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Neural Networks

Lecture 9

Expansion of hidden-layer dimension

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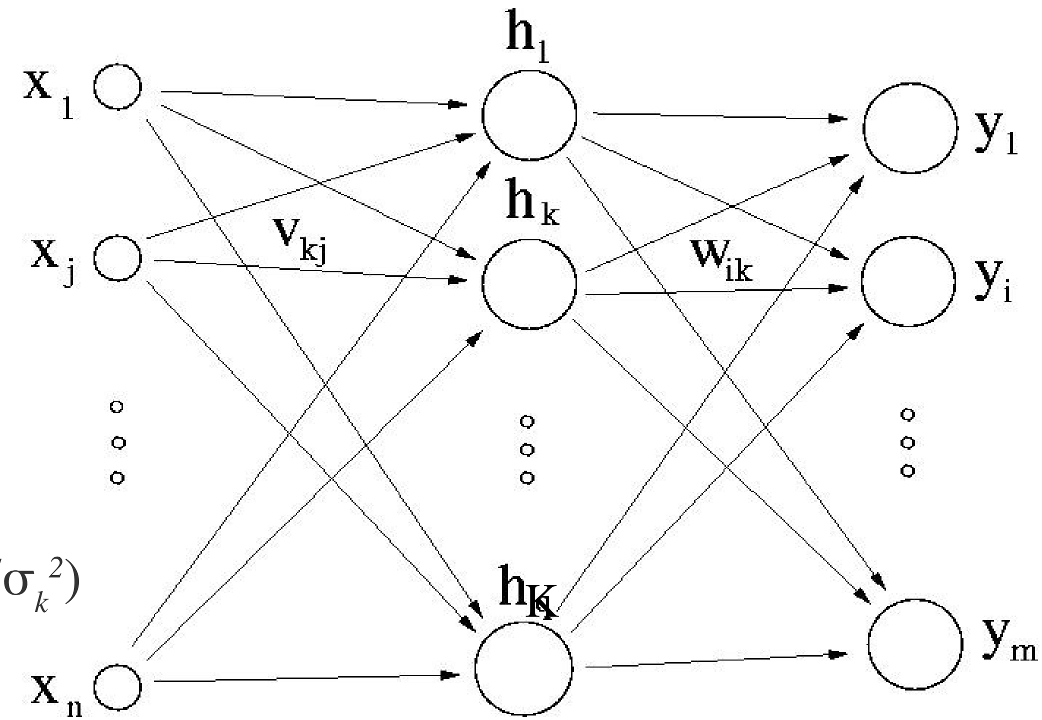
Changes in data dimensionality

- Neural networks process data by nonlinearly transforming them over layers
- Dimensionality reduction has many advantages:
  - allows to extract features
  - leads to abstraction(s)
  - allows robustness against noise
  - simplifies agent’s control (in RL)
- Dimensionality expansion leads to what?
  - supports better linear separability of inputs
  - enables to encode temporal dependences

Combined learning in NN models

- combination of unsupervised (or no learning) and supervised learning
- independent optimization, can be much faster than gradient descent, with similar results
- unsupervised learning → clustering
- more hidden units may be needed (compared to a fully supervised model)
- Examples:
  - learning vector quantization (Kohonen, 1990)
    - classifier on top of trained SOM
  - radial-basis-function networks (Moody & Darken, 1989)
  - semi-supervised learning → transductive learning
  - reservoir computing (e.g. echo-state networks)

Part 1: Radial-Basis-Function neural network



- Inputs $\boldsymbol{x}$, weights $\boldsymbol{w}$, outputs $\boldsymbol{y}$
- Output activation:

$$y_i = \sum_{k=1}^{K} w_{ik} h_k(\boldsymbol{x}) + w_{i0}$$

- h_k = radial activ. function, e.g.

  $h_k(\boldsymbol{x}) = \varphi_k(\|\boldsymbol{x}-\boldsymbol{v}_k\|) = \exp(-\|\boldsymbol{x}-\boldsymbol{v}_k\|^2/\sigma_k^2)$

  $\boldsymbol{v}_k$ ~ center k, σ_k ~ its width

  $\varphi(d)$ are (usually) local functions because for $d \to \infty$ $\varphi(d) \to 0$

  σ affects generalization

- $\boldsymbol{v}_k$ used for approximation of unconditional probability density of input data $p(\boldsymbol{x})$
- RBF as a neuron's receptive field (easier than that of an MLP)

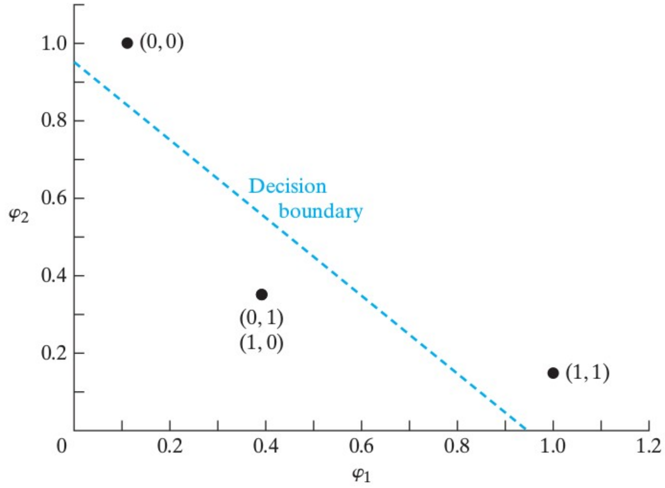
Separability of patterns

- Data projection into high-dim. space:
  A complex pattern classification problem cast in a high-dim. space nonlinearly is more likely to be linearly separable than in a low-dim. space (*Cover, 1965*).

- Consider binary partitioning (dichotomy) for $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N$ (classes C_1, C_2). Dichotomy $\{C_1, C_2\}$ is $\boldsymbol{\phi}$-separable, where $\boldsymbol{\phi}(\boldsymbol{x}) = [\varphi_1(\boldsymbol{x}), \varphi_2(\boldsymbol{x}), \ldots, \varphi_K(\boldsymbol{x})]$, if $\exists \boldsymbol{w} \in \Re^K$ such that for $\forall \boldsymbol{x} \in C_1$: $\boldsymbol{w}^{\mathrm{T}}.\boldsymbol{\phi}(\boldsymbol{x}) > 0$ and for $\forall \boldsymbol{x} \in C_2$: $\boldsymbol{w}^{\mathrm{T}}.\boldsymbol{\phi}(\boldsymbol{x}) < 0$.

- $\{\varphi_k(\boldsymbol{x})\}$ – feature functions (hidden space), $k = 1, 2, \ldots, K$

- Sometimes, non-linear transformation can result in linear separability without having to increase data dimension (e.g. XOR problem):



$$\varphi_k(\boldsymbol{x}) = \exp(-\|\boldsymbol{x} - \boldsymbol{v}_k\|^2) \qquad \boldsymbol{v}_1 = [0\ 0]\,,\ \boldsymbol{v}_2 = [1\ 1]$$

Input Pattern $\mathbf{x}$	First Hidden Function $\varphi_1(\mathbf{x})$	Second Hidden Function $\varphi_2(\mathbf{x})$
(1,1)	1	0.1353
(0,1)	0.3678	0.3678
(0,0)	0.1353	1
(1,0)	0.3678	0.3678

Interpolation problem

- Mapping data into higher dimensions can be useful:
- Then we can deal with multivariate interpolation in high-dim. space (Davis, 1963):

  Given the sets $\{\boldsymbol{h}_i \in \Re^K, d_i \in \Re\}$, find a function F that satisfies the condition: $F(\boldsymbol{h}_i) = d_i$, $i=1,2,...,N.$ (in strict sense)

- For RBF, we get the set of linear equations: $\boldsymbol{w}^{\mathrm{T}} \boldsymbol{h}_i = d_i$, $i = 1,2,...,N.$
- If $\mathbf{H}^{-1}$ exists, the solution is $\boldsymbol{w} = \mathbf{H}^{-1} \boldsymbol{d}$
- How can we be sure that interpolation matrix $\mathbf{H}$ is nonsingular?

- Theorem: Let $\{\boldsymbol{x}_i \in \Re^n\}$ be a set of distinct points $(i=1,2,...,N)$. Then $\mathbf{H}$ $[N \times N]$ with elements $h_{ij} = \varphi_{ij}(\|\boldsymbol{x}_i - \boldsymbol{x}_j\|)$, is nonsingular. (Michelli, 1986)
- a large class of RBFs satisfies this condition

Training RBF networks

- two-stage process
- nonlinear (layer 1) and linear (layer 2) optimization strategies are applied to different learning tasks
- Approaches for layer 1:
  - fixed centers selected at random
  - self-organized selection of centers
- Approaches for layer 2
  - via pseudoinverse $\mathbf{H}^{+}$: then $\boldsymbol{w} = \mathbf{H}^{+}\boldsymbol{d}$
  - online stochastic optimization (delta rule),
  - online deterministic algorithm (RLS)
- Yet another method: supervised selection of centers and output weight setting (not described here)

Fixed centers selected at random

- "sensible" approach if training data are distributed in a representative manner:

$$G(\|\boldsymbol{x} - \boldsymbol{v}_j\|^2) = \exp(-K\|\boldsymbol{x} - \boldsymbol{v}_j\|^2/d^2_{\max})$$

K – number of centers, $d_{\max} = \max_{kl}\{\|\boldsymbol{v}_k - \boldsymbol{v}_l\|\}$, => $\sigma = d_{\max}/(2K)^{1/2}$

- RBFs become neither too flat nor too wide
- Alternative: individual widths σ_j, inversely proportional to density $p(\boldsymbol{x})$ – requires experimentation with data
- relatively insensitive to regularization, for larger data sets

Self-organized selection of centers

Self-organization: *K*-means clustering:

Initialization: randomize $\{\boldsymbol{v}_1(0), \boldsymbol{v}_2(0), \ldots, \boldsymbol{v}_K(0)\}$

Two steps: (until stopping criterion is met)

1. minimize $J(C) = min_{\{\boldsymbol{v}_k\}} \sum_{k=1}^{K} \sum_{C(i)=k} \|\boldsymbol{x}(i) - \boldsymbol{v}_k\|^2$ for given encoder *C*

– by updating cluster centers: $\{\boldsymbol{v}_k(t)\}$

2. optimize the encoder: $C(i) = arg\,min_k \|\boldsymbol{x}(i) - \boldsymbol{v}_k\|^2$

– by reassigning inputs to clusters

Given a set of N observations, find the encoder C that assigns these observations to the K clusters in such a way that, within each cluster, the average measure of dissimilarity of the assigned observations from the cluster mean is minimized.

- *no guarantee for finding an optimum*

Recursive Least Squares (RLS)

- RBF centers can be updated recursively
- How to compute optimal output weights, recursively, too?
- RLS algorithm summary: given $\{\boldsymbol{\phi}^{(p)}, d^{(p)}\}$, $p = 1,2,\ldots,N;\ \ x^{(p)} \equiv x(t)$
- *Initialize:* $\mathbf{w}(0) = \mathbf{0}$, $\mathbf{P}(0) = \lambda^{-1}\,\mathbf{I}$, with $\lambda > 0$, $\lambda \approx 0$, regularizer $\tfrac{1}{2}\lambda \,\|\, \mathbf{w} \,\|^2$
- *Repeat:*

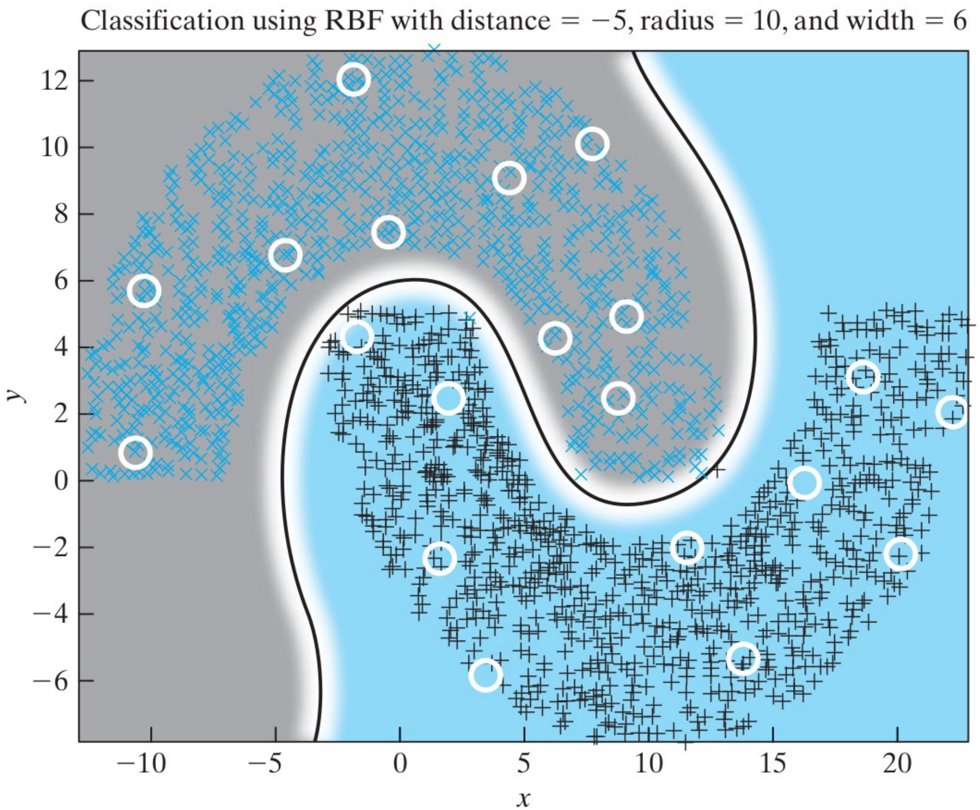
1. $\mathbf{P}(t) = \mathbf{P}(t-1) - \dfrac{\mathbf{P}(t-1)\boldsymbol{\Phi}(t)\boldsymbol{\Phi}^T(t)\mathbf{P}(t-1)}{1 + \boldsymbol{\Phi}^T(t)\mathbf{P}(t-1)\boldsymbol{\Phi}(t)}$
2. $\mathbf{g}(t) = \mathbf{P}(t).\boldsymbol{\phi}(t)$ (gain)
3. $a(t) = d(t) - \mathbf{w}^{\mathrm{T}}(t-1)\ \boldsymbol{\phi}(t)$ (prior estimation error)
4. $\mathbf{w}(t) = \mathbf{w}(t-1) + \mathbf{g}(t).a(t)$

Example using an RBF network

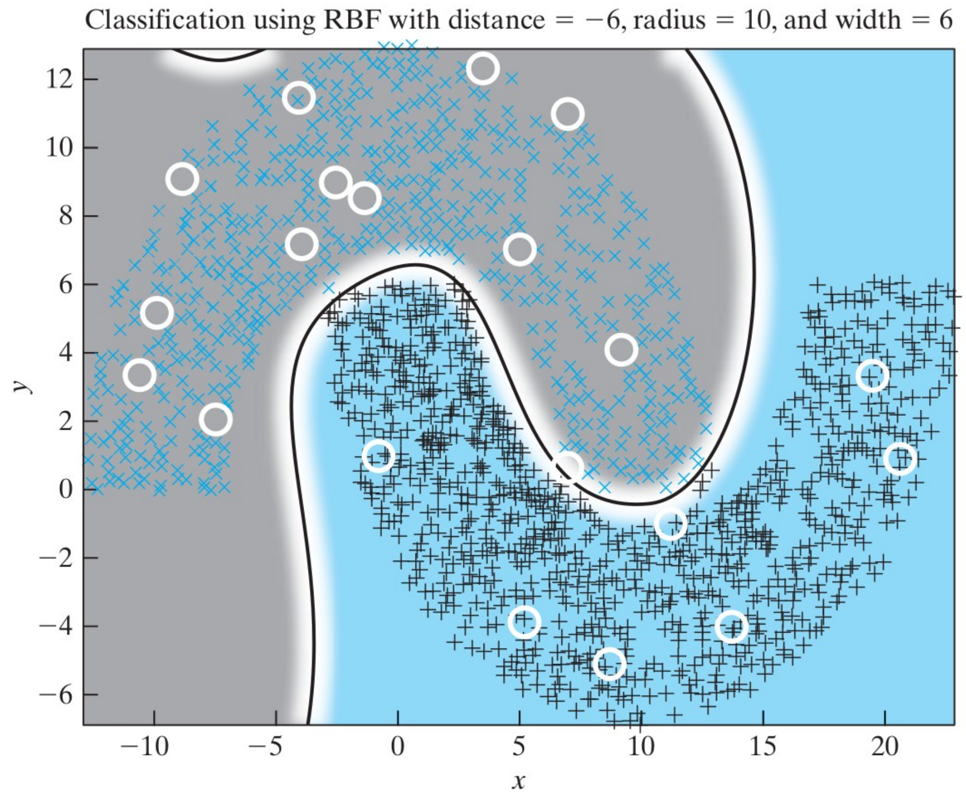
Two-moons classification task: 20 Gaussian units, 1000 points used for training, 2000 for testing. Different widths (σ) used.

$$\sigma = \frac{d_{\max}}{\sqrt{2K}}$$

$\sigma = 2.6$



$\sigma = 2.4$



Approximation properties of RBF networks

Theorem: (Park & Sandberg, 1991) Let $G: \Re^K \rightarrow \Re$ be an integrable bounded function such that G is continuous and $\int_{\Re^K} G(\boldsymbol{x})\, d\boldsymbol{x} \neq 0$. The family of RBF networks consists of functions $F: \Re^k \rightarrow \Re$:

$$F(\boldsymbol{x}) = \sum_{k=1}^{K} w_k\, G((\boldsymbol{x}-\boldsymbol{v}_k)/\sigma)$$

where $\sigma > 0$, $w_k \in \Re$ and $\boldsymbol{v}_k \in \Re^K$.

Then for any continuous function $f(\boldsymbol{x})$ there exists an RBF network with a set of centers $\boldsymbol{v}_k \in \Re^K$ and a common width $\sigma > 0$ such that $F(\boldsymbol{x})$ realized by RBF network is close to $f(\boldsymbol{x})$ in L_p norm, $p \in [1,\infty]$.

Note: Theorem does not require radial symmetry for kernel $G: \Re^K \rightarrow \Re$.

- Useful constraint in RBF design: *K* < *N* (number of patterns)
- Gaussian centers as kernels: $\int_{\Re^K} G(\boldsymbol{x})\, d\boldsymbol{x} = 1$

Kernel $G(\boldsymbol{x})$ = continuous, bounded, and real function of $\boldsymbol{x}$, symmetric about the origin, where it attains its maximum value.

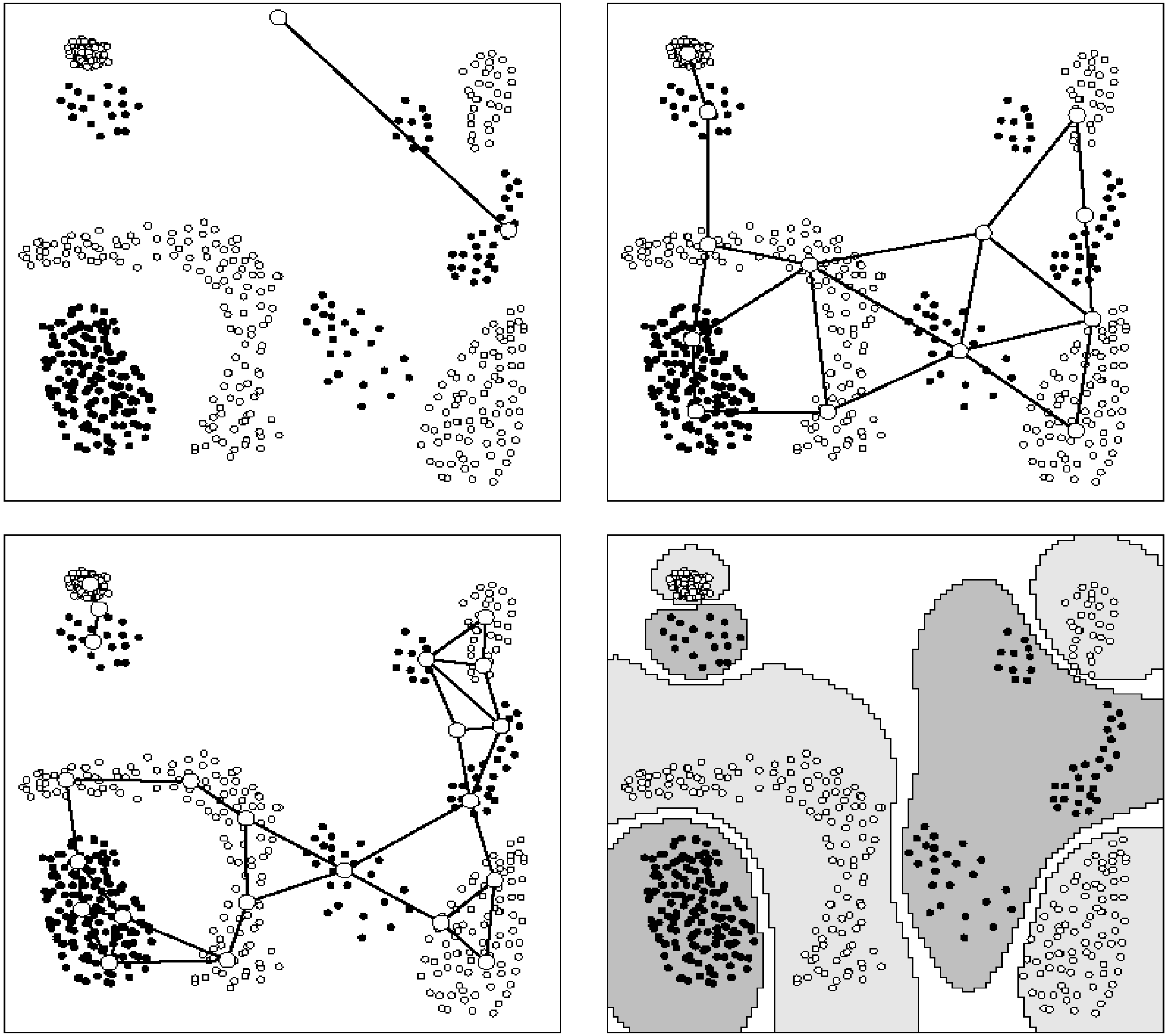
Comparison of RBF and MLP

- both are nonlinear layered feedforward networks
- both are universal approximators, using parametrized compositions of functions of single variables.
- localized vs. distributed representations on hidden layer =>
  - convergence of RBF may be faster
  - MLPs are global, RBF are local => MLP need fewer parameters (=> different consequences for generalization)
- different designs of a supervised network:
  - MLP = stochastic approximation problem
  - RBF = hypersurface-fitting problem in a high-dim. space
- one-stage (MLP) vs. two-stage (RBF) training scheme

Alternative self-organizing modules for center allocation

- Can be useful for input data
  - with varying dimensionality across input domain (e.g. Topology Representing Network)
  - with non-stationary data distributions – dynamic networks (Dynamic Cell Structures, Growing CS)
- to be coupled with dynamic linear part
- all based on (unsupervised) competitive learning

Example: binary classification with a growing RBF net



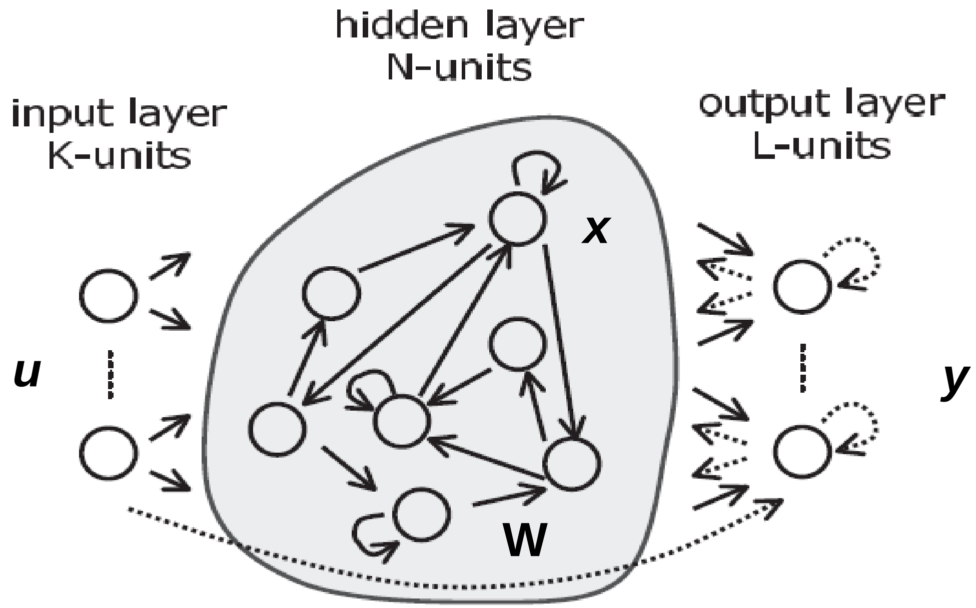
(Fritzke, 1994)

Part 2: Reservoir computing

- A relatively new framework for computation derived from a RNN that maps input signals into high-dimensional spaces through the dynamics of a fixed, non-linear system called a reservoir (Schrauwen et al, 2007).
- After the input signal is fed into the reservoir, which is treated as a "black box," a simple readout mechanism is trained to read the state of the reservoir and map it to the desired output.
- This has two benefits: (1) training is performed only at the readout stage, (2) computational efficiency, with very good accuracy in many tasks.
- Best known models are echo state network (with classical neurons) and liquid state machines (with spiking neurons).

Echo-state network

(Jaeger, 2001)



ESN can have an SRN architecture, but also additional connections are possible (useful for some tasks).

Reservoir units: usually nonlinear (tanh), can also be linear.

System equations:

$$\boldsymbol{x}(t) = f\left(\mathbf{W}\,\boldsymbol{x}(t-1) + \mathbf{W}^{\text{inp}}\boldsymbol{u}(t) + \underline{\mathbf{W}^{\text{fb}}\boldsymbol{y}}(t)\right)$$

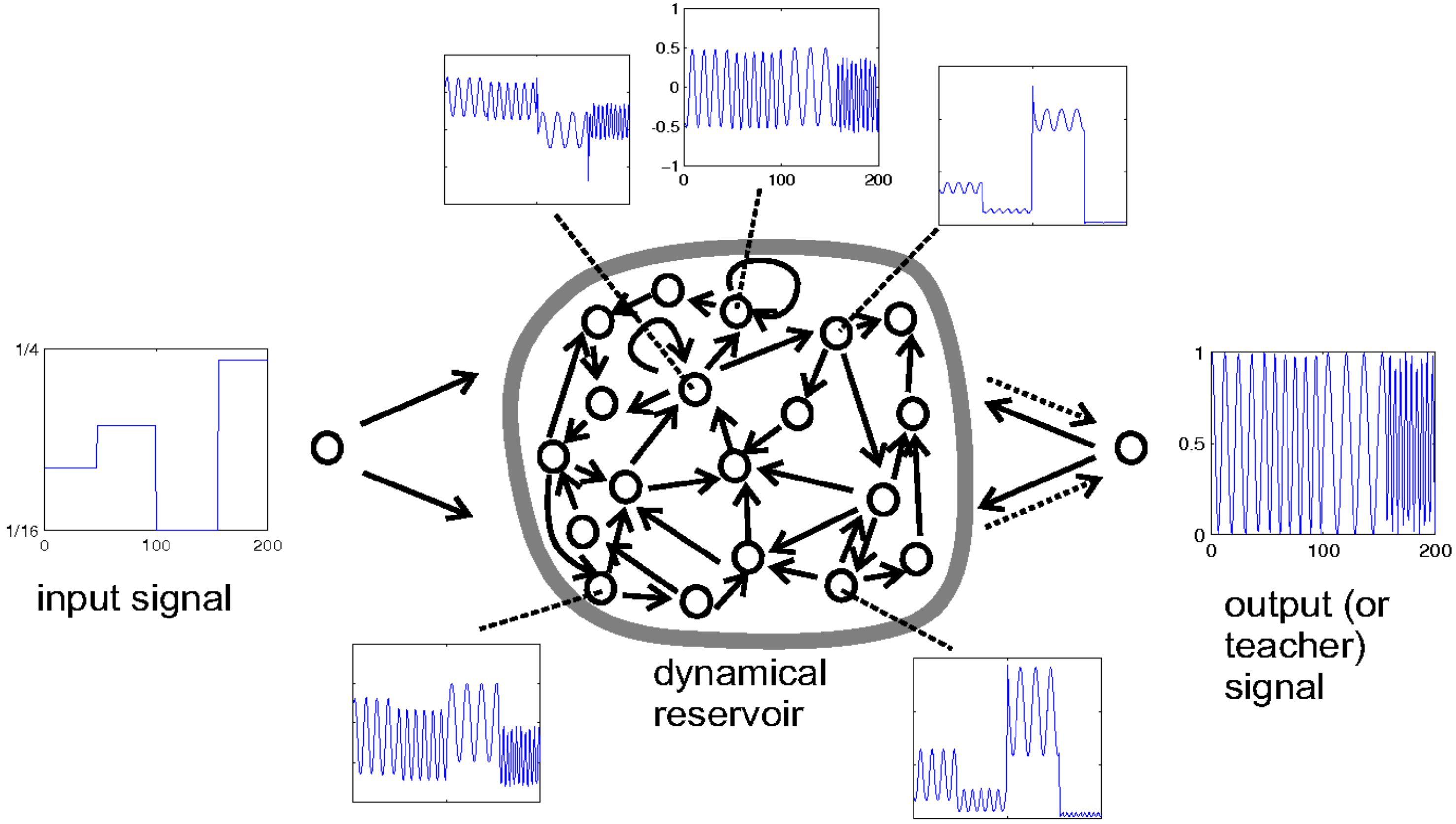
$$\boldsymbol{y}(t) = f^{out}\left(\mathbf{W}^{\text{out}}\boldsymbol{z}(t)\right)$$

$$\mathbf{W}^{out} \sim L \times (N+K)]$$

$$\boldsymbol{z}(t) = [\boldsymbol{x}(t);\underline{\boldsymbol{u}(t)}]$$

Note: these pathways (dotted lines in figure) are optional.

Echo State Network (ctd)



- studied issues: memory capacity, information transfer, ...
- edge of stability = interesting regime (may be optimal w.r.t. info processing)

ESN training

- Initialize the ESN
  - create the reservoir with echo-state property (asymptotic properties of reservoir dynamics are given by driving signal): (Jaeger, 2001)

    Network F: $X \times U \rightarrow X$ (with compactness condition) has the **echo state property** w.r.t. U, if for any left infinite input sequence $u^{-\infty} \in U^{-\infty}$ and any two state vector sequences $x^{-\infty}, y^{-\infty} \in X^{-\infty}$ compatible with $u^{-\infty}$, it holds that $x_0 = y_0$.
  - small random input weights (with uniform or gaussian distribution)
- Collect reservoir states
  - feed input sequence into network (recursively apply state eq.)
- Compute output weights
  - Supervised learning, via pseudoinverse of **X,** or RLS

- ESN reservoir has a Markov property (in symbolic dynamics)

ESN properties

Echo-state property (ESP): depends on spectral properties of $\boldsymbol{W}$ = (typically) random *sparse* matrix, measures:

- spectral radius: $\rho(\boldsymbol{W}) = |\lambda_{max}|$, i.e. largest absolute eigenvalue,
- spectral norm: $s_{max}(\boldsymbol{W})$ = largest singular value, relation: $0 \leq \rho(\boldsymbol{W}) \leq s_{max}(\boldsymbol{W})$

- Criteria for ESP: $s_{max}(\boldsymbol{W}) < 1$ → too strict, $\rho(\boldsymbol{W}) < 1$ not sufficient
- New recipe (Yildiz & Jaeger, 2012): (i) rnd $w_{ij} \geq 0$, (ii) scale $\boldsymbol{W}$ for $\rho(\boldsymbol{W}) < 1$, (iii) change the signs of a desired number of entries to get some $w_{ij} < 0$ as well.
- $\rho(\boldsymbol{W}) \approx 1$ tends to be a "turning point" in behavior (e.g. memory capacity)

Memory capacity (MC): reflects the ability to retrieve input data from reservoir

- scalar i.i.d. inputs assumed, MC depends on $\boldsymbol{W}$, $\boldsymbol{W}^{inp}$, reservoir size *N*, sparsity

$$\mathrm{MC} = \sum_{k=1}^{k_{\max}} \mathrm{MC}_k = \sum_{k=1}^{k_{\max}} \frac{cov^2(u(t-k), y_k(t))}{var(u(t)) \cdot var(y_k(t))}$$

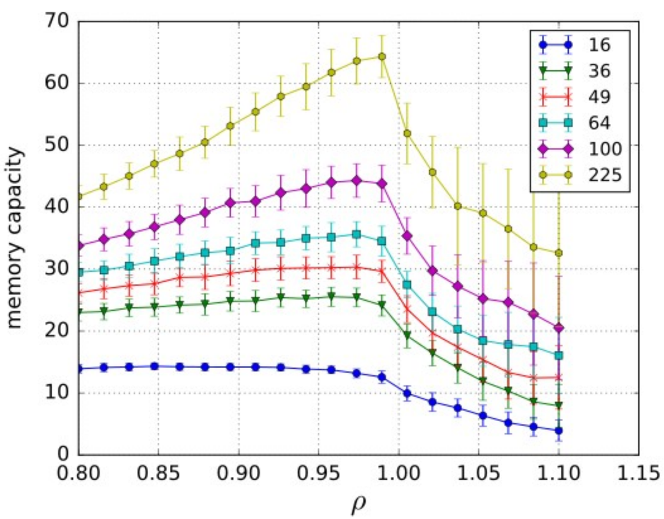
$$y_k(t) = \mathbf{w}_k^{\mathrm{out}} \mathbf{x}(t) = \tilde{u}(t-k)$$

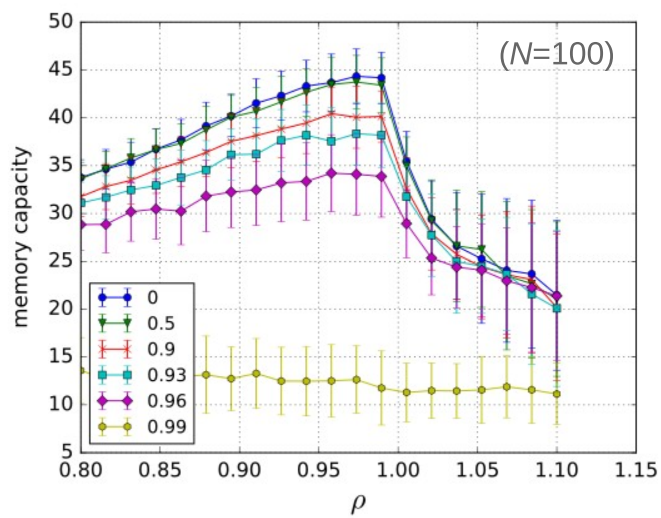
$$k_{\max} = L$$

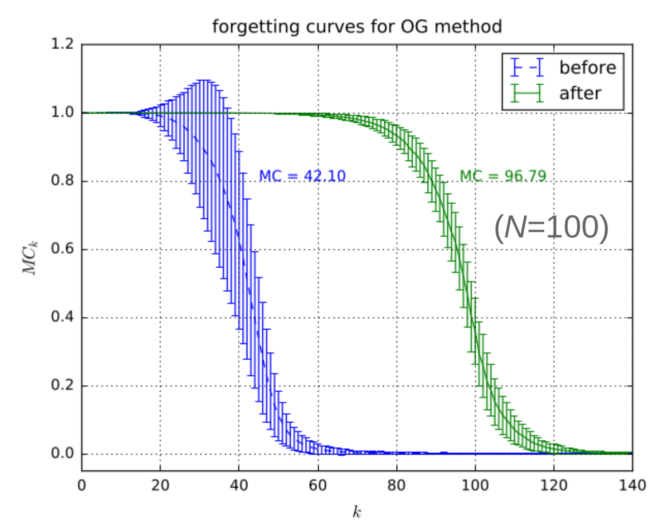
Reservoir stability – measured by characteristic Lyapunov exponent (Sprott, 2003), That quantifies average divergence of state space trajectories under perturbations.

Memory capacity – calculated

- MC depends on spectral radius ρ and grows with reservoir size *N* (left)
  - for ρ > 1 the dynamics may become unstable
- MC degrades very gracefully for sparse reservoirs (middle)
- MC can be increased by (iterative) reservoir orthogonalization (right)
  - reaching the theoretical limit (*N*)







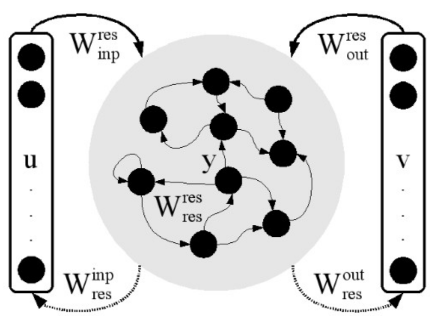
(Farkas et al, 2016)

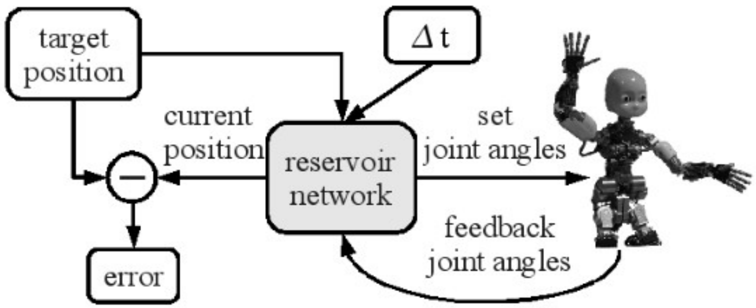
ESN behavior optimization

- trade-off b/w MC and predictive capacity (PC) in linear ESN (Marzen, 2019)
- small-world reservoir topology improves performance (both MC and PC) (Kawai,Park, Asada, 2019)
  - SW property = short average distance b/w nodes
- Importance of ESN operation at the “edge of criticality” (transition b/w stable regime and chaotic dynamics, ($\rho(\boldsymbol{W}) \approx 1$)
  - improves MC (but not PC)
  - supports efficient information integration (in complex systems)
  - flexibility (vs stability, exploration vs exploitation) (Atasoy, Deco, Kringelbach, 2019)

ESN applications

- time-series prediction
- Sequence classification, e.g. human gesture recognition (Jirak et al, 2020) – participants with smartphone and gesture recognition app →
- robot control – target reaching (Reinhart & Steil, 2009)





- Recent challenges for other tasks (speech recognition, machine translation, …) → randomized transformations work well with minimum effort
- Overview of applications and designs (Sun et al, 2020)

Summary

- RBF – hybrid feedforward NN model
  - hidden layer unsupervised (high-dim. projection), output layer supervised (linear readout)
  - various training algorithms for setting RBF centers
  - RLS for computing output weights, or pseudoinverse
  - universal approximator (like MLP)
  - applicable for function approximation and classification
- ESN – fast recurrent NN, only linear readout trained
  - reservoir = high-dim. spatio-temporal embedding
  - good for time series prediction and memory tasks with Markov properties