Basic introduction to machine learning

Jeffrey A. Fessler

EECS Department, BME Department, Dept. of Radiology
University of Michigan

ISMRM Educational Course:
Machine Learning: Everything You Wanted to Know but Were Afraid to Ask

2021-05-15

Declaration: No relevant financial interests or relationships to disclose

Outline

Outline

Slides and code

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https://tinyurl.com/ml2-18-jf

- Slides with bibliography
- Jupyter notebook
  - Julia code for all figures shown
  - Ju=Julia py=python r=R
  - Julia 1.0 released Aug. 2018
  - SIAM Review paper [1]
  - Convenience of scripting, performance of compiled code

Machine learning definitions

- `https://en.wikipedia.org/wiki/Machine_learning` 2021-04-16:

  Machine learning (ML) is the study of computer algorithms that improve automatically through experience and by the use of data.

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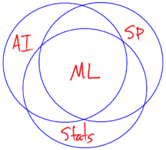
- Statistical perspective: "Machine learning is a field of study concerned with making quantitative inferences and predictions based on data." (Clay Scott, 2016)



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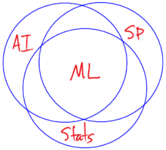
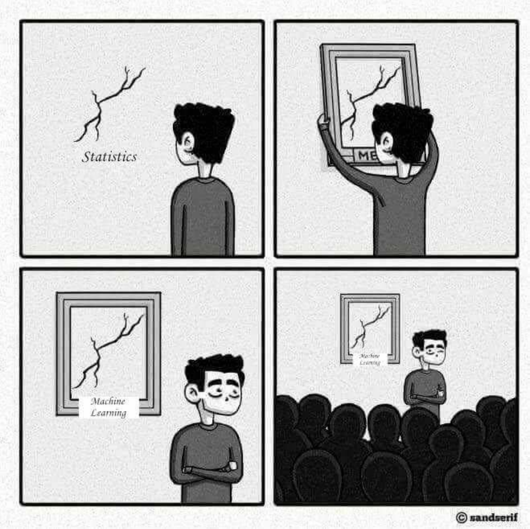


- ML is statistics without confidence intervals, p-values, or control of Type-I/II errors?

ML definitions

Image credit:

https://www.reddit.com/r/ProgrammerHumor/comments/88o6an/machine_learning/



Machine learning categories

Application:

- classification (labeling / detection / segmentation)
- regression (parameter estimation / quantification)

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Training method:

- supervised learning (labeled training data)
- unsupervised learning
- semi-supervised learning
- reinforcement learning

ML categories

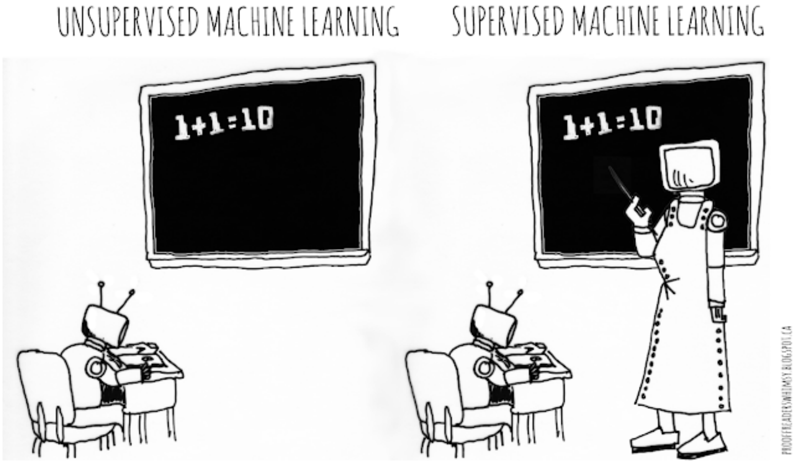

Image credit: `http://prooffreaderswhimsy.blogspot.com/2014/11/machine-learning.html`

Unsupervised vs Supervised Learning

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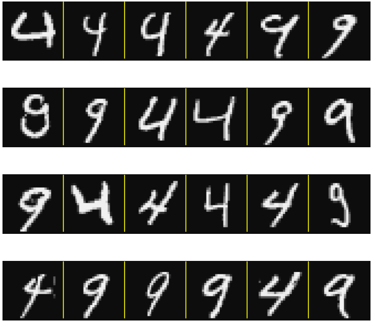
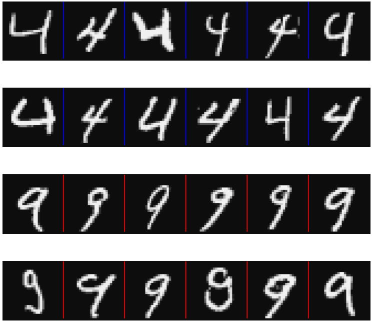
Unsupervised



Supervised



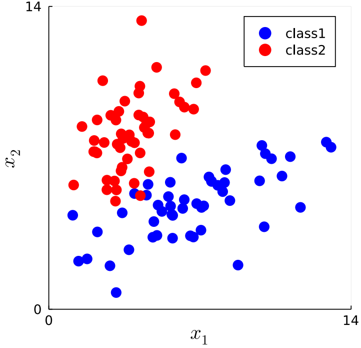
Domain experts needed...

Supervised learning overview: classification

Given paired (feature,label) training data: $(\boldsymbol{x}_1, y_1), \ldots (\boldsymbol{x}_N, y_N)$

Example:

- $\boldsymbol{x} \in \mathbb{R}^2$
- $y \in \{\text{class1=blue}, \text{class2=red}\}$

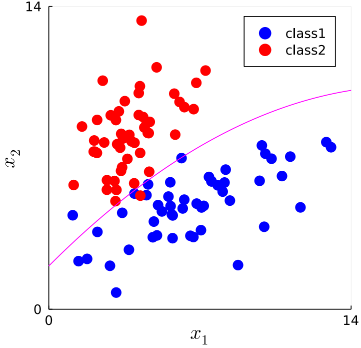


Supervised learning overview: classification

Given paired (feature,label) training data:
$(\boldsymbol{x}_1, y_1), \dots (\boldsymbol{x}_N, y_N)$

Goal: predict output (*e.g.*, class) y
for a subsequent test feature $\boldsymbol{x}$

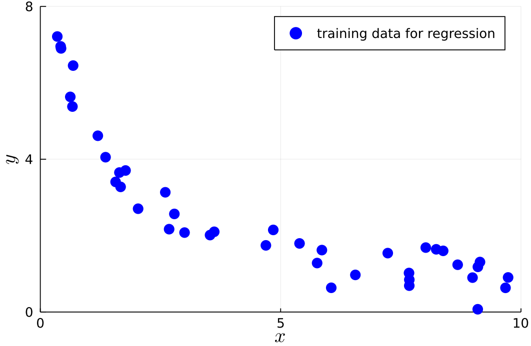
A classifier is a function $y = f(\boldsymbol{x})$ that maps
a feature vector into a class label,
i.e., $f : \mathbb{R}^d \mapsto \{1, \dots, K\}$.



Given paired (feature,label) training data: $(\boldsymbol{x}_1, y_1), \ldots (\boldsymbol{x}_N, y_N)$.

Example:

- $\boldsymbol{x} \in \mathbb{R}$
- $y \in \mathbb{R}$

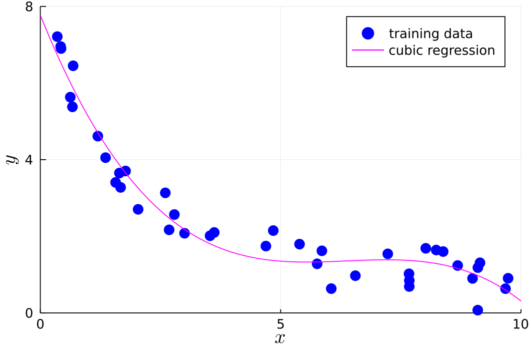


Supervised learning overview: regression

Given paired (feature,label) training data: $(\boldsymbol{x}_1, y_1), \ldots (\boldsymbol{x}_N, y_N)$.

Goal: predict output (*e.g.*, value) y for a subsequent test feature $\boldsymbol{x}$.

Key challenge in supervised learning is generalization beyond training data for future predictions.

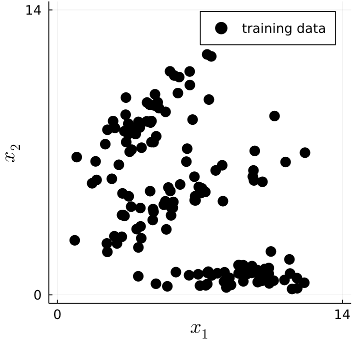


Unsupervised learning overview: clustering

No labels, just feature vector training data $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N$.

Example:

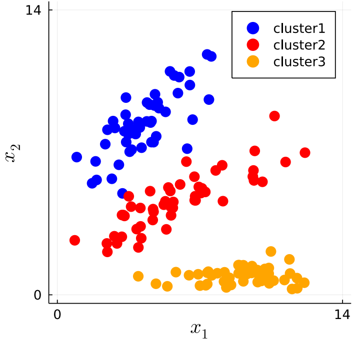
- $\boldsymbol{x} \in \mathbb{R}^2$



No labels, just feature vector training data $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N$.

Goal: understand data structure

- Clustering
- Dimensionality reduction
- Density estimation

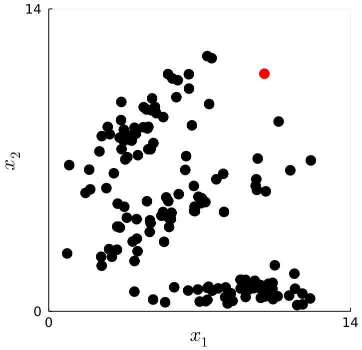


Unsupervised learning overview: clustering

No labels, just feature vector training data $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N$.

Another unsupervised learning problem: novelty detection.

Many other ML problems...



More categories of ML methods

Distribution assumptions

- Generative: full probabilistic model for data
- Discriminative: partial or no probabilistic model

Model type / complexity:

- parametric: number of model parameters is independent of sample size
- nonparametric: number of model parameters grows with sample size

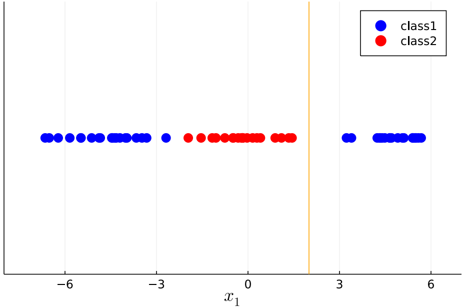
Computational form

- Linear: output y is a linear / affine function of input $\boldsymbol{x}$
- Nonlinear

Why nonlinearity? (Classification)

Example: supervised classifier learning

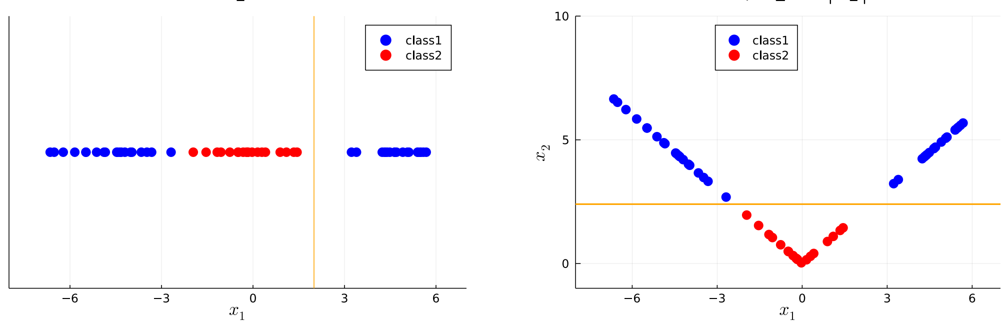
$$\boldsymbol{x} = x_1 \in \mathbb{R}$$



Why nonlinearity? (Classification)

Example: supervised classifier learning

$\boldsymbol{x} = x_1 \in \mathbb{R}$ $\qquad$ $\boldsymbol{x} \in \mathbb{R}^2, \; x_2 \triangleq |x_1|$



In this (simple, synthetic) example, nonlinear "lifting" from 1D to 2D enables a basic "linear" classifier from $(x_1, x_2) = (x_1, |x_1|)$.

(Inspired by `https://www.youtube.com/watch?v=3liCbRZPrZA`)

Why nonlinearity? (2D Classification case)

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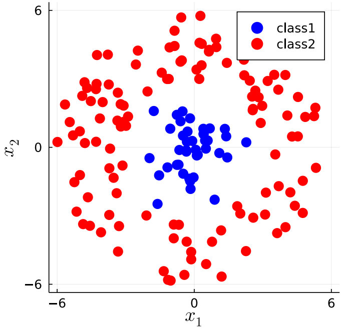
$$\boldsymbol{x} = (x_1, x_2) \in \mathbb{R}^2$$



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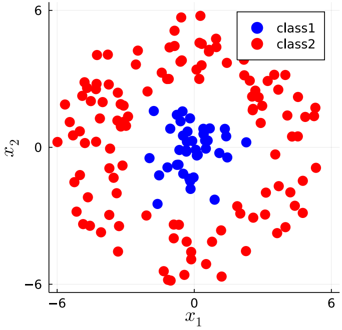
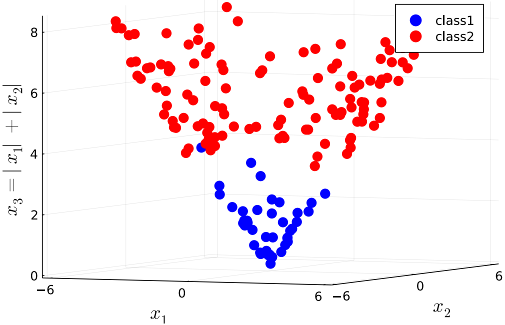


$\boldsymbol{x} \in \mathbb{R}^3,\ x_3 \triangleq |x_1| + |x_2|$



One additional nonlinear "feature" enables linear separation: $\boldsymbol{x} = (x_1, x_2, |x_1| + |x_2|)$

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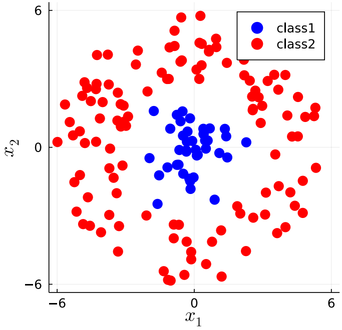

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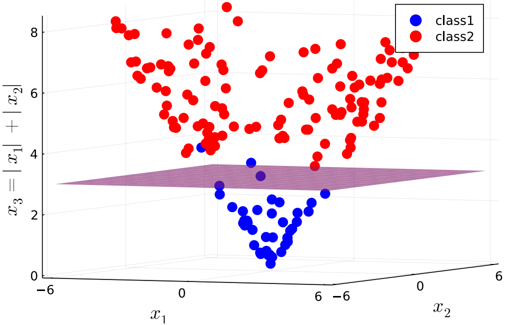

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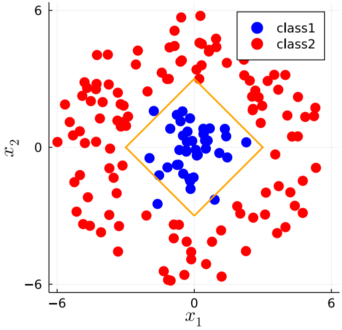

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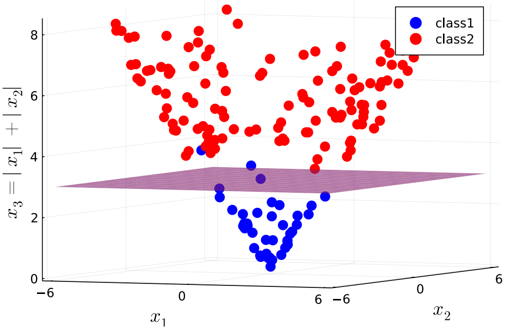

One additional nonlinear "feature" enables linear separation: $\boldsymbol{x} = (x_1, x_2, |x_1| + |x_2|)$

Many artificial neural nets (ANNs) use nonlinear rectified linear unit:

$\text{ReLU}(x) = \max(x, 0)$, where $|x| = \text{ReLU}(x) + \text{ReLU}(-x)$.

Why nonlinearity? (Regression)

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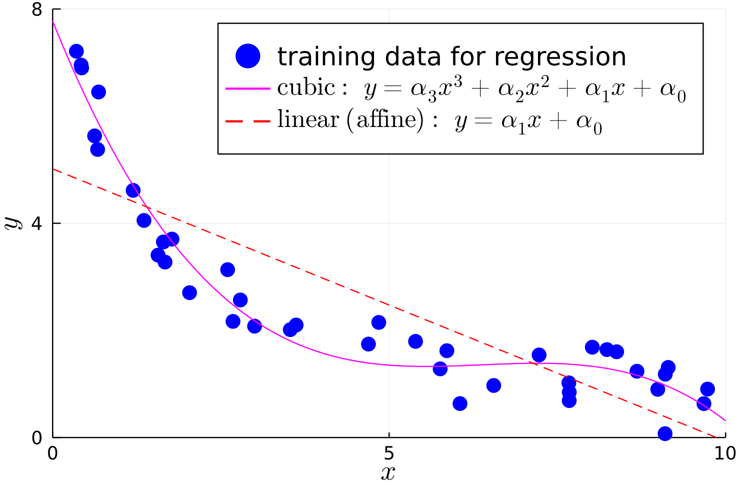
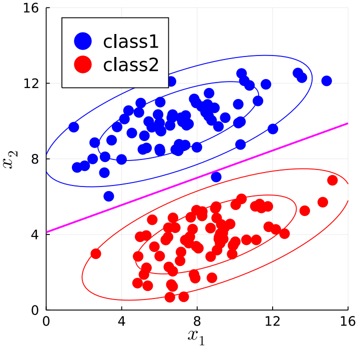


Assuming:
- Normal distributions
- Equal covariances

Optimal decision boundary is a line in 2D (hyperplane in general)

Optimal classifier is (mostly) linear:

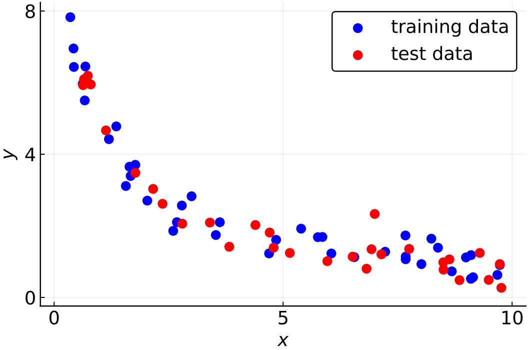
$$y = \begin{cases} \text{class1}, & \boldsymbol{w}'\boldsymbol{x} < \text{threshold} \\ \text{class2}, & \text{otherwise} \end{cases}$$



https://en.wikipedia.org/wiki/Linear_discriminant_analysis

Outline

- Most ML methods lack p-values, confidence intervals, Type I/II error formulae, ...
- Performance evaluation is performed *empirically* using testing data,
- after training the method ("learning") using training data.

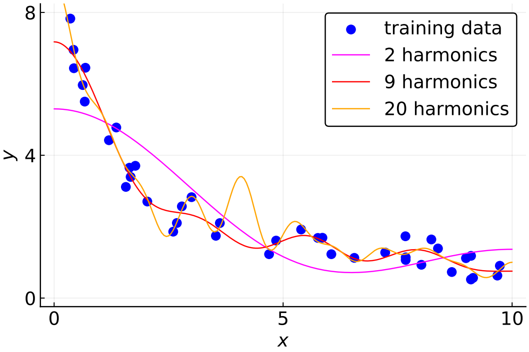


Model-order selection

ML methods have two categories of design choices:

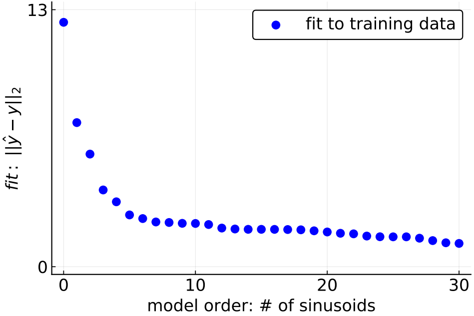
- Architecture / model order
- Tunable parameters (coefficients)

  We can learn the coefficients from training data for any given model order:



Training data: not for model selection

Fitting "error" with various numbers of sinusoids:



- More sinusoids (more degrees of freedom / larger model order) $\Longrightarrow$ "better" fit to the training data

Training data: not for model selection

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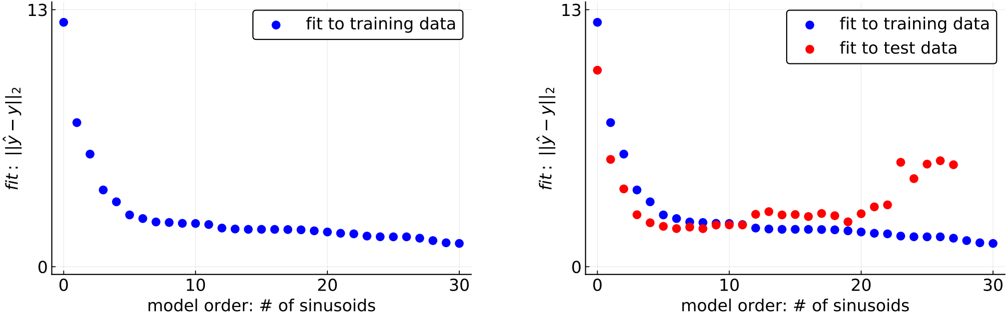

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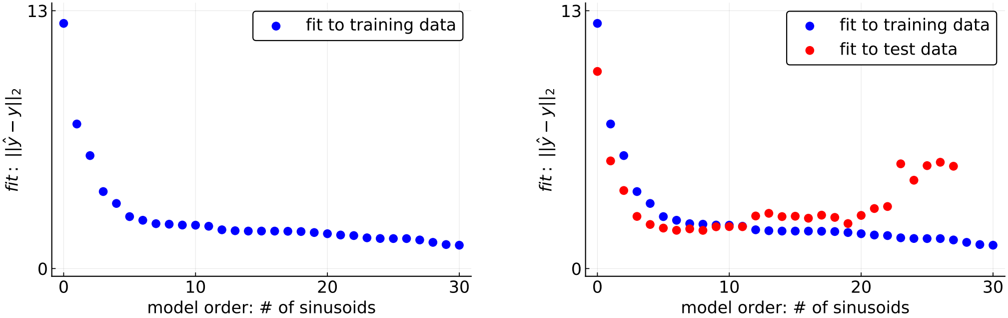
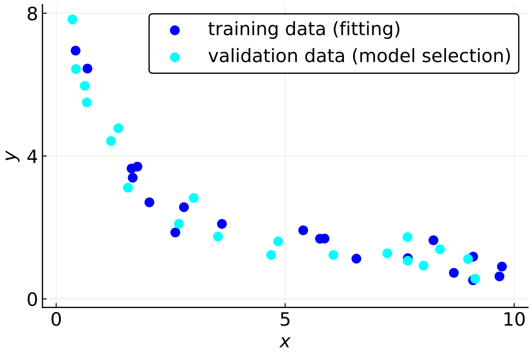


- More sinusoids (more degrees of freedom / larger model order) $\Longrightarrow$ "better" fit to the training data
- Over-fit if model order is "too high" $\Longrightarrow$ poor generalization / test results
- Cannot use the test data for training / model-order selection!

Validation data (e.g., cross validation)

Separate training data into two groups:

- training data
  for fitting parameters (coefficients)
- validation data
  for selecting model order / architecture



- (50-50% holdout shown here; one of many **cross validation** options)

Validation data for model-order selection

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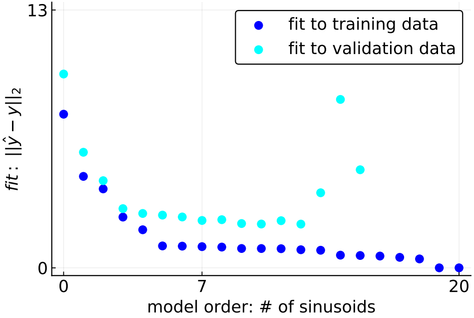

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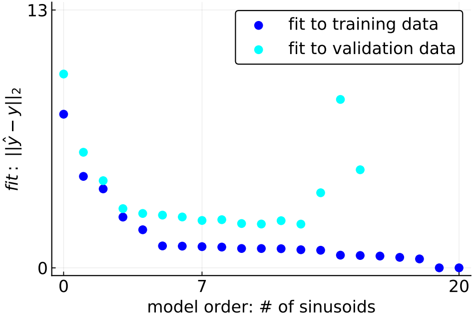

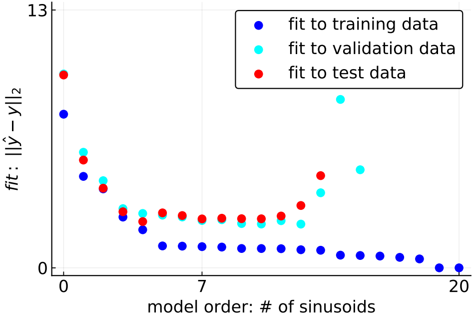

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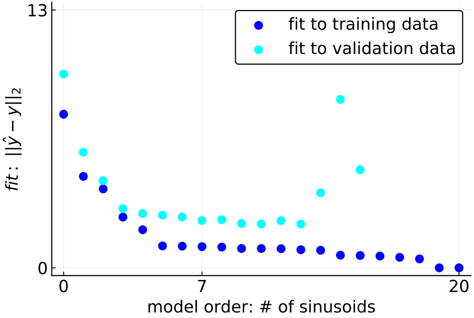

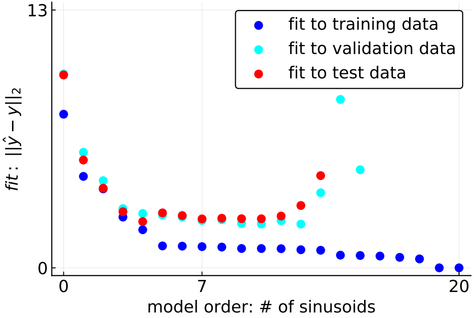

- Options for model-order selection:
  - Choose minimum of validation loss curve
  - Stop increasing model order when validation loss first increases (first sign of over-fitting)
- Attempts to assess how well the results will generalize to new data (red vs cyan)

Outline

Training an artificial neural network: overview

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Input: features $\rightarrow$ artificial NN $\rightarrow$ Output: prediction

Goal (supervised learning):
train NN so that output closely matches training data, without over fitting

(requires math...)

Training an artificial neural network: details

Input: features $\boldsymbol{x} \in \mathbb{R}^d$ $\rightarrow$ NN parameters $\boldsymbol{\theta}$ $\rightarrow$ Output: prediction: response (regression) $\hat{\boldsymbol{y}} = f(\boldsymbol{x}; \boldsymbol{\theta}) \in \mathbb{R}^m$

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- Supervised training problem: given training data $(\boldsymbol{x}_1, \boldsymbol{y}_1), \ldots, (\boldsymbol{x}_N, \boldsymbol{y}_N)$, learn parameters $\boldsymbol{\theta}$ of NN so that $\hat{\boldsymbol{y}}_n \triangleq f(\boldsymbol{x}_n; \boldsymbol{\theta}) \approx \boldsymbol{y}_n$.

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- Quantify "≈" using a loss function $\ell(\hat{\boldsymbol{y}}_n, \boldsymbol{y}_n)$ such as $\ell(\hat{\boldsymbol{y}}, \boldsymbol{y}) = \|\hat{\boldsymbol{y}} - \boldsymbol{y}\|_2^2$.

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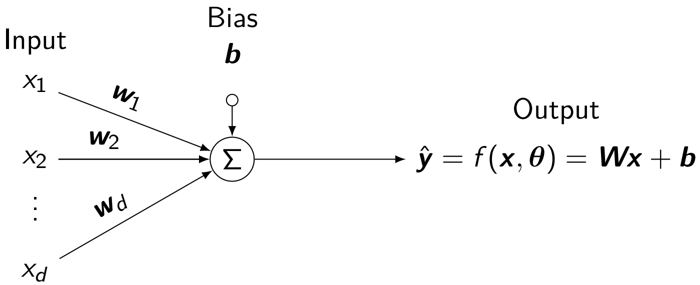
- Quantify "$\approx$" using a loss function $\ell(\hat{\boldsymbol{y}}_n, \boldsymbol{y}_n)$ such as $\ell(\hat{\boldsymbol{y}}, \boldsymbol{y}) = \|\hat{\boldsymbol{y}} - \boldsymbol{y}\|_2^2$.
- Training is an optimization problem (minimize average loss):

$$\boldsymbol{\theta}_* = \arg\min_{\boldsymbol{\theta}} L(\boldsymbol{\theta}; \boldsymbol{X}, \boldsymbol{Y}), \qquad L(\boldsymbol{\theta}; \boldsymbol{X}, \boldsymbol{Y}) \triangleq \frac{1}{N} \sum_{n=1}^{N} \ell(f(\boldsymbol{x}_n; \boldsymbol{\theta}), \boldsymbol{y}_n).$$

Simplest example: affine NN (dense / fully connected)



- $\boldsymbol{x} \in \mathbb{R}^d$ is input
- $\boldsymbol{W} \in \mathbb{R}^{m \times d}$ are weights
- $\boldsymbol{b} \in \mathbb{R}^m$ is offset or bias
- $\boldsymbol{y} \in \mathbb{R}^m$ is output (response / prediction)
- NN parameters are weights and bias: $\boldsymbol{\theta} = (\boldsymbol{W}, \boldsymbol{b})$

Training an affine NN

Squared error loss: $\ell(\hat{\boldsymbol{y}}, \boldsymbol{y}) = \|\hat{\boldsymbol{y}} - \boldsymbol{y}\|_2^2 \implies$ training cost function is:

$$L(\theta; \boldsymbol{X}, \boldsymbol{Y}) = \left\| \begin{bmatrix} \boldsymbol{y}_1 & \dots & \boldsymbol{y}_N \end{bmatrix} - \boldsymbol{W} \begin{bmatrix} \boldsymbol{x}_1 & \dots & \boldsymbol{x}_N \end{bmatrix} - \boldsymbol{b}\mathbf{1}_N' \right\|_{\mathrm{F}}^2 .$$

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Optimization has analytical solution from $\nabla_{\boldsymbol{\theta}} L = \boldsymbol{0}$, leads to MMSE form:

$$\hat{\boldsymbol{y}} = f(\boldsymbol{x}, \boldsymbol{\theta}_*) = \boldsymbol{\mu}_y + \underbrace{\boldsymbol{K}_{yx} \boldsymbol{K}_x^{-1}}_{\boldsymbol{W}_*} (\boldsymbol{x} - \boldsymbol{\mu}_x), \quad \boldsymbol{\mu}_x = \frac{1}{N} \sum_{n=1}^N \boldsymbol{x}_n, \quad \boldsymbol{\mu}_y = \frac{1}{N} \sum_{n=1}^N \boldsymbol{y}_n,$$

$$\boldsymbol{K}_x = \frac{1}{N} \sum_{n=1}^N (\boldsymbol{x}_n - \boldsymbol{\mu}_x)(\boldsymbol{x}_n - \boldsymbol{\mu}_x)', \quad \boldsymbol{K}_{yx} = \frac{1}{N} \sum_{n=1}^N (\boldsymbol{y}_n - \boldsymbol{\mu}_y)(\boldsymbol{x}_n - \boldsymbol{\mu}_x)'.$$

Training an affine NN

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Squared error loss: $\ell(\hat{\boldsymbol{y}}, \boldsymbol{y}) = \|\hat{\boldsymbol{y}} - \boldsymbol{y}\|_2^2 \Longrightarrow$ training cost function is:

$$L(\boldsymbol{\theta}; \boldsymbol{X}, \boldsymbol{Y}) = \left\| \begin{bmatrix} \boldsymbol{y}_1 & \dots & \boldsymbol{y}_N \end{bmatrix} - \boldsymbol{W} \begin{bmatrix} \boldsymbol{x}_1 & \dots & \boldsymbol{x}_N \end{bmatrix} - \boldsymbol{b}\boldsymbol{1}_N' \right\|_{\mathrm{F}}^2 .$$

Optimization has analytical solution from $\nabla_{\boldsymbol{\theta}} L = \boldsymbol{0}$, leads to MMSE form:

$$\hat{\boldsymbol{y}} = f(\boldsymbol{x}, \boldsymbol{\theta}_*) = \boldsymbol{\mu}_y + \underbrace{\boldsymbol{K}_{yx} \, \boldsymbol{K}_x^{-1}}_{\boldsymbol{W}_*} (\boldsymbol{x} - \boldsymbol{\mu}_x), \quad \boldsymbol{\mu}_x = \frac{1}{N} \sum_{n=1}^N \boldsymbol{x}_n, \quad \boldsymbol{\mu}_y = \frac{1}{N} \sum_{n=1}^N \boldsymbol{y}_n,$$

$$\boldsymbol{K}_x = \frac{1}{N} \sum_{n=1}^N (\boldsymbol{x}_n - \boldsymbol{\mu}_x)(\boldsymbol{x}_n - \boldsymbol{\mu}_x)', \quad \boldsymbol{K}_{yx} = \frac{1}{N} \sum_{n=1}^N (\boldsymbol{y}_n - \boldsymbol{\mu}_y)(\boldsymbol{x}_n - \boldsymbol{\mu}_x)'.$$

- Need $N \geq d$ so that feature covariance matrix $\boldsymbol{K}_x$ is invertible (more training samples N than feature dimension d). Otherwise some regularization of weights is needed.

Training an affine NN

Squared error loss: $\ell(\hat{\boldsymbol{y}}, \boldsymbol{y}) = \|\hat{\boldsymbol{y}} - \boldsymbol{y}\|_2^2 \implies$ training cost function is:

$$L(\boldsymbol{\theta}; \boldsymbol{X}, \boldsymbol{Y}) = \left\| \begin{bmatrix} \boldsymbol{y}_1 & \dots & \boldsymbol{y}_N \end{bmatrix} - \boldsymbol{W} \begin{bmatrix} \boldsymbol{x}_1 & \dots & \boldsymbol{x}_N \end{bmatrix} - \boldsymbol{b}\boldsymbol{1}_N' \right\|_{\mathrm{F}}^2 .$$

Optimization has analytical solution from $\nabla_{\boldsymbol{\theta}} L = \boldsymbol{0}$, leads to MMSE form:

$$\hat{\boldsymbol{y}} = f(\boldsymbol{x}, \boldsymbol{\theta}_*) = \boldsymbol{\mu}_y + \underbrace{\boldsymbol{K}_{yx} \boldsymbol{K}_x^{-1}}_{\boldsymbol{W}_*} (\boldsymbol{x} - \boldsymbol{\mu}_x), \quad \boldsymbol{\mu}_x = \frac{1}{N} \sum_{n=1}^N \boldsymbol{x}_n, \quad \boldsymbol{\mu}_y = \frac{1}{N} \sum_{n=1}^N \boldsymbol{y}_n,$$

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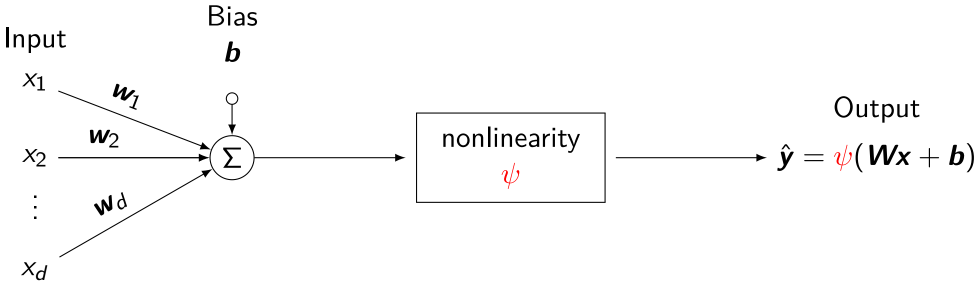
- Need $N \geq d$ so that feature covariance matrix $\boldsymbol{K}_x$ is invertible (more training samples N than feature dimension d). Otherwise some regularization of weights is needed.
- This simple case is one of very few with analytical (noniterative) solution for $\boldsymbol{\theta}_*$

Nonlinear artificial neuron

Perceptron: Rosenblatt, 1957 [2]



- No analytical solution for training NN parameters $\boldsymbol{W}, \boldsymbol{b}$
- Iterative methods required

Kernel ridge regression (nonlinearity)

$$\boldsymbol{x} \to \boxed{\begin{array}{c}\text{Nonlinear}\\ \text{function}\\ \phi : \mathbb{R}^d \mapsto \mathbb{R}^D\end{array}} \to \boldsymbol{z} \to \boxed{\begin{array}{c}\text{Affine}\\ \text{function}\\ \boldsymbol{W}\boldsymbol{z} + \boldsymbol{b}\end{array}} \to \hat{\boldsymbol{y}} = f(\boldsymbol{x}; \boldsymbol{\theta}) = \boldsymbol{W}\phi(\boldsymbol{x}) + \boldsymbol{b} \in \mathbb{R}^m$$

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For MSE training loss and fixed ϕ, MMSE estimator is

$$\hat{\boldsymbol{y}} = \boldsymbol{\mu}_y + \boldsymbol{K}_{yz}\, \boldsymbol{K}_z^{-1}\, (\boldsymbol{z} - \boldsymbol{\mu}_z) = \boldsymbol{\mu}_y + \boldsymbol{K}_{yz}\, \boldsymbol{K}_z^{-1}\, (\phi(\boldsymbol{x}) - \boldsymbol{\mu}_z), \quad \boldsymbol{\mu}_z = \frac{1}{N} \sum_{n=1}^{N} \boldsymbol{z}_n,$$

$$\boldsymbol{z}_n \triangleq \phi(\boldsymbol{x}_n), \quad \boldsymbol{K}_z = \frac{1}{N} \sum_{n=1}^{N} (\boldsymbol{z}_n - \boldsymbol{\mu}_z)(\boldsymbol{z}_n - \boldsymbol{\mu}_z)', \quad \boldsymbol{K}_{yz} = \frac{1}{N} \sum_{n=1}^{N} (\boldsymbol{y}_n - \boldsymbol{\mu}_y)(\boldsymbol{z}_n - \boldsymbol{\mu}_z)'.$$

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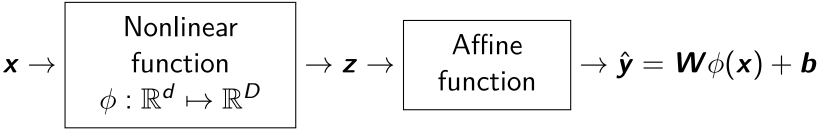
- Typically $D = \dim(\boldsymbol{z}) \gg d = \dim(\boldsymbol{x})$, so even more samples N could be needed.
- Solution is to use ridge regression: replace $\boldsymbol{K}_z^{-1}$ with $(\boldsymbol{K}_z + \alpha \boldsymbol{I})^{-1}$; choose α by cross validation.

Kernel ridge regression universality

J. Fessler



- Affine function $\boldsymbol{W}\boldsymbol{z} + \boldsymbol{b}$ is same as a fully connected NN layer without nonlinearity.
- Choosing a nonlinear function ϕ based on a Gaussian kernel is universal:
  can approximate regular functions to arbitrary accuracy as N increases [3, 4] using:

$$\phi(\boldsymbol{x}) = \begin{bmatrix} \mathrm{e}^{-\|\boldsymbol{x}-\boldsymbol{x}_1\|_{\boldsymbol{\Lambda}}^2} & \dots & \mathrm{e}^{-\|\boldsymbol{x}-\boldsymbol{x}_N\|_{\boldsymbol{\Lambda}}^2} \end{bmatrix}^T.$$

- Training is very easy and fast because only free parameters are linear ones: $\boldsymbol{W}$ and $\boldsymbol{b}$
- Shallow learning
- Suitable for low-dimensional problems like parameter quantification.

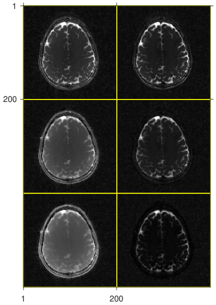
Quantitative MRI example

Quantitative MRI: images $\rightarrow$ estimation $\rightarrow$ parameters (T1,T2,. . .)

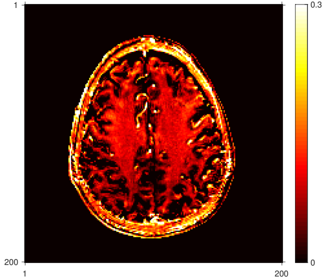
- Traditional nonlinear estimation methods:
  - nonlinear least squares
  - dictionary matching (quantized maximum likelihood via variable projection)
- Machine-learning methods
  - deep neural network regression [5–8]
    typically long training times
  - parameter estimation via kernel regression (PERK)
    Gopal Nataraj et al., ISBI 2017 [9], IEEE T-MI 2018 [3], arXiv 1809.08908 [10],

MWF PERK example

Myelin water fraction (MWF) estimated from 3 DESS scans
with optimized flip angles 33.0, 18.3, 15.1° and TRs 17.5, 30.2, 60.3 ms. [10–12]



→ PERK →



$$\text{Input} \quad \rightarrow \boxed{\text{NN with parameters } \boldsymbol{\theta}} \rightarrow \quad \text{Output}$$

Learning NN parameters (training) requires optimization (minimize average loss):

$$\boldsymbol{\theta}_* = \arg\min_{\boldsymbol{\theta}} L(\boldsymbol{\theta}; \boldsymbol{X}, \boldsymbol{Y}), \quad L(\boldsymbol{\theta}; \boldsymbol{X}, \boldsymbol{Y}) \triangleq \frac{1}{N} \sum_{n=1}^N \ell(f(\boldsymbol{x}_n; \boldsymbol{\theta}), \boldsymbol{y}_n)$$

Input $\rightarrow$ | NN with parameters $\boldsymbol{\theta}$ | $\rightarrow$ Output

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- Cannot solve $\nabla_{\boldsymbol{\theta}} L = \mathbf{0}$ analytically in general.

Training as an optimization problem

J. Fessler

Input $\rightarrow$ | NN with parameters $\boldsymbol{\theta}$ | $\rightarrow$ Output

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- Cannot solve $\nabla_{\boldsymbol{\theta}} L = \mathbf{0}$ analytically in general.
- Natural approach is (slow!) gradient descent iteration for $k = 0, 1, \ldots$

$$\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - \alpha \nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}_k),$$

  - step size $\alpha > 0$ aka "learning rate"
  - the gradient $\nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}_k)$ is the vector of partial derivatives of the loss function w.r.t. every NN parameter.
  - Initializer $\boldsymbol{\theta}_0$ often random

Accelerating training

- Use mini-batch approximation to gradient of loss:

$$\nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}_k) = \underbrace{\frac{1}{N}\sum_{n=1}^{N}}_{\text{all data}} \nabla_{\boldsymbol{\theta}} \ell(f(\boldsymbol{x}_n; \boldsymbol{\theta}_k), \boldsymbol{y}_n) \approx \underbrace{\frac{1}{|\mathcal{S}_k|}\sum_{n \in \mathcal{S}_k}}_{\text{some data}} \nabla_{\boldsymbol{\theta}} \ell(f(\boldsymbol{x}_n; \boldsymbol{\theta}_k), \boldsymbol{y}_n),$$

where $\mathcal{S}_k$ is a (often random) subset of the data at kth iteration.
  - Mini-batch size often matched to # of compute threads.
  - Aka **stochastic gradient descent** (SGD) or incremental gradients.

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  - Mini-batch size often matched to # of compute threads.
  - Aka **stochastic gradient descent** (SGD) or incremental gradients.
- Momentum
- Automated step-size selection [13]
- Use GPUs...

The gradient operation looks simple on paper:

$$\nabla_{\boldsymbol{\theta}} \ell(f(\boldsymbol{x}; \boldsymbol{\theta}), \boldsymbol{y}) = \begin{bmatrix} \frac{\partial}{\partial \theta_1} \ell(f(\boldsymbol{x}; \boldsymbol{\theta}), \boldsymbol{y}) \\ \vdots \\ \frac{\partial}{\partial \theta_K} \ell(f(\boldsymbol{x}; \boldsymbol{\theta}), \boldsymbol{y}) \end{bmatrix},$$

but for deep networks the model is a cascade of many functions, one per layer:

$$\boldsymbol{x} \to \boxed{f_1(\cdot; \boldsymbol{\theta})} \to \boxed{f_2(\cdot; \boldsymbol{\theta})} \to \cdots \to \boxed{f_L(\cdot; \boldsymbol{\theta})} \to f(\boldsymbol{x}; \boldsymbol{\theta}) = f_L(\cdots f_2(f_1(\boldsymbol{x}; \boldsymbol{\theta}); \boldsymbol{\theta}); \boldsymbol{\theta}).$$

- In practice most layers have different parameters, but some parameters may affect multiple layers (especially RNN)

Backpropagation

The gradient operation looks simple on paper:

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- In practice most layers have different parameters, but some parameters may affect multiple layers (especially RNN)
- Backpropagation = chain rule for differentiation, hopefully efficiently coded [14] [15]
- Convenient software tools provide automatic differentiation (Python: TensorFlow, PyTorch, ...) (Julia: Flux, ...) (Matlab: MatConvNet?)

Backpropagation illustration (1)

Consider a two-layer NN with a single weight to be learned in the first layer:

$$\begin{array}{c} \text{Input} \\ x \end{array} \to \boxed{\begin{array}{c} \text{Layer1} \\ h_w(\cdot) \end{array}} \xrightarrow{h_w(x)} \boxed{\begin{array}{c} \text{Layer2} \\ g(\cdot) \end{array}} \xrightarrow{g(h_w(x))} \begin{array}{c} \text{Output} \\ \hat{y} = g(h_w(x)) \end{array} \to \boxed{\begin{array}{c} \text{Loss} \\ L(w) \end{array}}$$

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Loss function for a single training sample:

$$L(w) = \ell(g(h_w(x)), y).$$

Consider a two-layer NN with a single weight to be learned in the first layer:

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Loss function for a single training sample:

$$L(w) = \ell(g(h_w(x)), y).$$

Chain rule for derivative of loss w.r.t. weight w:

$$\frac{\partial}{\partial w} L(w) = \dot{L}(w) = \frac{\partial}{\partial w} \ell(f_w(x), y) = \dot{\ell}(g(h_w(x)), y) \, \dot{g}(h_w(x)) \, \dot{h}_w(x).$$

Two key ingredients two compute:

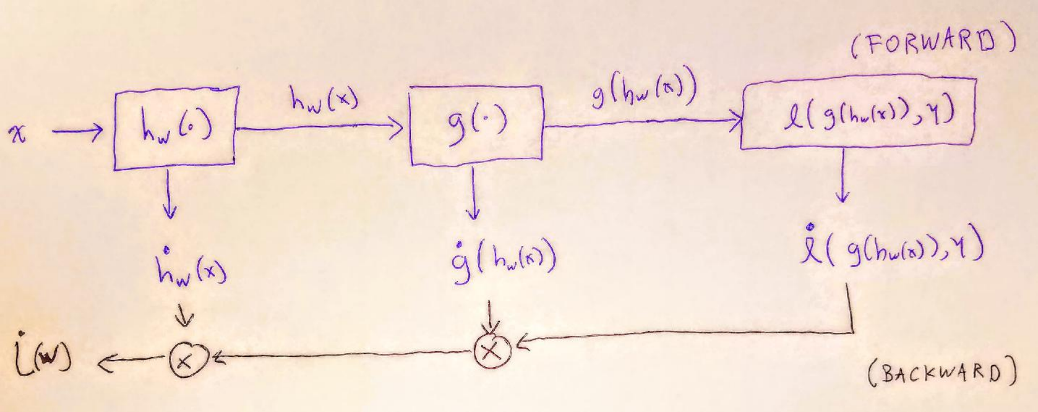
- Model at each layer of NN
- Derivatives of model at each layer, evaluated at layer input

Backpropagation illustration (2)

$$\dot{L}(w) = \dot{\ell}(g(h_w(x)), y) \quad \dot{g}(h_w(x)) \quad \dot{h}_w(x)$$
$$= \dot{h}_w(x) \quad \dot{g}(h_w(x)) \quad \dot{\ell}(g(h_w(x)), y).$$

Backpropagation illustration (2)

$$\dot{L}(w) = \dot{\ell}(g(h_w(x)), y) \quad \dot{g}(h_w(x)) \quad \dot{h}_w(x)$$
$$= \dot{h}_w(x) \quad \dot{g}(h_w(x)) \quad \dot{\ell}(g(h_w(x)), y).$$



Backpropagation illustration (2)

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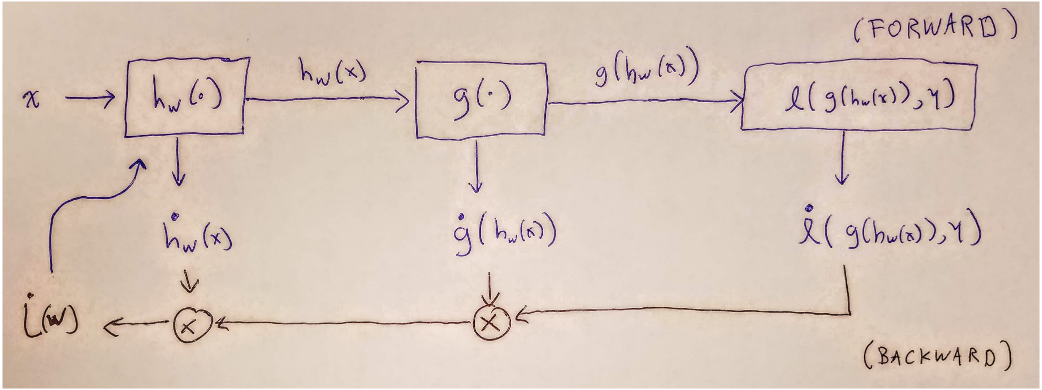

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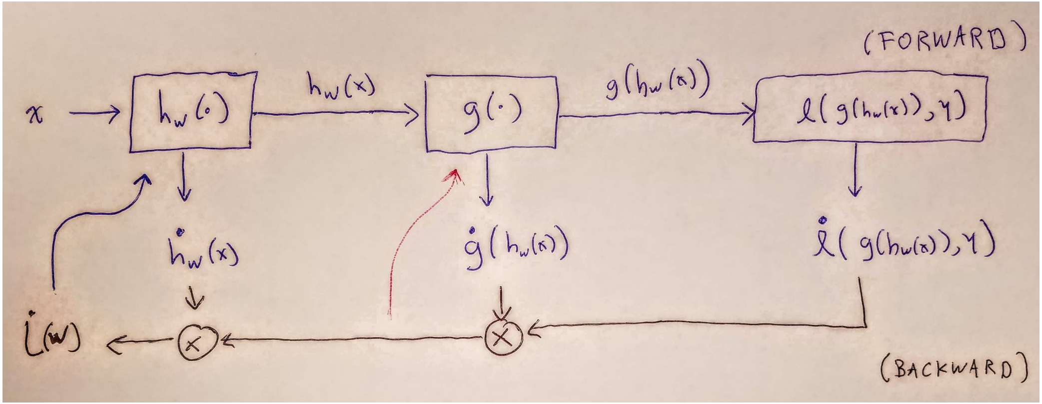
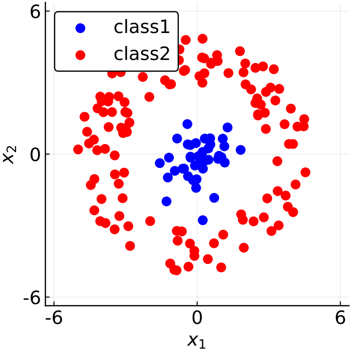


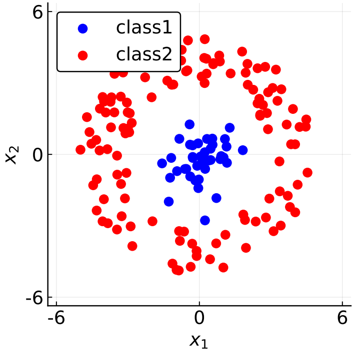
Supervised NN training example: binary classification

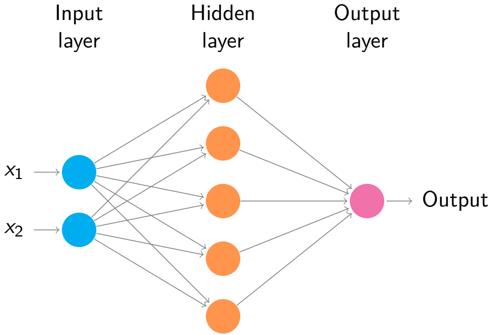
J. Fessler



- Nonlinearity is essential here

Supervised NN training example: binary classification





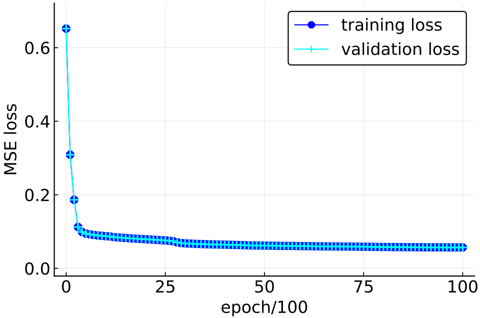
- Nonlinearity is essential here
- Each hidden node is a perceptron with $\text{ReLU}(x) = \max(x, 0)$
- Train output to be 1 for class2 and -1 for class1.

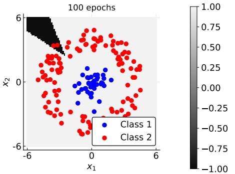
Example Flux code

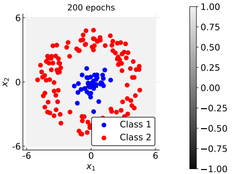
- Julia's Flux library [16] `http://fluxml.ai/Flux.jl`
- ML ingredients: training data $(\boldsymbol{X}, \boldsymbol{Y})$, model/architecture, loss function, optimizer
- For full Jupyter notebook see `https://tinyurl.com/ml2-18-jf`

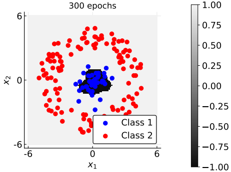
```
nhidden = 10 # neurons in hidden layer
model = Chain(Dense(2,nhidden,relu), Dense(nhidden,1)) # NN arch
loss(x, y) = mse(model(x), y)
iters = 10000 # hand crafted...
dataset = Base.Iterators.repeated((X, Y), iters)
Flux.train!(loss, dataset, ADAM(params(model)))
```

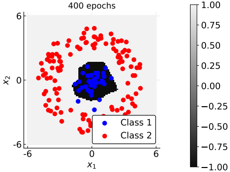
Flux NN training

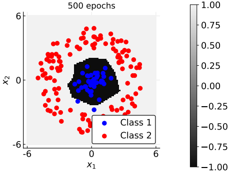


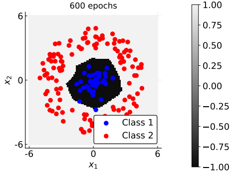












Flux results for binary classification

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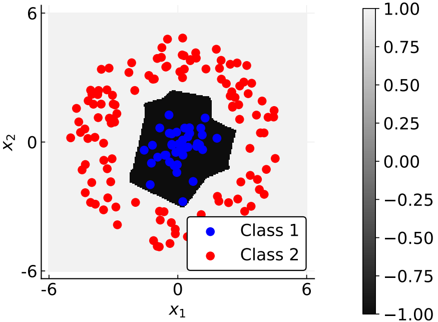
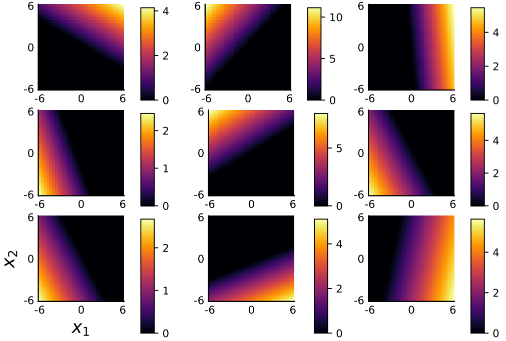
Classifier results



Hidden layer functions



Principles generalize from binary classification to multiclass problems.

NN-based denoising example

See `https://tinyurl.com/ml2-18-jf`

Outline

Roles for machine learning in medical imaging

- Image analysis (post-processing):
  - classification: diagnosis / segmentation / treatment planning, ...
  - regression: localization / registration / quantification, ...
    (object size, e.g., vessel diameter, contrast concentration, T1, T2, ...)
- Image reconstruction
- Image acquisition

Machine learning in medical image interpretation

Most obvious place for machine learning is post-processing:

reconstructed images $\hat{\boldsymbol{x}}$ → ML-based image processing (classification or regression) → interpretation

Special issue of IEEE Trans. on Med. Imaging, May 2016 [17]

IEEE TRANSACTIONS ON MEDICAL IMAGING, VOL. 35, NO. 5, MAY 2016 1153

Guest Editorial

Deep Learning in Medical Imaging: Overview and Future Promise of an Exciting New Technique raw data $\boldsymbol{y}$ → ML-based image reconstruction → images $\hat{\boldsymbol{x}}$

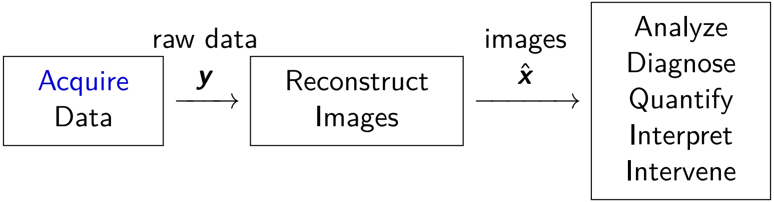
Special issue of IEEE Trans. on Medical Imaging, June 2018 [18]

IEEE TRANSACTIONS ON MEDICAL IMAGING, VOL. 37, NO. 6, JUNE 2018 1289

Image Reconstruction Is a New Frontier of Machine Learning

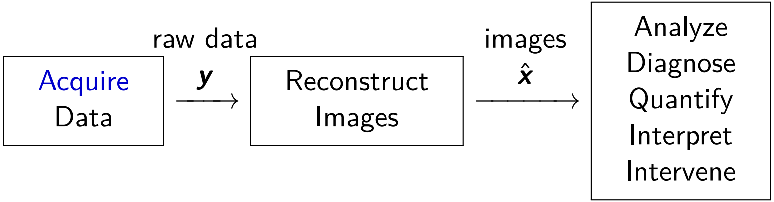
Ge Wang, *Fellow, IEEE*, Jong Chu Ye, *Senior Member, IEEE*, Klaus Mueller, *Senior Member, IEEE*, and Jeffrey A. Fessler, *Fellow, IEEE*

Machine learning in medical imaging: scan design



- Choose best k-space phase encoding locations based on training images:
  - "Learning-based compressive MRI" [19, 20]
    (Volkan Cevher group, June 2018 IEEE T-MI)
  - Yue Cao and David Levin, MRM Sep. 1993 "Feature recognizing MRI" [21–23]

Machine learning in medical imaging: scan design



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  - "Learning-based compressive MRI" [19, 20]
    (Volkan Cevher group, June 2018 IEEE T-MI)
  - Yue Cao and David Levin, MRM Sep. 1993 "Feature recognizing MRI" [21–23]
- Process fMRI data in real time, provide brain-state feedback to subject [24, 25]

Recommended reading (incomplete lists)

- Machine learning books: [26] [27] [28] [29] [30] [31] [32] [33]
- Survey paper(s) [34]
- Optimization: [35]
- DL overviews: [36–38]
- Generative models: [39, 40]:
- Deep learning myths [41]
- NN complexity analysis / function approximation [42–44] [45]
- Application to MR fingerprinting [5, 8]
- MR reconstruction / enhancement using CNN [46–54]
- Dynamic MR reconstruction using CNN [55]
- ...

Talk and code available online at
`https://tinyurl.com/ml2-18-jf`

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