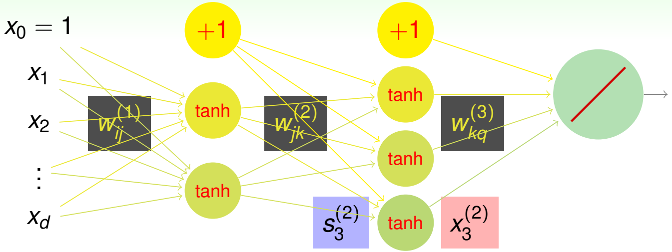

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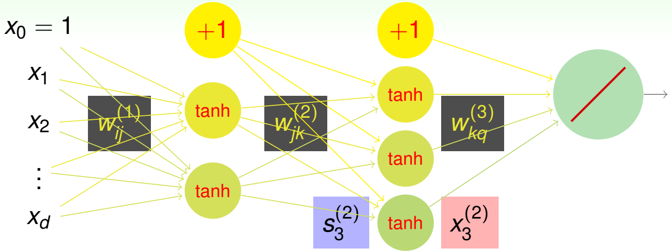

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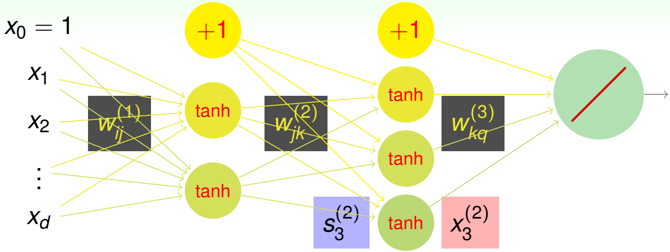

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structural decisions:
key issue for applying NNet

Shallow versus Deep Neural Networks

shallow: few (hidden) layers; deep: many layers

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deep NNet (**deep learning**)
gaining attention in recent years

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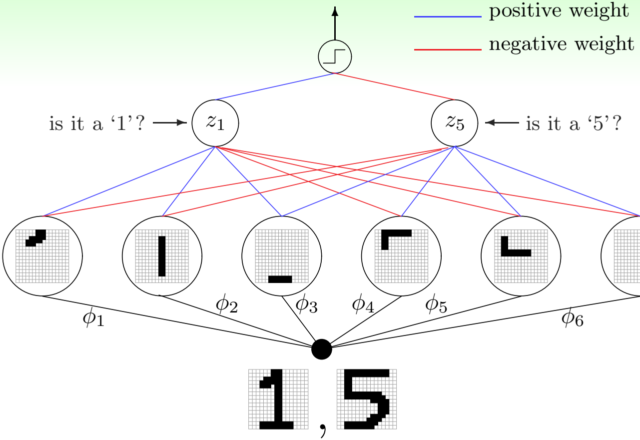

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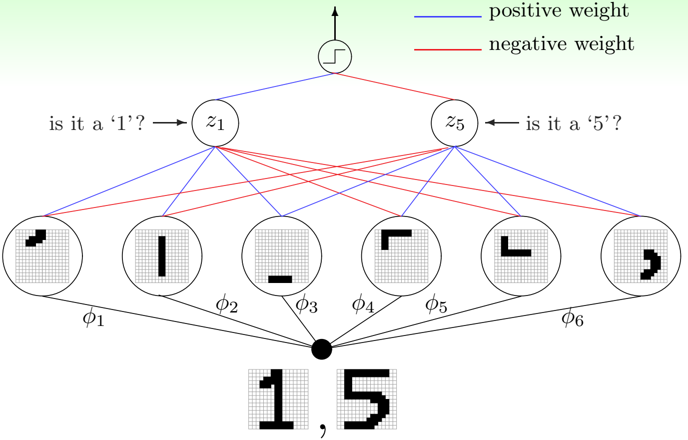

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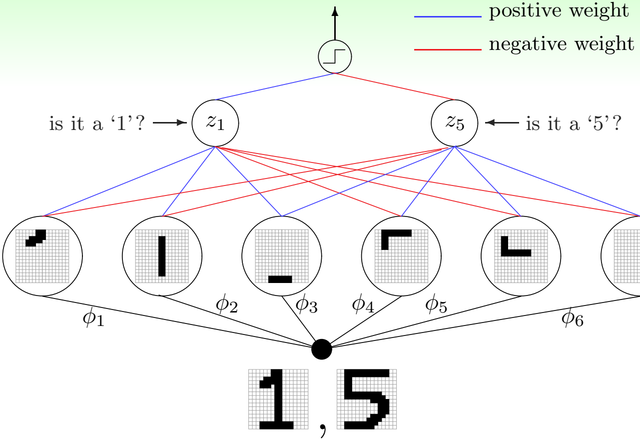

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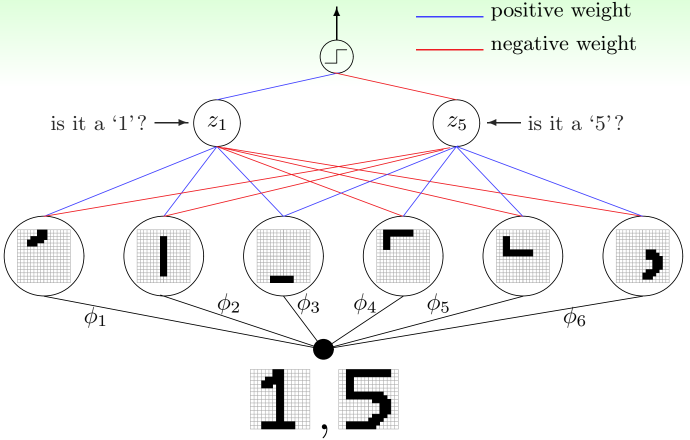

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deep NNet: currently popular in
vision/speech/...

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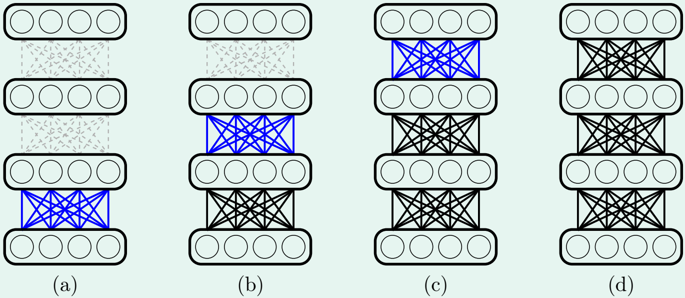
IMHO, careful **regularization** and **initialization** are key techniques

A Two-Step Deep Learning Framework

Simple Deep Learning

1. for $\ell = 1, \ldots, L$, **pre-train** $\left\{w_{ij}^{(\ell)}\right\}$ assuming $w_*^{(1)}, \ldots w_*^{(\ell-1)}$ fixed



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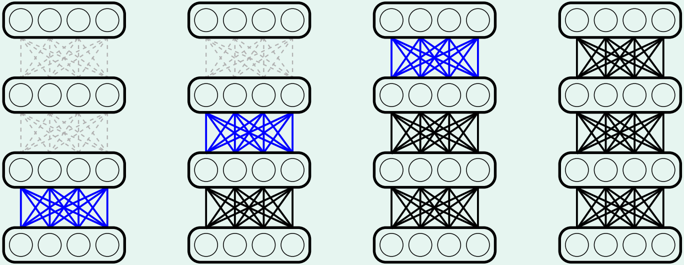

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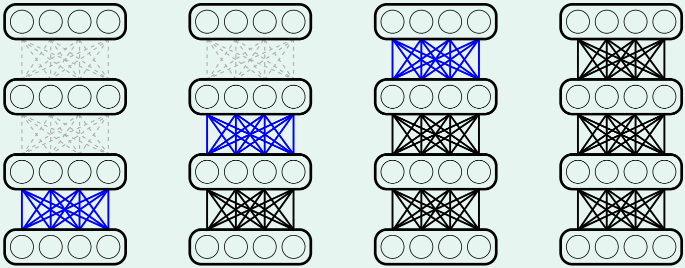

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will focus on **simplest pre-training** technique along with **regularization**

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1. pixels
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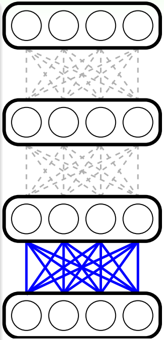
Reference Answer: 2

Simple strokes are likely the 'next-level' features that can be extracted from raw pixels.

Information-Preserving Encoding

- **weights**: feature transform, i.e. **encoding**



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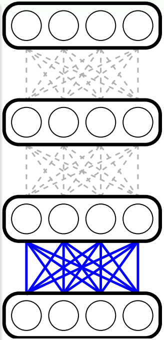

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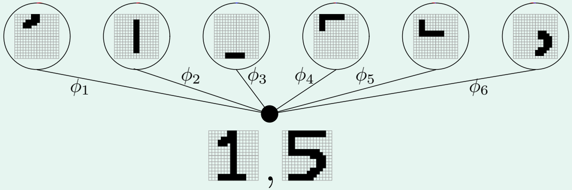

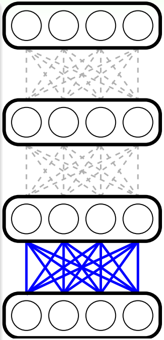

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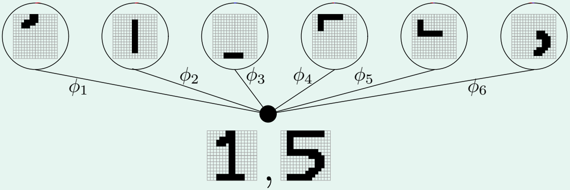
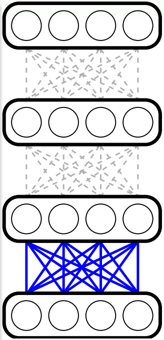
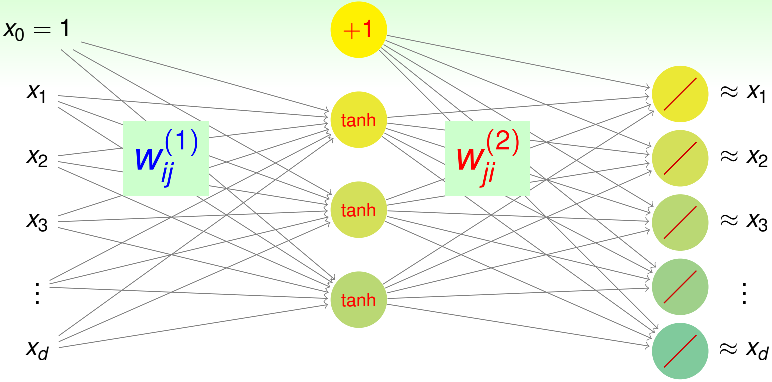




idea: **pre-train weights** towards
information-preserving encoding

Information-Preserving Neural Network



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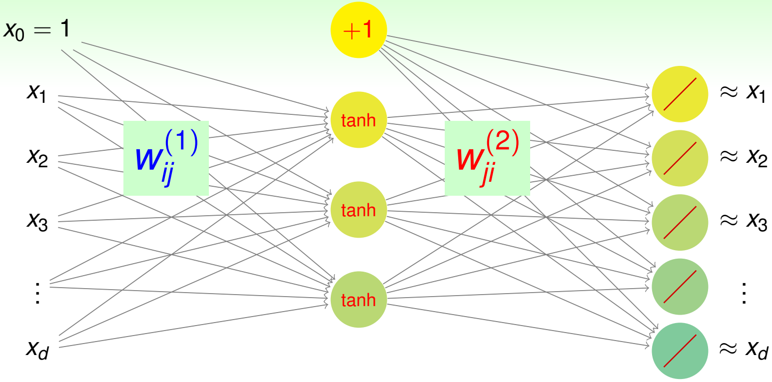

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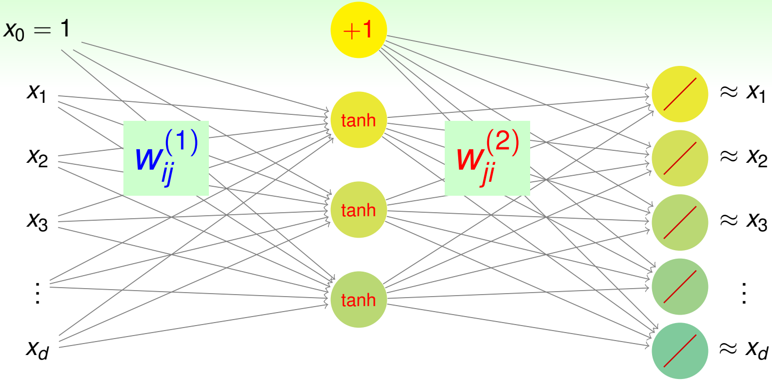

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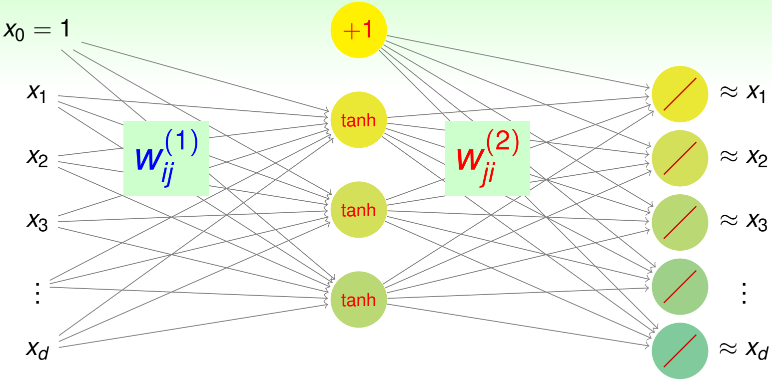

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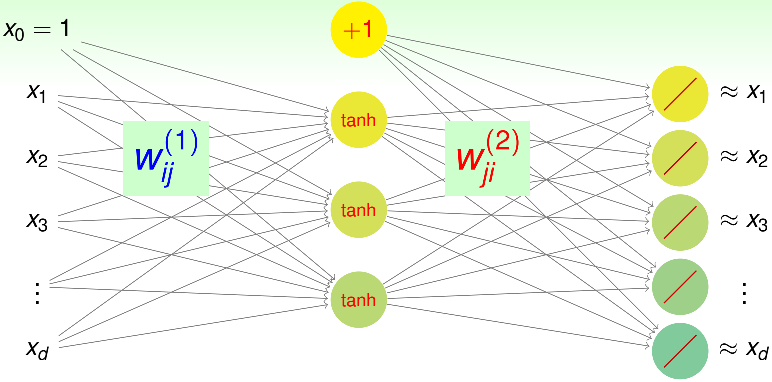

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why **approximating identity function**?

Usefulness of Approximating Identity Function

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- for supervised learning:

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autoencoder:

representation-learning through approximating identity function

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basic **autoencoder**:

d—$\tilde{d}$—d NNet with error function $\sum_{i=1}^{d}(g_i(\mathbf{x}) - x_i)^2$

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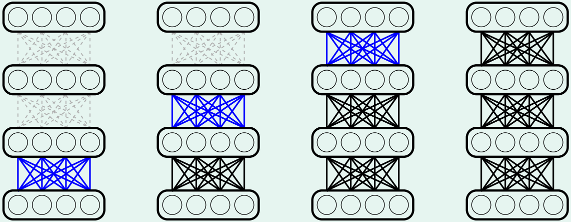
basic **autoencoder** in basic deep learning:
$\left\{w_{ij}^{(1)}\right\}$ taken as shallowly pre-trained weights

Pre-Training with Autoencoders

Deep Learning

1. for $\ell = 1, \ldots, L$, **pre-train** $\left\{ w_{ij}^{(\ell)} \right\}$ assuming $w_*^{(1)}, \ldots w_*^{(\ell-1)}$ fixed



(a) (b) (c) (d)

2. **train with backprop** on **pre-trained** NNet to **fine-tune** all $\left\{ w_{ij}^{(\ell)} \right\}$

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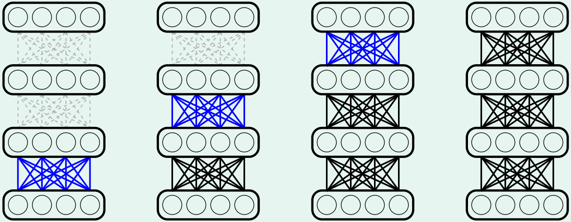

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by **training basic autoencoder on** $\left\{ \mathbf{x}_n^{(\ell-1)} \right\}$ **with** $\tilde{d} = d^{(\ell)}$

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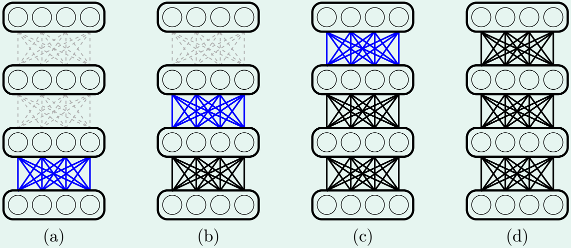

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many successful **pre-training** techniques take **'fancier' autoencoders** with different **architectures** and **regularization schemes**

Fun Time

Suppose training a d-$\tilde{d}$-d autoencoder with backprop takes approximately $c \cdot d \cdot \tilde{d}$ seconds. Then, what is the total number of seconds needed for pre-training a d-$d^{(1)}$-$d^{(2)}$-$d^{(3)}$-1 deep NNet?

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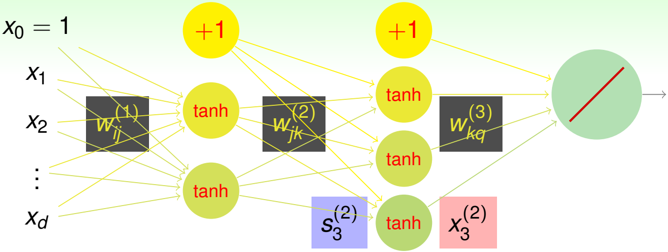
Reference Answer: 3

Each $c \cdot d^{(\ell-1)} \cdot d^{(\ell)}$ represents the time for pre-training with one autoencoder to determine one layer of the weights.

Regularization in Deep Learning



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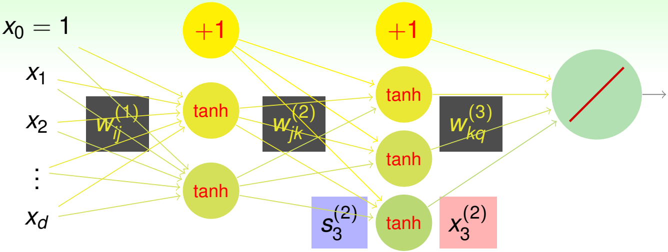

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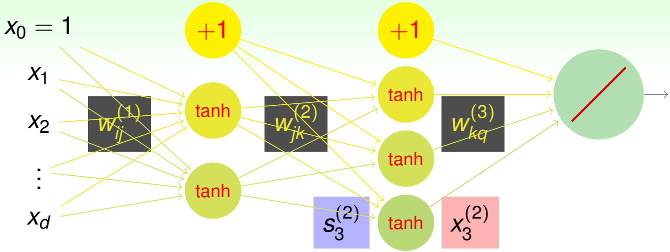

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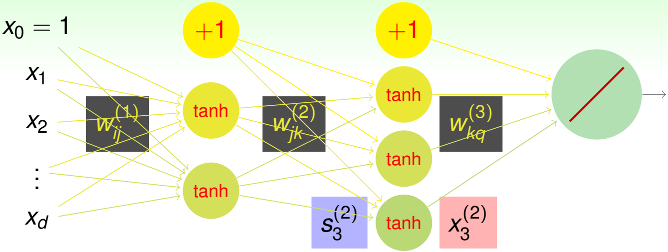

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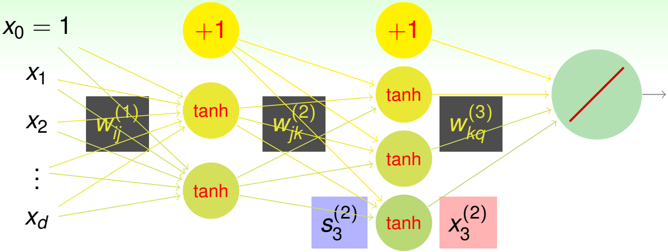

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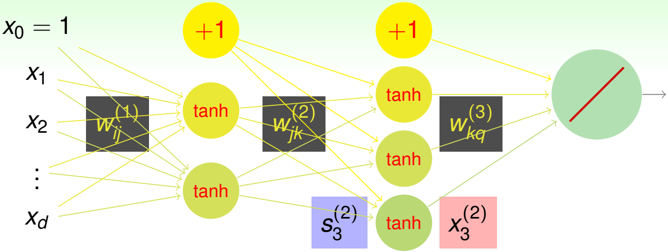

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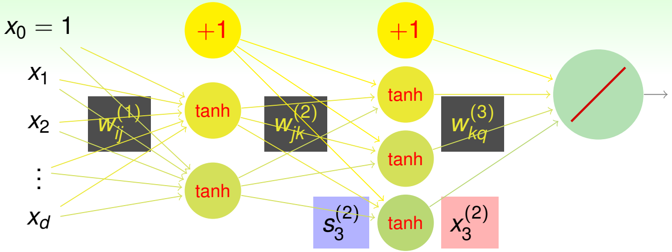

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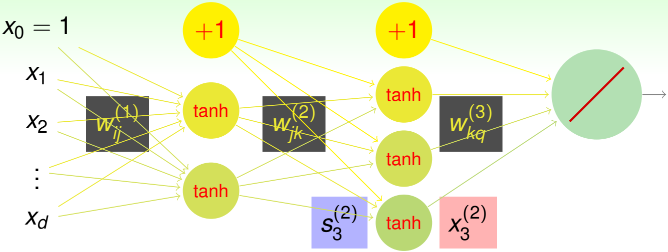

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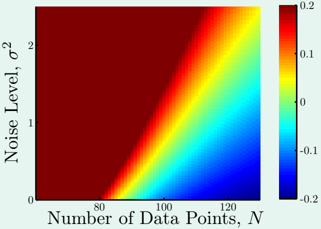
next: another **regularization** technique

Reasons of Overfitting Revisited

stochastic noise



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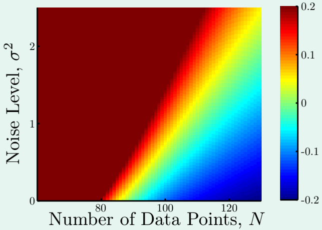

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how to deal with **noise**?

Dealing with Noise

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artificial noise/**hint** as **regularization**!
—practically also useful for other NNet/models

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Reference Answer: (4)

(1) is our new friend for regularization, while (2) and (3) are old friends.

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consider three special conditions:

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- $\mathrm{W}\mathrm{W}^T\mathbf{x}_n =$ $\mathbf{x}_n$

Linear Autoencoder Error Function

$$E_{\text{in}}(\mathbf{h}) = E_{\text{in}}(\mathrm{W}) = \frac{1}{N}\sum_{n=1}^{N}\left\|\mathbf{x}_n - \mathrm{W}\mathrm{W}^T\mathbf{x}_n\right\|^2 \text{ with } d \times \tilde{d} \text{ matrix } \mathrm{W}$$

—analytic solution to minimize E_{in}? but **4-th order polynomial of w_{ij}**

let's familiarize the problem with linear algebra (**be brave! :-)**)

- eigen-decompose $\mathrm{W}\mathrm{W}^T = \mathrm{V}\Gamma\mathrm{V}^T$
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  - $\mathrm{V}(\cdots)$: reconstruct by coefficients and basis (**back-rotate**)

Linear Autoencoder Error Function

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- $\mathbf{x}_n = \mathrm{V}\mathrm{I}\mathrm{V}^T\mathbf{x}_n$: **rotate** and **back-rotate** cancel out

next: minimize E_{in} **by optimizing Γ and V**

The Optimal Γ

$$\min_{\mathrm{V}} \min_{\Gamma} \frac{1}{N} \sum_{n=1}^{N} \left\| \underbrace{\mathrm{V}\mathrm{I}\mathrm{V}^T \mathbf{x}_n}_{\mathbf{x}_n} - \underbrace{\mathrm{V}\Gamma\mathrm{V}^T \mathbf{x}_n}_{\mathrm{W}\mathrm{W}^T \mathbf{x}_n} \right\|^2$$

- **back-rotate** not affecting length: ~~V~~

The Optimal Γ

$$\min_{\mathrm{V}} \min_{\Gamma} \frac{1}{N} \sum_{n=1}^{N} \left\| \underbrace{\mathrm{V}\mathrm{I}\mathrm{V}^T \mathbf{x}_n}_{\mathbf{x}_n} - \underbrace{\mathrm{V}\Gamma\mathrm{V}^T \mathbf{x}_n}_{\mathrm{W}\mathrm{W}^T \mathbf{x}_n} \right\|^2$$

- **back-rotate** not affecting length: ~~V~~
- $\min_{\Gamma} \sum \|(\mathrm{I} - \Gamma)(\text{some vector})\|^2$: **want many** within $(\mathrm{I} - \Gamma)$

The Optimal Γ

$$\min_{\mathrm{V}} \min_{\Gamma} \frac{1}{N} \sum_{n=1}^{N} \left\| \underbrace{\mathrm{V}\mathrm{I}\mathrm{V}^T \mathbf{x}_n}_{\mathbf{x}_n} - \underbrace{\mathrm{V}\Gamma\mathrm{V}^T \mathbf{x}_n}_{\mathrm{W}\mathrm{W}^T\mathbf{x}_n} \right\|^2$$

- **back-rotate** not affecting length: $\not{\mathrm{V}}$
- $\min_{\Gamma} \sum \|(\mathrm{I} - \Gamma)(\text{some vector})\|^2$: **want many** 0 within $(\mathrm{I} - \Gamma)$

The Optimal Γ

$$\min_{\mathrm{V}} \min_{\Gamma} \frac{1}{N} \sum_{n=1}^{N} \left\| \underbrace{\mathrm{V I V}^T \mathbf{x}_n}_{\mathbf{x}_n} - \underbrace{\mathrm{V} \Gamma \mathrm{V}^T \mathbf{x}_n}_{\mathrm{W W}^T \mathbf{x}_n} \right\|^2$$

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- optimal diagonal Γ with rank $\leq \tilde{d}$:

$$\left\{ \begin{array}{c} \tilde{d} \textbf{ diagonal components} \\ \text{other components} \end{array} \right\}$$

The Optimal Γ

$$\min_{\mathrm{V}} \min_{\Gamma} \frac{1}{N} \sum_{n=1}^{N} \left\| \underbrace{\mathrm{V}\mathrm{I}\mathrm{V}^T \mathbf{x}_n}_{\mathbf{x}_n} - \underbrace{\mathrm{V}\Gamma\mathrm{V}^T \mathbf{x}_n}_{\mathrm{W}\mathrm{W}^T \mathbf{x}_n} \right\|^2$$

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- optimal diagonal Γ with rank $\leq \tilde{d}$:

$$\left\{ \begin{array}{c} \tilde{d} \textbf{ diagonal components } 1 \\ \text{other components } 0 \end{array} \right\}$$

The Optimal Γ

$$\min_{\mathrm{V}} \min_{\Gamma} \frac{1}{N} \sum_{n=1}^{N} \left\| \underbrace{\mathrm{V}\mathrm{I}\mathrm{V}^T \mathbf{x}_n}_{\mathbf{x}_n} - \underbrace{\mathrm{V}\Gamma\mathrm{V}^T \mathbf{x}_n}_{\mathrm{W}\mathrm{W}^T \mathbf{x}_n} \right\|^2$$

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$$\left\{ \begin{array}{c} \tilde{d} \textbf{ diagonal components } 1 \\ \text{other components } 0 \end{array} \right\} \Longrightarrow \text{without loss of gen.} \begin{bmatrix} \mathrm{I}_{\tilde{d}} & 0 \\ 0 & 0 \end{bmatrix}$$

The Optimal Γ

$$\min_{\mathrm{V}} \min_{\Gamma} \frac{1}{N} \sum_{n=1}^{N} \left\| \underbrace{\mathrm{V}\mathrm{I}\mathrm{V}^T \mathbf{x}_n}_{\mathbf{x}_n} - \underbrace{\mathrm{V}\Gamma\mathrm{V}^T \mathbf{x}_n}_{\mathrm{W}\mathrm{W}^T \mathbf{x}_n} \right\|^2$$

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$$\text{next: } \min_{\mathrm{V}} \sum_{n=1}^{N} \left\| \underbrace{\begin{bmatrix} 0 & 0 \\ 0 & \mathrm{I}_{d-\tilde{d}} \end{bmatrix}}_{\mathrm{I}-\text{optimal } \Gamma} \mathrm{V}^T \mathbf{x}_n \right\|^2$$

The Optimal V

$$\min_{\mathrm{V}} \sum_{n=1}^{N} \left\| \begin{bmatrix} 0 & 0 \\ 0 & \mathrm{I}_{d-\tilde{d}} \end{bmatrix} \mathrm{V}^T \mathbf{x}_n \right\|^2 \equiv \max_{\mathrm{V}} \sum_{n=1}^{N} \left\| \begin{bmatrix} \quad & \quad \end{bmatrix} \mathrm{V}^T \mathbf{x}_n \right\|^2$$

The Optimal V

$$\min_{\mathrm{V}} \sum_{n=1}^{N} \left\| \begin{bmatrix} 0 & 0 \\ 0 & \mathrm{I}_{d-\tilde{d}} \end{bmatrix} \mathrm{V}^T \mathbf{x}_n \right\|^2 \equiv \max_{\mathrm{V}} \sum_{n=1}^{N} \left\| \begin{bmatrix} \mathrm{I}_{\tilde{d}} & 0 \\ 0 & 0 \end{bmatrix} \mathrm{V}^T \mathbf{x}_n \right\|^2$$

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- $\tilde{d} = 1$: only first row $\mathbf{v}^T$ of V^T matters

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  $\max_{\mathbf{v}} \sum_{n=1}^{N} \mathbf{v}^T \mathbf{x}_n \mathbf{x}_n^T \mathbf{v}$ subject to

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$$\max_{\mathbf{v}} \sum_{n=1}^{N} \mathbf{v}^T \mathbf{x}_n \mathbf{x}_n^T \mathbf{v} \text{ subject to } \mathbf{v}^T \mathbf{v} = 1$$

The Optimal V

$$\min_{\mathrm{V}} \sum_{n=1}^{N} \left\| \begin{bmatrix} 0 & 0 \\ 0 & \mathrm{I}_{d-\tilde{d}} \end{bmatrix} \mathrm{V}^T \mathbf{x}_n \right\|^2 \equiv \max_{\mathrm{V}} \sum_{n=1}^{N} \left\| \begin{bmatrix} \mathrm{I}_{\tilde{d}} & 0 \\ 0 & 0 \end{bmatrix} \mathrm{V}^T \mathbf{x}_n \right\|^2$$

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  - optimal $\mathbf{v}$ satisfies $\sum_{n=1}^{N} \mathbf{x}_n \mathbf{x}_n^T \mathbf{v} = \lambda \mathbf{v}$

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    —using Lagrange multiplier λ, remember? :-)

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  - optimal $\mathbf{v}$: eigenvector of $\mathrm{X}^T\mathrm{X}$

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  - optimal $\mathbf{v}$: 'topmost' eigenvector of $\mathrm{X}^T \mathrm{X}$

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- general $\tilde{d}$: $\{\mathbf{v}_j\}_{j=1}^{\tilde{d}}$ 'topmost' eigenvector**S** of $\mathrm{X}^T\mathrm{X}$

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  —optimal $\{\mathbf{w}_j\} = \{\mathbf{v}_j$ with $[\![\gamma_j = 1]\!]\}$ = **top eigenvectors**

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linear autoencoder: projecting to orthogonal patterns $\mathbf{w}_j$ **that 'matches' $\{\mathbf{x}_n\}$ most**

Principal Component Analysis

Linear Autoencoder

2. calculate $\tilde{d}$ top eigenvectors $\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_{\tilde{d}}$ of $\mathrm{X}^T\mathrm{X}$

- linear autoencoder:
  maximize $\sum$(maginitude after projection)^2

Principal Component Analysis

Linear Autoencoder

2. calculate $\tilde{d}$ top eigenvectors $\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_{\tilde{d}}$ of $\mathrm{X}^T\mathrm{X}$
3. return feature transform $\mathbf{\Phi}(\mathbf{x}) = \mathrm{W}(\mathbf{x} \quad)$

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Principal Component Analysis

Linear Autoencoder

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- principal component analysis (PCA) from statistics:
  maximize $\sum$(variance after projection)

Principal Component Analysis

Linear Autoencoder or **PCA**

1. let $\bar{\mathbf{x}} = \frac{1}{N}\sum_{n=1}^{N} \mathbf{x}_n$, and let $\mathbf{x}_n \leftarrow \mathbf{x}_n - \bar{\mathbf{x}}$
2. calculate $\tilde{d}$ top eigenvectors $\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_{\tilde{d}}$ of $\mathrm{X}^T\mathrm{X}$
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- both useful for **linear dimension reduction**

though PCA more popular

Principal Component Analysis

Linear Autoencoder or **PCA**

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- principal component analysis (PCA) from statistics:
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- both useful for **linear dimension reduction**
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linear dimension reduction:
useful for **data processing**

Fun Time

When solving the optimization problem

$$\max_{\mathbf{v}} \sum_{n=1}^{N} \mathbf{v}^T \mathbf{x}_n \mathbf{x}_n^T \mathbf{v} \text{ subject to } \mathbf{v}^T \mathbf{v} = 1,$$

we know that the optimal $\mathbf{v}$ is the 'topmost' eigenvector that corresponds to the 'topmost' eigenvalue λ of $\mathrm{X}^T\mathrm{X}$. Then, what is the optimal objective value of the optimization problem?

1. λ^1
2. λ^2
3. λ^3
4. λ^4

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Reference Answer: 1

The objective value of the optimization problem is simply $\mathbf{v}^T\mathrm{X}^T\mathrm{X}\mathbf{v}$, which is $\lambda\mathbf{v}^T\mathbf{v}$ and you know what $\mathbf{v}^T\mathbf{v}$ must be.

Summary

1. Embedding Numerous Features: Kernel Models
2. Combining Predictive Features: Aggregation Models
3. Distilling Implicit Features: Extraction Models

Lecture 13: Deep Learning

- Deep Neural Network

  difficult hierarchical feature extraction problem
- Autoencoder

  unsupervised NNet learning of representation
- Denoising Autoencoder

  using noise as hints for regularization
- Principal Component Analysis

  linear autoencoder variant for data processing

- **next: extracting 'prototype' instead of pattern**