02450: Introduction to Machine Learning and Data Mining

Artificial Neural Networks and Bias/Variance

Jes Frellsen

DTU Compute, Technical University of Denmark (DTU)

DTU Compute
Department of Applied Mathematics and Computer Science

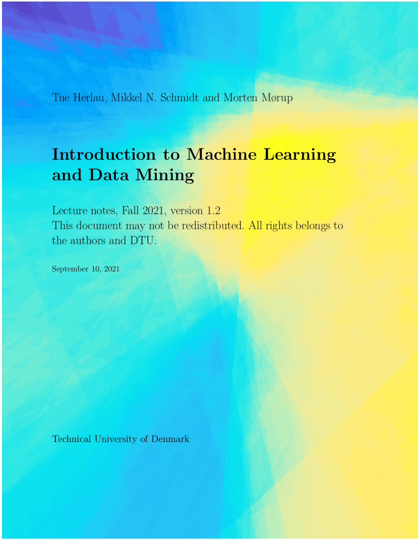
Today

Feedback Groups of the day:

Luke Patrick Chardon Labrie-Cleary, Nok Ching Lai, Kasper Kruse Lange, Lucia Larraona, Nicolai Overgaard Larsen, Jonas Dahl Larsen, Niels Jakob Larsen, Cheuk Yin Lau, Nathaly Yessenia Leon Yupa, Daniel Lewis, Xinchen Li, Alexander Li, Chen Liang, Kalliopi Lianou, Anne Birgitte Lillelund, Seunghwan Lim, Jirapa Limsuriwong, Anders Skott Lind, Emma Victoria Vendel Lind, Jens Valdemar Lindegaard, Mikkel Koefoed Lindtner, Yifan Liu, Yuzhong Liu, Samuel Lonneman, Cheng-Liang Lu, Mathias Herløv Lund, Christian Carlstedt Lundgreen, Michlas Cliff Lund-Mouritzen, Victor Gouveia de Menezes Lyra, Liting Ma, Nada Riad Maarouf, Laura Sofia Machado Gonzalez, Maggie Henry Madsen, Asbjørn Utoft Madsen, Lukás Málek, Ioannis Manganas, Maria Maniati, Beatrice Costanza Marrano, Caroline Uldahl Martensen, Iker Martinez Montoya, Dávid Martini, Rut Mas de Les Valls Cierco

Reading material:

Chapter 14, Chapter 15


Tue Herlau, Mikkel N. Schmidt and Morten Mørup

Introduction to Machine Learning and Data Mining

Lecture notes, Fall 2021, version 1.2
This document may not be redistributed. All rights belongs to the authors and DTU.

September 10, 2021

Technical University of Denmark

Schedule

1. Introduction
   1 February: C1

Data: Feature extraction, and visualization

2. Data, feature extraction and PCA
   8 February: C2, C3
3. Measures of similarity, summary statistics and probabilities
   15 February: C4, C5
4. Probability densities and data visualization
   22 February: C6, C7

Supervised learning: Classification and regression

5. Decision trees and linear regression
   1 March: C8, C9
6. Overfitting, cross-validation and Nearest Neighbor
   8 March: C10, C12 **(Project 1 due before 13:00)**
7. Performance evaluation, Bayes, and Naive Bayes
   15 March: C11, C13
8. **Artificial Neural Networks and Bias/Variance**
   22 March: C14, C15
9. AUC and ensemble methods
   29 March: C16, C17

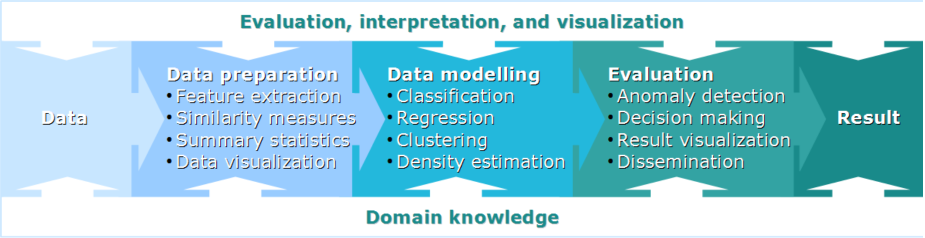
Unsupervised learning: Clustering and density estimation

10. K-means and hierarchical clustering
    5 April: C18
11. Mixture models and density estimation
    19 April: C19, C20 **(Project 2 due before 13:00)**
12. Association mining
    26 April: C21

Recap

13. Recap and discussion of the exam
    3 May: C1-C21

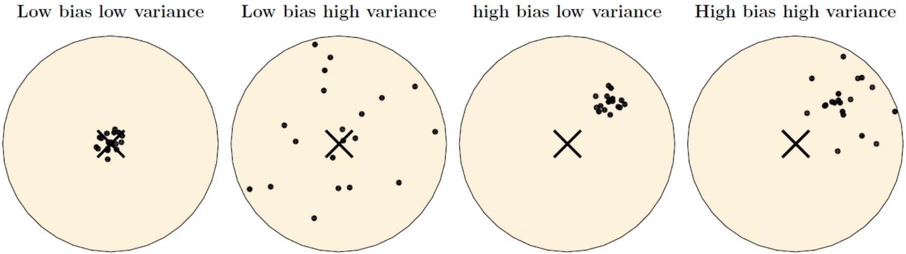
Lecture stream: See DTU Learn
Q&A during lectures: Zoom chat or Piazza
Lecture recordings: `https://video.dtu.dk`
Online assistance (exercises): Microsoft Teams
Online assistance (24/7): Piazza forum



Learning Objectives

- Understand the Bias-Variance decomposition
- Understand and apply regularized least squares regression (i.e. ridge regression)
- Understand the principles behind artificial neural networks (ANNs) and how ANNs can be used for classification and regression
- Understand how logistic regression and ANNs can be extended to multi-class classification

What is bias and what is variance?



Regularized least squares

- Recall cost function from linear regression

$$E(\boldsymbol{w}) = \left\|\boldsymbol{y} - \tilde{\boldsymbol{X}}\boldsymbol{w}\right\|^2$$

- A parsimonious model can be obtained by **forcing** parameters towards zero.
- Problem: Columns of $\boldsymbol{X}$ have very different scale (i.e. require large/small values of $\boldsymbol{w}$)
- Therefore, standardize $\boldsymbol{X}$:

$$\hat{X}_{ij} = \frac{X_{ij} - \mu_j}{\hat{s}_j}, \quad \mu_j = \frac{1}{N}\sum_{i=1}^{N} X_{kj}, \quad \hat{s}_j = \sqrt{\frac{1}{N-1}\sum_{i=1}^{N}(X_{ij} - \mu_j)^2}$$

- Note $\hat{\boldsymbol{X}}$ contains no constant term.

- Introduce regularization term $\lambda\|\boldsymbol{w}\|^2$ to penalize large weights:

$$E_\lambda(\boldsymbol{w}, w_0) = \sum_{i=1}^{N}(y_i - w_0 - \hat{\boldsymbol{x}}^\top \boldsymbol{w})^2 + \lambda\|\boldsymbol{w}\|^2 = \left\|\boldsymbol{y} - w_0\mathbf{1} - \hat{\boldsymbol{X}}\boldsymbol{w}\right\|^2 + \lambda\|\boldsymbol{w}\|^2$$

- We can solve for w_0 and $\boldsymbol{w}$:

$$\frac{dE_\lambda}{dw_0} = \sum_{i=1}^{N} -2(y_i - w_0 - \hat{\boldsymbol{x}}_{\boldsymbol{i}}^\top \boldsymbol{w}) = -2N\mathbb{E}[y] - 2Nw_0 - N\left(\frac{1}{N}\sum_{i=1}^{N}\hat{\boldsymbol{x}}_{\boldsymbol{i}}^\top\right)\boldsymbol{w}$$

$$\Rightarrow w_0 = \mathbb{E}[y]$$

- With $\hat{y}_i = y_i - \mathbb{E}[y]$

$$E_\lambda = \left\|\hat{\boldsymbol{y}} - \hat{\boldsymbol{X}}\boldsymbol{w}\right\|^2 + \lambda\|\boldsymbol{w}\|^2$$

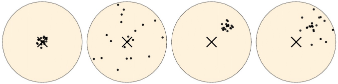
- Setting the derivative wrt. $\boldsymbol{w}$ equal to zero and solving for $\boldsymbol{w}$ yields

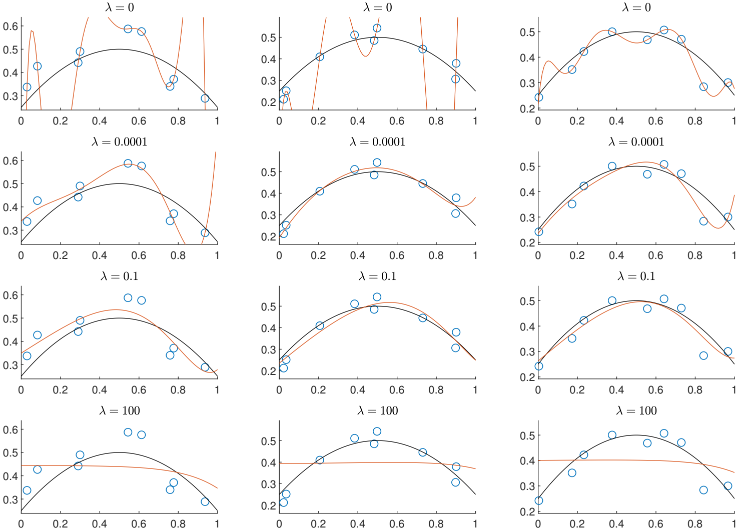
$$\boldsymbol{w}^* = (\hat{\boldsymbol{X}}^\top\hat{\boldsymbol{X}} + \lambda\boldsymbol{I})\backslash(\hat{\boldsymbol{X}}^\top\hat{\boldsymbol{y}})$$

Selecting λ

- Suppose
$$\boldsymbol{w}^* = (\hat{\boldsymbol{X}}^\top \hat{\boldsymbol{X}} + \lambda \boldsymbol{I}) \backslash (\hat{\boldsymbol{X}}^\top \hat{\boldsymbol{y}}) \propto \frac{Xy}{X^2 + \lambda}$$
- So if $\lambda = 0$ then no effect, else if $\lambda \to \infty$ then $\boldsymbol{w}^* \to 0$
- λ controls complexity of model. Select λ using cross-validation

How does different values of λ (vertical) affect the bias/variance of learned function (red lines)





The Bias-Variance decomposition

$$\mathbb{E}_{\mathcal{D}}\left[E^{\text{gen}}\right] = \mathbb{E}_{\mathcal{D},(\boldsymbol{x},y)}\left[\left(y - f_{\mathcal{D}}(\boldsymbol{x})\right)^2\right]$$

We first consider $\boldsymbol{x}$ fixed

$$\bar{y}(\boldsymbol{x}) = \mathbb{E}_{y|\boldsymbol{x}}\left[y\right]$$

$$\begin{aligned}
&\mathbb{E}_{\mathcal{D},y|\boldsymbol{x}}\left[\left(y - f_{\mathcal{D}}(\boldsymbol{x})\right)^2\right] \\
&= \mathbb{E}_{\mathcal{D},y|\boldsymbol{x}}\left[\left(y - \bar{y}(\boldsymbol{x}) + \bar{y}(\boldsymbol{x}) - f_{\mathcal{D}}(\boldsymbol{x})\right)^2\right] \\
&= \mathbb{E}_{y|\boldsymbol{x}}\left[\left(y - \bar{y}(\boldsymbol{x})\right)^2\right] + \mathbb{E}_{\mathcal{D}}\left[\left(\bar{y}(\boldsymbol{x}) - f_{\mathcal{D}}(\boldsymbol{x})\right)^2\right] + 2\mathbb{E}_{\mathcal{D},y|\boldsymbol{x}}\left[\left(y - \bar{y}(\boldsymbol{x})\right)\left(\bar{y}(\boldsymbol{x}) - f_{\mathcal{D}}(\boldsymbol{x})\right)\right]
\end{aligned}$$

https://commons.wikimedia.org/wiki/File:Frustrated_man_at_a_desk_(cropped).jpg

The Bias-Variance decomposition

$$\mathbb{E}_{\mathcal{D}}\left[E^{\text{gen}}\right] = \mathbb{E}_{\mathcal{D},(\boldsymbol{x},y)}\left[\left(y - f_{\mathcal{D}}(\boldsymbol{x})\right)^2\right]$$

We first consider $\boldsymbol{x}$ fixed

$$\bar{y}(\boldsymbol{x}) = \mathbb{E}_{y|\boldsymbol{x}}\left[y\right]$$

$$\mathbb{E}_{\mathcal{D},y|\boldsymbol{x}}\left[\left(y - f_{\mathcal{D}}(\boldsymbol{x})\right)^2\right]$$

$$= \mathbb{E}_{\mathcal{D},y|\boldsymbol{x}}\left[\left(y - \bar{y}(\boldsymbol{x}) + \bar{y}(\boldsymbol{x}) - f_{\mathcal{D}}(\boldsymbol{x})\right)^2\right]$$

$$= \mathbb{E}_{y|\boldsymbol{x}}\left[\left(y - \bar{y}(\boldsymbol{x})\right)^2\right] + \mathbb{E}_{\mathcal{D}}\left[\left(\bar{y}(\boldsymbol{x}) - f_{\mathcal{D}}(\boldsymbol{x})\right)^2\right] + \cancel{2\mathbb{E}_{\mathcal{D},y|\boldsymbol{x}}\left[\left(y - \bar{y}(\boldsymbol{x})\right)\left(\bar{y}(\boldsymbol{x}) - f_{\mathcal{D}}(\boldsymbol{x})\right)\right]}$$

https://commons.wikimedia.org/wiki/File:Frustrated_man_at_a_desk_(cropped).jpg

The Bias-Variance decomposition

$$\mathbb{E}_{\mathcal{D},y|\boldsymbol{x}}\left[\left(y - f_{\mathcal{D}}(\boldsymbol{x})\right)^2\right] = \mathbb{E}_{y|\boldsymbol{x}}\left[\left(y - \bar{y}(\boldsymbol{x})\right)^2\right] + \mathbb{E}_{\mathcal{D}}\left[\left(\bar{y}(\boldsymbol{x}) - f_{\mathcal{D}}(\boldsymbol{x})\right)^2\right]$$

$$\bar{f}(\boldsymbol{x}) = \mathbb{E}_{\mathcal{D}}\left[f_{\mathcal{D}}(\boldsymbol{x})\right]$$

$$\begin{aligned}
&\mathbb{E}_{\mathcal{D}}\left[\left(\bar{y}(\boldsymbol{x}) - f_{\mathcal{D}}(\boldsymbol{x})\right)^2\right] \\
&= \mathbb{E}_{\mathcal{D}}\left[\left(\bar{y}(\boldsymbol{x}) - \bar{f}(\boldsymbol{x}) + \bar{f}(\boldsymbol{x}) - f_{\mathcal{D}}(\boldsymbol{x})\right)^2\right] \\
&= \mathbb{E}_{\mathcal{D}}\left[\left(\bar{y}(\boldsymbol{x}) - \bar{f}(\boldsymbol{x})\right)^2\right] + \mathbb{E}_{\mathcal{D}}\left[\left(\bar{f}(\boldsymbol{x}) - f_{\mathcal{D}}(\boldsymbol{x})\right)^2\right] + 2\mathbb{E}_{\mathcal{D}}\left[\left(\bar{y}(\boldsymbol{x}) - \bar{f}(\boldsymbol{x})\right)\left(\bar{f}(\boldsymbol{x}) - f_{\mathcal{D}}(\boldsymbol{x})\right)\right]
\end{aligned}$$

https://commons.wikimedia.org/wiki/File:Frustrated_man_at_a_desk_(cropped).jpg

The Bias-Variance decomposition

$$\mathbb{E}_{\mathcal{D},y|\boldsymbol{x}}\left[\left(y-f_{\mathcal{D}}(\boldsymbol{x})\right)^2\right]=\mathbb{E}_{y|\boldsymbol{x}}\left[\left(y-\bar{y}(\boldsymbol{x})\right)^2\right]+\mathbb{E}_{\mathcal{D}}\left[\left(\bar{y}(\boldsymbol{x})-f_{\mathcal{D}}(\boldsymbol{x})\right)^2\right]$$

$$\bar{f}(\boldsymbol{x})=\mathbb{E}_{\mathcal{D}}\left[f_{\mathcal{D}}(\boldsymbol{x})\right]$$

$$\begin{aligned}
&\mathbb{E}_{\mathcal{D}}\left[\left(\bar{y}(\boldsymbol{x})-f_{\mathcal{D}}(\boldsymbol{x})\right)^2\right]\\
&=\mathbb{E}_{\mathcal{D}}\left[\left(\bar{y}(\boldsymbol{x})-\bar{f}(\boldsymbol{x})+\bar{f}(\boldsymbol{x})-f_{\mathcal{D}}(\boldsymbol{x})\right)^2\right]\\
&=\mathbb{E}_{\mathcal{D}}\left[\left(\bar{y}(\boldsymbol{x})-\bar{f}(\boldsymbol{x})\right)^2\right]+\mathbb{E}_{\mathcal{D}}\left[\left(\bar{f}(\boldsymbol{x})-f_{\mathcal{D}}(\boldsymbol{x})\right)^2\right]+\xcancel{2\mathbb{E}_{\mathcal{D}}\left[\left(\bar{y}(\boldsymbol{x})-\bar{f}(\boldsymbol{x})\right)\left(\bar{f}(\boldsymbol{x})-f_{\mathcal{D}}(\boldsymbol{x})\right)\right]}
\end{aligned}$$

$$\begin{aligned}
&\mathbb{E}_{\mathcal{D},y|\boldsymbol{x}}\left[\left(y-f_{\mathcal{D}}(\boldsymbol{x})\right)^2\right]\\
&=\mathbb{E}_{y|\boldsymbol{x}}\left[\left(y-\bar{y}(\boldsymbol{x})\right)^2\right]+\left(\bar{y}(\boldsymbol{x})-\bar{f}(\boldsymbol{x})\right)^2+\mathbb{E}_{\mathcal{D}}\left[\left(\bar{f}(\boldsymbol{x})-f_{\mathcal{D}}(\boldsymbol{x})\right)^2\right]\\
&=\mathrm{Var}_{y|\boldsymbol{x}}\left[y\right]+\left(\bar{y}(\boldsymbol{x})-\bar{f}(\boldsymbol{x})\right)^2+\mathrm{Var}_{\mathcal{D}}\left[f_{\mathcal{D}}(\boldsymbol{x})\right]
\end{aligned}$$

The Bias-Variance decomposition

$$\mathbb{E}_{\mathcal{D}}\left[E^{\text{gen}}\right] = \mathbb{E}_{\boldsymbol{x}}\left[\mathbb{E}_{\mathcal{D},y|\boldsymbol{x}}\left[\left(y - f_{\mathcal{D}}(\boldsymbol{x})\right)^2\right]\right]$$

$$\mathbb{E}_{\mathcal{D}}\left[E^{\text{gen}}\right] = \mathbb{E}_{\boldsymbol{x}}\left[\text{Var}_{y|\boldsymbol{x}}\left[y\right] + \left(\bar{y}(\boldsymbol{x}) - \bar{f}(\boldsymbol{x})\right)^2 + \text{Var}_{\mathcal{D}}\left[f_{\mathcal{D}}(\boldsymbol{x})\right]\right]$$

https://commons.wikimedia.org/wiki/File:Frustrated_man_at_a_desk_(cropped).jpg

The Bias-Variance decomposition

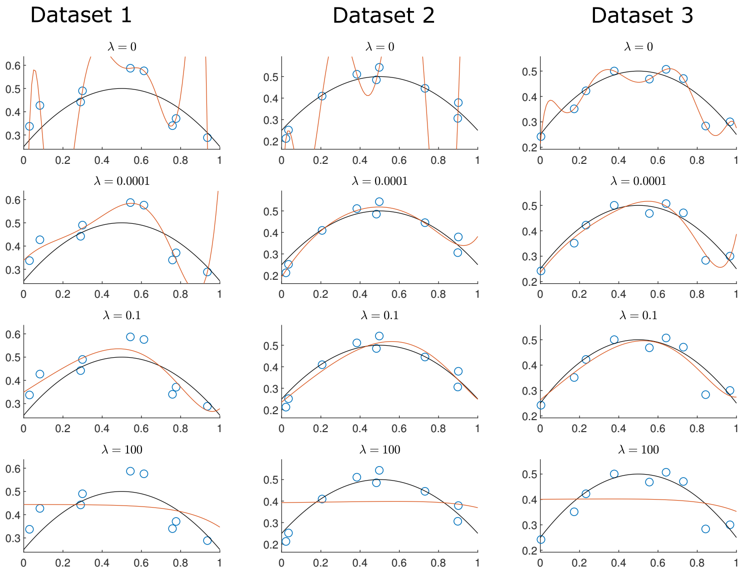
$$\mathbb{E}_{\mathcal{D}}\left[E^{\text{gen}}\right] = \mathbb{E}_{\boldsymbol{x}}\left[\boxed{\mathrm{Var}_{y|\boldsymbol{x}}\left[y\right]} + \boxed{\left(\bar{y}(\boldsymbol{x}) - \bar{f}(\boldsymbol{x})\right)^2} + \boxed{\mathrm{Var}_{\mathcal{D}}\left[f_{\mathcal{D}}(\boldsymbol{x})\right]}\right]$$

The first term does not depend at all upon our choice of model but simply represents the intrinsic difficulty of the problem. We cannot make this term any larger or smaller by selecting one model over another.

The second term is the **bias** term. It tells us how much the average values of models trained on different training datasets differ compared to the true mean of the data.

The third term is the **variance** term. It tells us how much the model wiggles when trained on different sets of training data. That is, when you train the models on N different (random) sets of training data and the models (the prediction curves) are nearly the same this term is small.

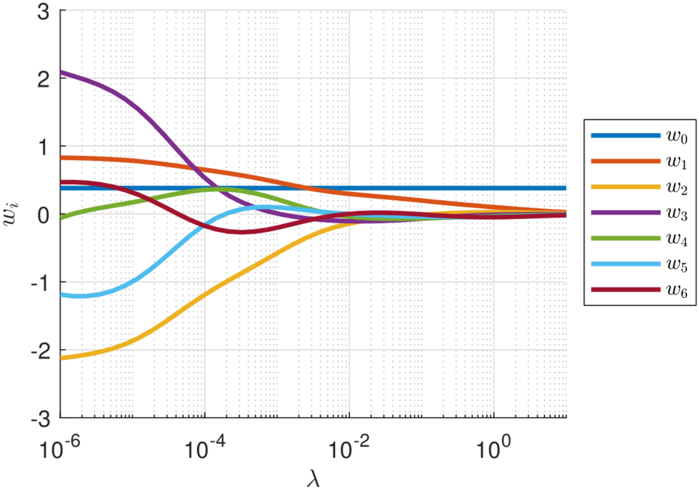
The bias variance decomposition



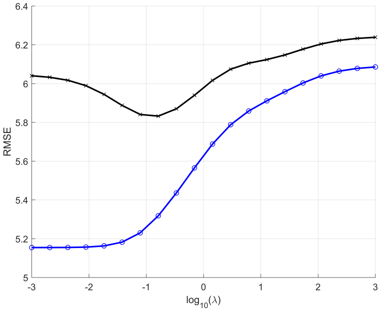
By regularization we can tradeoff bias and variance, in particular, we can hope to substantially reduce variance without introducing too much bias!

Parameters w^* as function of λ

$$E_\lambda(\boldsymbol{w}) = \sum_{i=1}^{N} (\hat{y}_i - w_0 - \hat{\boldsymbol{x}}_i{}^\top \boldsymbol{w})^2 + \lambda \|\boldsymbol{w}\|^2$$



Quiz 1, Bias-variance (Fall 2017)



Using 54 observations of a dataset about Basketball, we would like to predict the average points scored per game (y) based on the four features. For this purpose we consider regularized least squares regression which minimizes with respect to $\boldsymbol{w}$ the following cost function:

$$E(\boldsymbol{w}) = \sum_n (y_n - [1\ x_{n1}\ x_{n2}\ x_{n3}\ x_{n4}]\boldsymbol{w})^2 + \lambda \boldsymbol{w}^\top \boldsymbol{w},$$

We consider 20 different values of λ and use leave-one-out cross-validation to estimate the performance (measured by mean-squared error) of each of these different values of λ and plot the result in the figure. For the value of $\lambda = 0.6952$ the following model is identified:

$$f(\boldsymbol{x}) = 2.76 - 0.37x_1 + 0.01x_2 + 7.67x_3 + 7.67x_4.$$

Which one of the following statements is correct?

A. In the figure the blue curve with circles corresponds to the training error whereas the black curve with crosses corresponds to the test error.

B. According to the model defined for $\lambda = 0.6952$ increasing a players height x_1 will increase his average points scored per game.

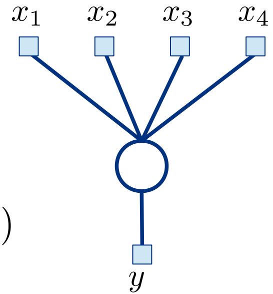
C. There is no optimal way of choosing λ since increasing λ reduces the variance but increases the bias.

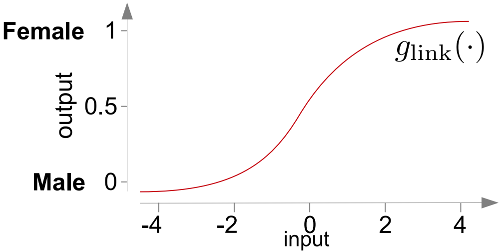
D. As we increase λ the 2-norm of the weight vector $\boldsymbol{w}$ will also increase.

E. Don't know.

General linear model

- **Remember the generalized linear model?**
  - Data $\{\boldsymbol{x}_n, y_n\}_{n=1}^N$
  - Model $f(\boldsymbol{x}) = g_{\text{link}}(\boldsymbol{x}^\top \boldsymbol{w})$
  - Cost function $d\big(y, f(\boldsymbol{x})\big)$
  - Parameters $\boldsymbol{w} = \arg\min_{\boldsymbol{w}} \sum_{n=1}^N d\big(y_n, f(\boldsymbol{x}_n)\big)$

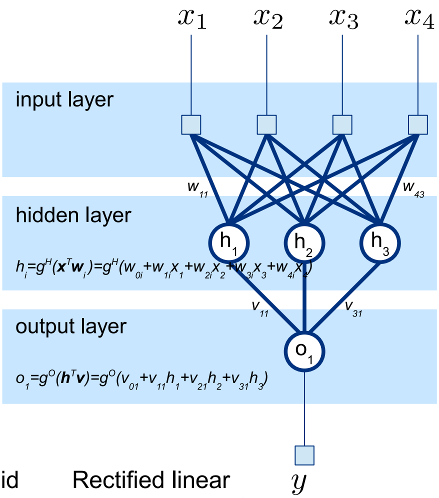




Artificial neural networks

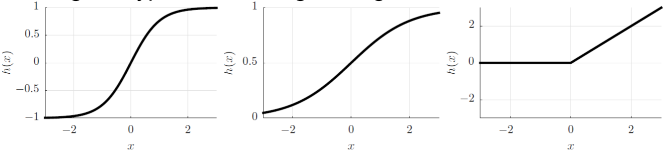
Feed forward network

- Each "neuron"
  - Computes a non-linear function of the sum of its inputs
  - Is just like a generalized linear model
  - Has its own set of parameters
- Modeling choices
  - Cost function
  - Non-linearities
  - Number of neurons and hidden layers
  - Selection of inputs
- Parameter estimation using numerical optimization methods
- Very flexible model: Can easily overfit



Example of non-linearities:

Tangent hyperbolic | Logistic sigmoid | Rectified linear

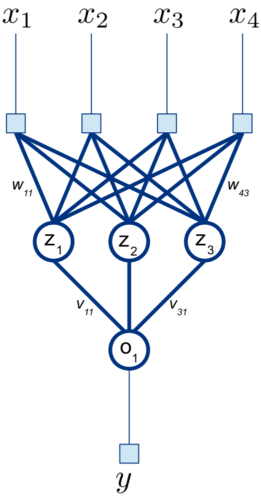


Data: $\{\boldsymbol{x}_i, y_i\}$

Model: $f(\boldsymbol{x}) = h^{(2)}\left(v_{10} + \sum_{j=1}^{H} v_{1j} h^{(1)}\left(\tilde{\boldsymbol{x}}^\top \boldsymbol{w}_j\right)\right)$

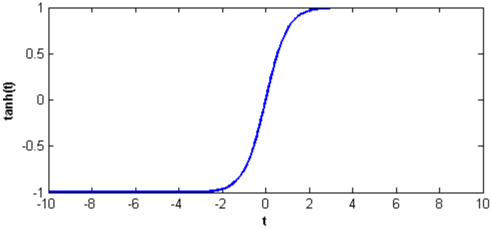
Distance: $d(y, f(\boldsymbol{x}))$

Cost: $E = \sum_{i=1}^{N} d(y_i, f(\boldsymbol{x}_i))$



Common choices

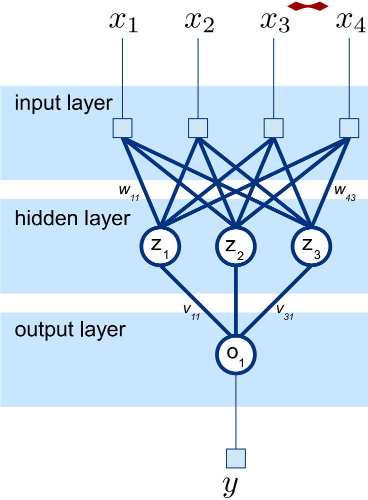
$$h^{(1)}(x) = \tanh(x)$$
$$h^{(2)}(x) = x$$
$$d(y, f(\boldsymbol{x})) = (y - f(\boldsymbol{x}))^2$$



Neurons and layers

Recall:

$$f(\boldsymbol{x}) = h^{(2)}\left(v_{10} + \sum_{j=1}^{H} v_{1j} h^{(1)}\left(\tilde{\boldsymbol{x}}^\top \boldsymbol{w}_j\right)\right)$$



- Let $z_j^{(1)}$ be output of j'th hidden unit

$$z_j^{(1)} = h^{(1)}\left(\boldsymbol{w}_j^{(1)\top} \tilde{x}\right)$$

Abbreviated $\boldsymbol{z}^{(1)} = h^{(1)}\left(\boldsymbol{W}^{(1)} \tilde{x}\right)$

- Output

$$f(\boldsymbol{x}) = h^{(2)}\left(v_{10} + \sum_{j=1}^{H} v_{1j} z_j^{(1)}\right) = h^{(2)}\left(\boldsymbol{W}^{(2)} \boldsymbol{z}^{(1)}\right)$$

We consider each $z_j^{(1)}$ a neuron and $\boldsymbol{z}^{(1)}$ a (hidden) layer

Quiz 2, Artificial Neural Network (Fall 2017)

We will consider an artificial neural network (ANN) trained to predict the average score of a player (i.e., y). The ANN is based on the model:

$$f(\boldsymbol{x}, \boldsymbol{w}) = w_0^{(2)} + \sum_{j=1}^{2} w_j^{(2)} h^{(1)}([1\ \boldsymbol{x}]\boldsymbol{w}_j^{(1)}).$$

where $h^{(1)}(x) = \max(x, 0)$ is the rectified linear function used as activation function in the hidden layer (i.e., positive values are returned and negative values are set to zero). We will consider an ANN with two hidden units in the hidden layer defined by:

$$\boldsymbol{w}_1^{(1)} = \begin{bmatrix} 21.78 \\ -1.65 \\ 0 \\ -13.26 \\ -8.46 \end{bmatrix}, \boldsymbol{w}_2^{(1)} = \begin{bmatrix} -9.60 \\ -0.44 \\ 0.01 \\ 14.54 \\ 9.50 \end{bmatrix},$$

and $w_0^{(2)} = 2.84$, $w_1^{(2)} = 3.25$, and $w_2^{(2)} = 3.46$.

What is the predicted average score of a basketball player with observation vector $\boldsymbol{x}^* = [6.8\ 225\ 0.44\ 0.68]$?

A. 1.00

B. 3.74

C. 8.21

D. 11.54

E. Don't know.

Generalization 1: Multiple outputs

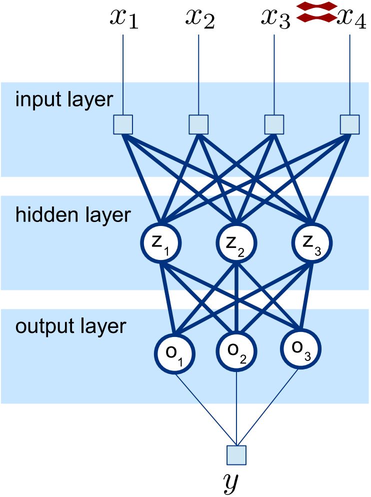
- As before define: $\boldsymbol{z}^{(1)} = h^{(1)}\left(\boldsymbol{W}^{(1)}\tilde{x}\right)$
- Now let $\boldsymbol{W}^{(2)}$ be a $C \times H$ matrix then:

$$\boldsymbol{y} = \boldsymbol{f}(\boldsymbol{x}) = h^{(2)}\left(\boldsymbol{W}^{(2)}\boldsymbol{z}^{(1)}\right)$$

  will be C-dimensional

- Re-define error function

$$E = \sum_{i=1}^{N} \|\boldsymbol{y}_i - \boldsymbol{f}(\boldsymbol{x}_i)\|_2^2$$



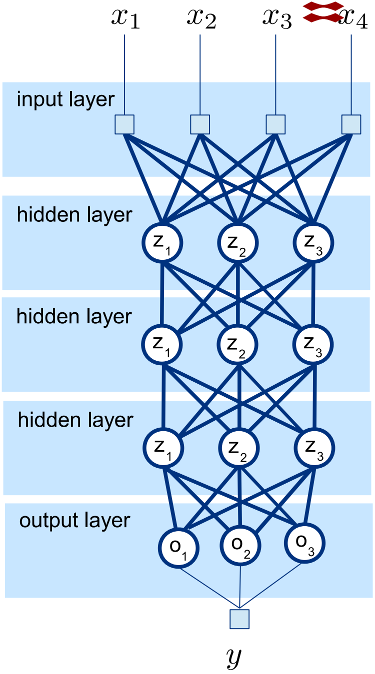
Generalization 2: Multiple layers

- Define $\boldsymbol{z}^{(0)} = \boldsymbol{x}$
- For each layer $l = 1, \ldots, L$ compute

$$z_j^{(l)} = h^{(l)} \left(\boldsymbol{W}^{(l)} \boldsymbol{z}^{(l-1)} \right)$$

- Output is simply

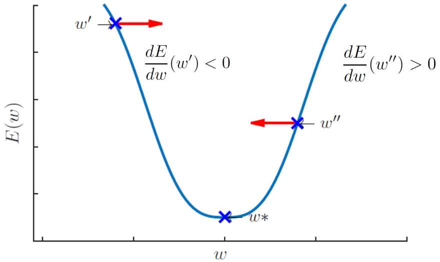
$$\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{z}^{(L)}$$

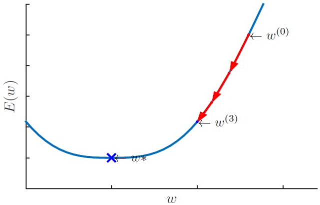


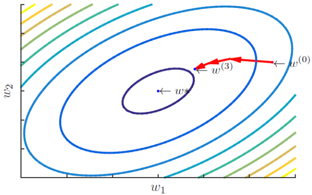
Gradient descent

- Start from an initial guess at $\boldsymbol{w}^*$, $\boldsymbol{w}^{(0)}$
- At step t of the algorithm, modify $\boldsymbol{w}^{(t-1)}$ to produce a better guess $\boldsymbol{w}^{(t)}$:

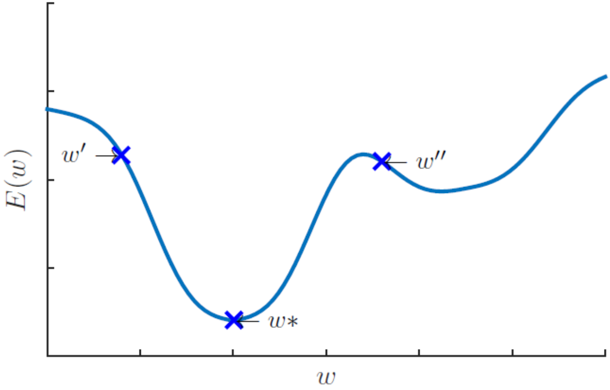
$$\boldsymbol{w}^{(t)} = \boldsymbol{w}^{(t-1)} - \epsilon \frac{dE}{d\boldsymbol{w}}(\boldsymbol{w}^{(t-1)})$$







Contrary to least-squares linear regression and logistic regression ANNs have issues of local minima



Single and multi-class: One out of K coding

Nationality

TXT= 'Sweden' 'Sweden' 'Sweden' 'Sweden' 'Norway' 'Norway' 'Norway' 'Norway' 'Norway' 'Sweden' 'Norway' 'Denmark' 'Denmark' 'Sweden' 'Sweden' 'Sweden' 'Denmark' 'Sweden' 'Norway' 'Denmark'

$\longrightarrow$

X_tmp=

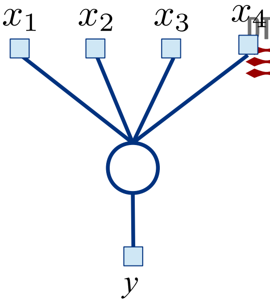
Denmark	Norway	Sweden
0	0	1
0	0	1
0	0	1
0	0	1
0	1	0
0	1	0
0	1	0
0	1	0
0	1	0
0	0	1
0	1	0
1	0	0
1	0	0
0	0	1
0	0	1
0	0	1
1	0	0
0	0	1
0	1	0
1	0	0

One-out-of-K coding

Multi-class classification

- Logistic regression, $y = 0, 1$:

$$p(y|\theta) = \theta^y (1-\theta)^{1-y}$$
$$\theta = \sigma(\boldsymbol{x}^\top \boldsymbol{w})$$



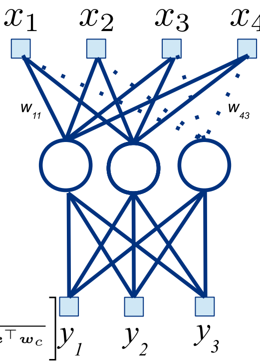
- Multinomial regression, $y = 1, 2, \ldots, K$

z_k : one-of-K encoding of y,

$$p(y|\boldsymbol{\theta}) = \prod_{i=1}^{K} \theta_k^{z_k}$$

$$\boldsymbol{\theta} = \mathrm{softmax}\left(\begin{bmatrix} \boldsymbol{x}^\top \boldsymbol{w}_1 & \cdots & \boldsymbol{x}^\top \boldsymbol{w}_K \end{bmatrix}\right)$$
$$= \begin{bmatrix} \frac{e^{\boldsymbol{x}^\top \boldsymbol{w}_1}}{\sum_{c=1}^{K} e^{\boldsymbol{x}^\top \boldsymbol{w}_c}} & \cdots & \frac{e^{\boldsymbol{x}^\top \boldsymbol{w}_{K-1}}}{\sum_{c=1}^{K} e^{\boldsymbol{x}^\top \boldsymbol{w}_c}} & \frac{e^{\boldsymbol{x}^\top \boldsymbol{w}_K}}{\sum_{c=1}^{K} e^{\boldsymbol{x}^\top \boldsymbol{w}_c}} \end{bmatrix}$$

or: $\boldsymbol{\theta} = \begin{bmatrix} \frac{e^{\boldsymbol{x}^\top \boldsymbol{w}_1}}{1+\sum_{c=1}^{K-1} e^{\boldsymbol{x}^\top \boldsymbol{w}_c}} & \cdots & \frac{e^{\boldsymbol{x}^\top \boldsymbol{w}_{K-1}}}{1+\sum_{c=1}^{K-1} e^{\boldsymbol{x}^\top \boldsymbol{w}_c}} & \frac{1}{1+\sum_{c=1}^{K-1} e^{\boldsymbol{x}^\top \boldsymbol{w}_c}} \end{bmatrix}$



Connection to neural networks

Multinomial regression:

- Define:

$$\boldsymbol{\theta} = \left[\frac{e^{\boldsymbol{x}^\top \boldsymbol{w}_1}}{1+\sum_{c=1}^{K-1} e^{\boldsymbol{x}^\top \boldsymbol{w}_c}} \quad \cdots \quad \frac{1}{1+\sum_{c=1}^{K-1} e^{\boldsymbol{x}^\top \boldsymbol{w}_c}} \right]$$

- Cost function is ($z_{i\cdot}$ is one-of-K encoding of y_i)

$$E = -\sum_{i=1}^{N} \log p(y_i|\boldsymbol{x}_i) = -\sum_{i=1}^{N}\sum_{c=1}^{K} z_{ic} \log \theta_{ic}$$

Multi-class neural network:

- Suppose $\tilde{y}_1, \ldots, \tilde{y}_K$ are outputs of a neural network
- Define

$$\boldsymbol{\theta} = \left[\frac{e^{\tilde{\boldsymbol{y}}^\top \boldsymbol{w}_1}}{\sum_{c=1}^{K} e^{\tilde{\boldsymbol{y}}^\top \boldsymbol{w}_c}} \quad \cdots \quad \frac{e^{\tilde{\boldsymbol{y}}^\top \boldsymbol{w}_K}}{\sum_{c=1}^{K} e^{\tilde{\boldsymbol{y}}^\top \boldsymbol{w}_c}} \right]$$

- Cost function is:

$$E = -\sum_{i=1}^{N} \log p(y_i|\tilde{\boldsymbol{y}}_i) = -\sum_{i=1}^{N}\sum_{c=1}^{K} z_{ic} \log \theta_{ic}$$

Quiz 3, Multinomial Regression (Spring 2016)

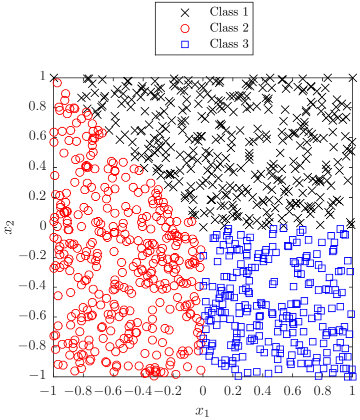


Figure 1: Observations labelled with the most probable class

Consider a multinomial regression classifier for a three-class problem where for each point $\boldsymbol{x} = \begin{bmatrix} x_1 & x_2 \end{bmatrix}^\top$ we compute the class-probability using the softmax function

$$P(\hat{y} = k) = \frac{e^{\boldsymbol{w}_k^\top \boldsymbol{x}}}{e^{\boldsymbol{w}_1^\top \boldsymbol{x}} + e^{\boldsymbol{w}_2^\top \boldsymbol{x}} + e^{\boldsymbol{w}_3^\top \boldsymbol{x}}}.$$

A dataset of $N = 1000$ points where each point is labeled according to the maximum class-probability is shown in Figure 1. Which setting of the weights was used?

A. $w_1 = \begin{bmatrix} -1 \\ -1 \end{bmatrix}$, $w_2 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$, $w_3 = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$

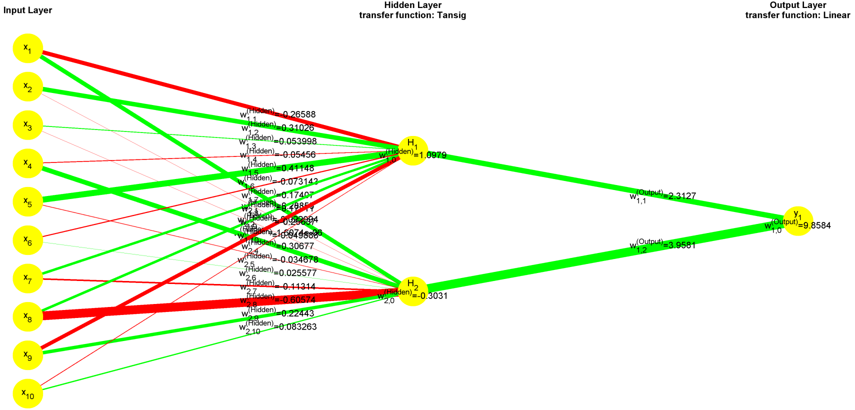
B. $w_1 = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$, $w_2 = \begin{bmatrix} -1 \\ -1 \end{bmatrix}$, $w_3 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$

C. $w_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$, $w_2 = \begin{bmatrix} -1 \\ -1 \end{bmatrix}$, $w_3 = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$

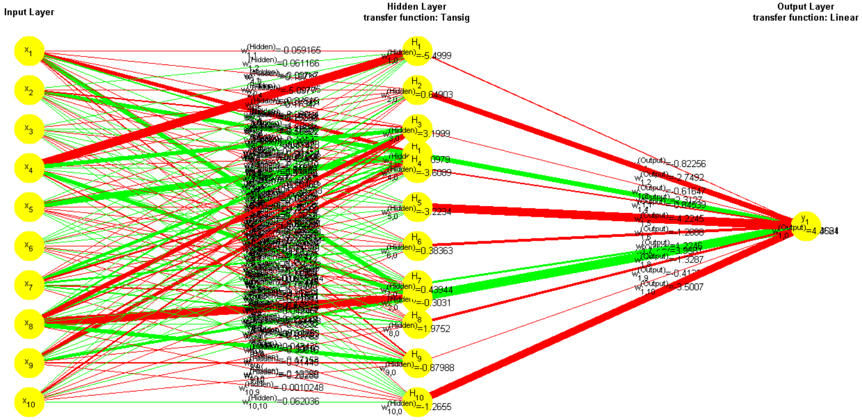
D. $w_1 = \begin{bmatrix} -1 \\ -1 \end{bmatrix}$, $w_2 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$, $w_3 = \begin{bmatrix} -1 \\ 1 \end{bmatrix}$

E. Don't know.

Interpreting neural networks can be difficult



Interpreting neural networks can be difficult



Resources

https://www.youtube.com Exellent video resource explaining the concepts behind neural networks (https://www.youtube.com/watch?v=aircAruvnKk&list=PLZHQObOWTQDNU6R1_67000Dx_ZCJB-3pi)

http://playground.tensorflow.org Sleek interactive neural network example where you can examine the effect of different number of hidden neurons, activation functions, and many other things on training (http://playground.tensorflow.org/)

https://www.tensorflow.org Most popular and well-documented deep learning framework. While well documented, notice it requires some python knowledge (https://www.tensorflow.org/)

https://pytorch.org Upcoming (and in some ways slightly simpler) framework for deep learning; alternative to tensorflow (https://pytorch.org/)