Machine Learning in Healthcare

#C04 Linear Models for Regression

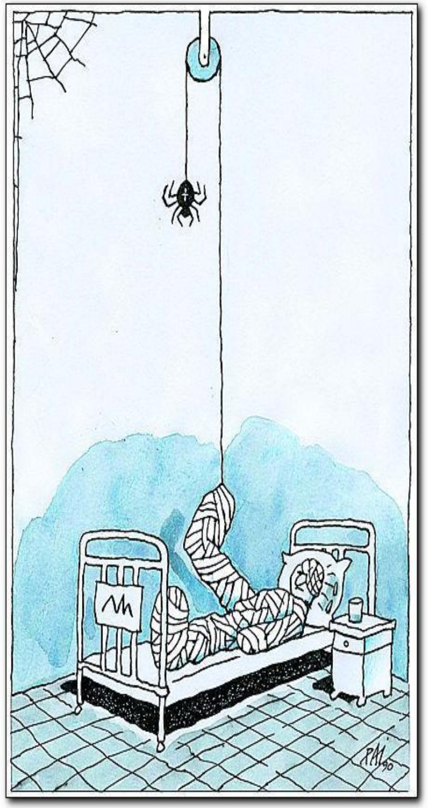
Technion-IIT, Haifa, Israel

Assist. Prof. Joachim Behar
Biomedical Engineering Faculty
Technion-IIT

AIMLab.

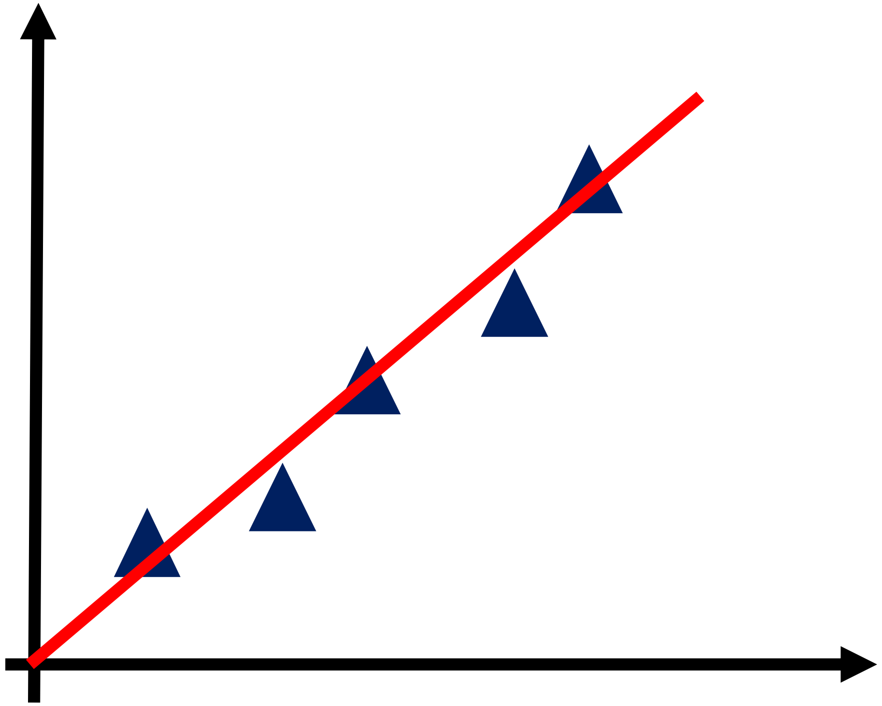
The Problem

- Given the information x, we want to predict event y
- E.g. Our patient's respiration rate is 14, heart rate is 72, GCS is 15.
  - *How long will this patient stay in the hospital?*

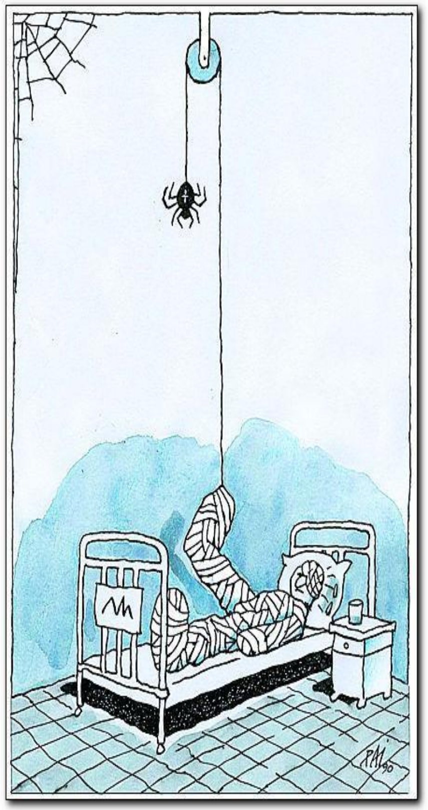


The Problem

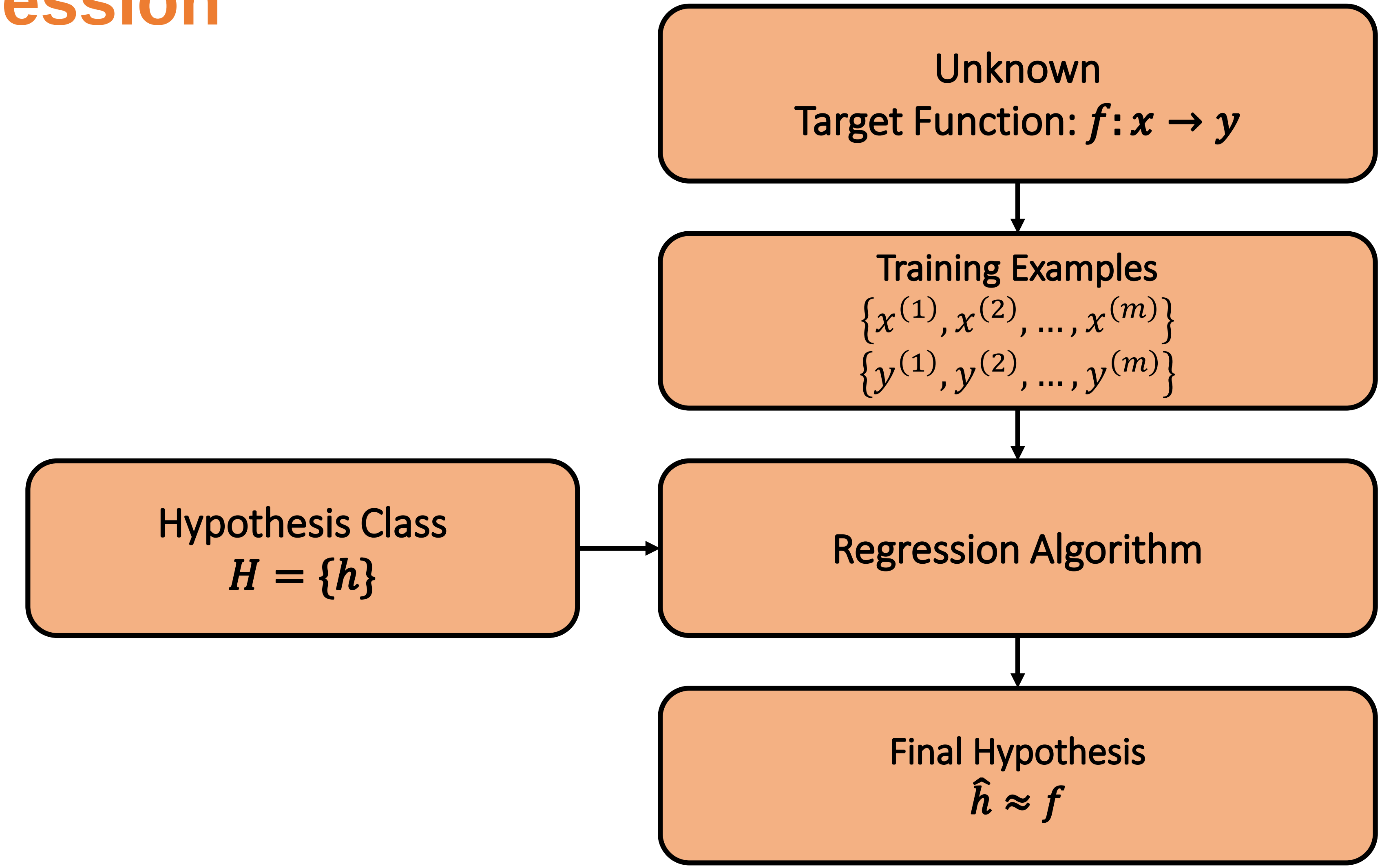
Regression



Estimate relationships among usually continuous variables.

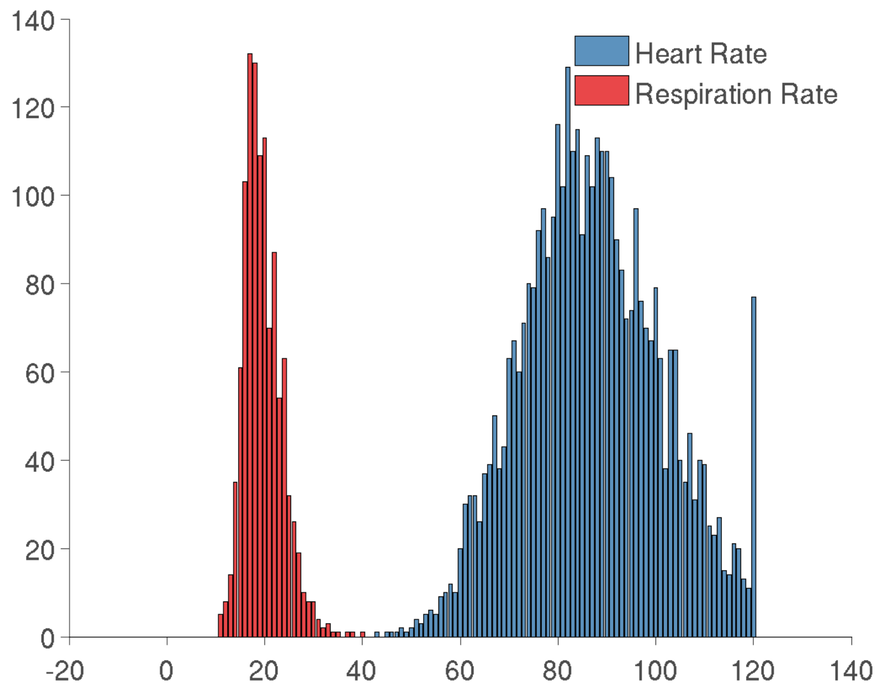


Regression

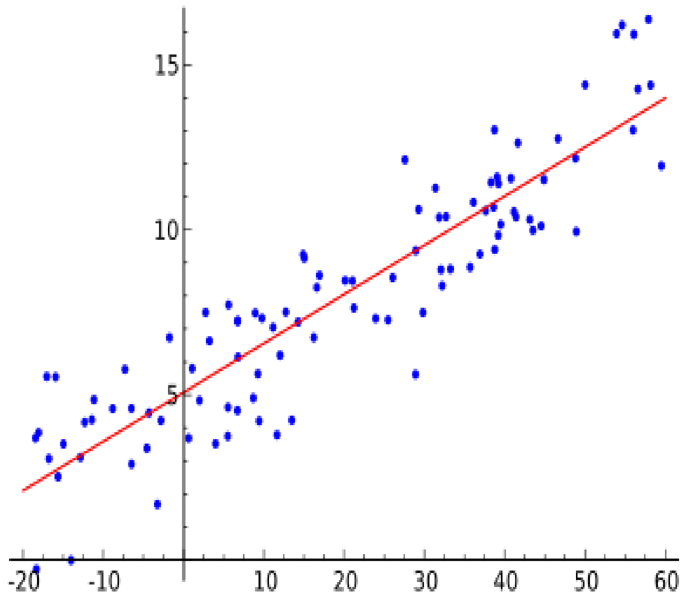

Unknown
Target Function: $\boldsymbol{f}: \boldsymbol{x} \rightarrow \boldsymbol{y}$
Training Examples
$\{x^{(1)}, x^{(2)}, \dots, x^{(m)}\}$
$\{y^{(1)}, y^{(2)}, \dots, y^{(m)}\}$
Hypothesis Class
$\boldsymbol{H} = \{\boldsymbol{h}\}$
Regression Algorithm
Final Hypothesis
$\hat{\boldsymbol{h}} \approx \boldsymbol{f}$

Defining the Problem

- Features, targets, function:
  - Features: $X = \begin{bmatrix} HR_1^{(1)} & RR_{n_x}^{(1)} \\ \dots & \dots \\ HR_1^{(m)} & RR_{n_x}^{(m)} \end{bmatrix} \in \mathbb{R}^{m \times n_x}$
  - Target: $\underline{y} = [y^{(1)}, \dots, y^{(n)}]$
  - Function: $\underline{y} = f(X)$
- Here the hypothesis functions is assumed **linear**.
- On the example:
  - We can imagine that say, higher heart rates (HR) are bad.
  - We can also imagine that lower respiration rates (RR) are bad.
    - $y = w_1 HR + w_2 RR$
    - How do you imagine w_1 and w_2 to look like?



Linear Regression - Intuition



- More generally:
  - $\underline{y} = f(X) = Xw$
    - $w \in \mathbb{R}^{n_x}$
    - $X \in \mathbb{R}^{m \times n_x}$
- Linear regression aims to predict *an independent variable* from one or more *dependent variables*.

Linear Regression - Intuition

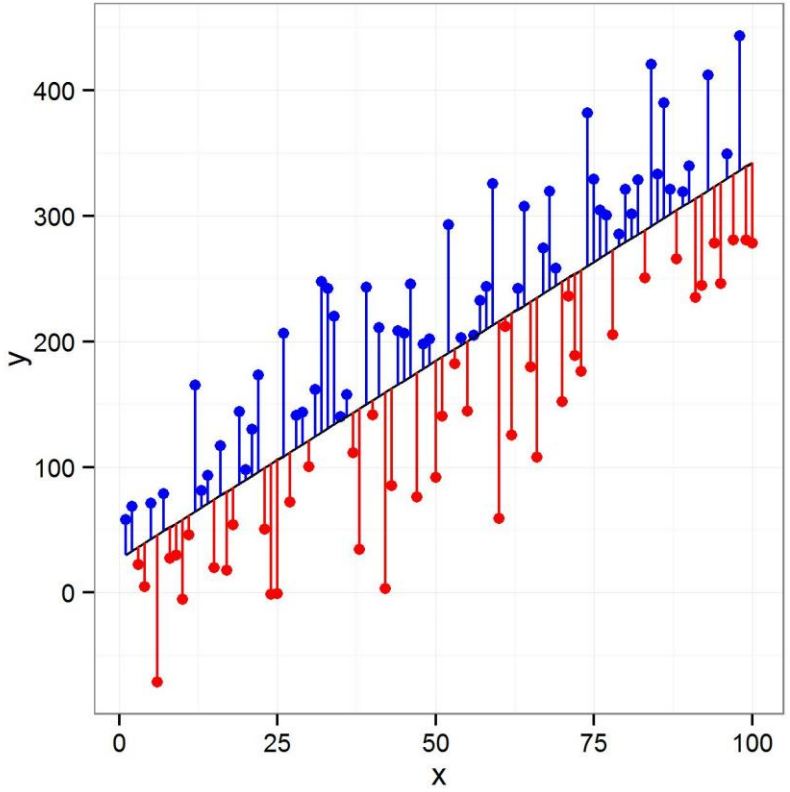
- Formally, **linear regression** involves solving for w:
  - $\underline{y} = w_0 + w_1 x_1 + w_2 x_2 + \cdots + w_n x_n$
- We need a set of m examples for that purpose:
  - $x^{(i)} = [x_1, \dots, x_n] \rightarrow y^{(i)}$
  - This is our **training set**!

Linear Regression - Intuition

- How do we estimate the coefficients?
- Intuitively, we can consider an example:
  - $\begin{bmatrix} 3 \\ 7 \end{bmatrix} = \begin{bmatrix} 3 & 8 \\ -1 & 4 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}$
- Simple enough with matrix math: invert X and solve:
  - $\begin{bmatrix} w_1 \\ w_2 \end{bmatrix} = \begin{bmatrix} 3 & 8 \\ -1 & 4 \end{bmatrix}^{-1} \begin{bmatrix} 3 \\ 7 \end{bmatrix}$
- But it’s not always so simple!
  - $\begin{bmatrix} 1 \\ 3 \end{bmatrix} = \begin{bmatrix} 2 & 3 \\ 6 & 9 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}.$

Linear Regression - Intuition

- How do we estimate the coefficients without directly inverting X?
- The best we can do is minimize some kind or error.
- For example we like **the mean square error (MSE)!**
  - $min_w \left(\left\| \underline{y} - Xw \right\|_2^2 \right)$
  - $J(w) = \frac{1}{m} \sum_{i=1}^{m} (y^{(i)} - w^T x^{(i)})^2$



Mathematical Proof

Linear Regression – Normal Equation

- In the situation where the matrix is not square, we can't directly take the inverse:
  - $\underline{y} = Xw$
- But because we're clever, we noted that $X^T\, X$ is a **positive semi definite** matrix and that these matrices are invertible!
  - $X^T\, X\, w = X^T \underline{y}$
  - $w = (X^T\, X)^{-1} X^T \underline{y}$
  - $(X^T\, X)^{-1} X^T$: pseudo inverse of X
- Turns out minimizing the mean square error is equivalent solving the "**Normal equation**"*
- We will demonstrate that now.

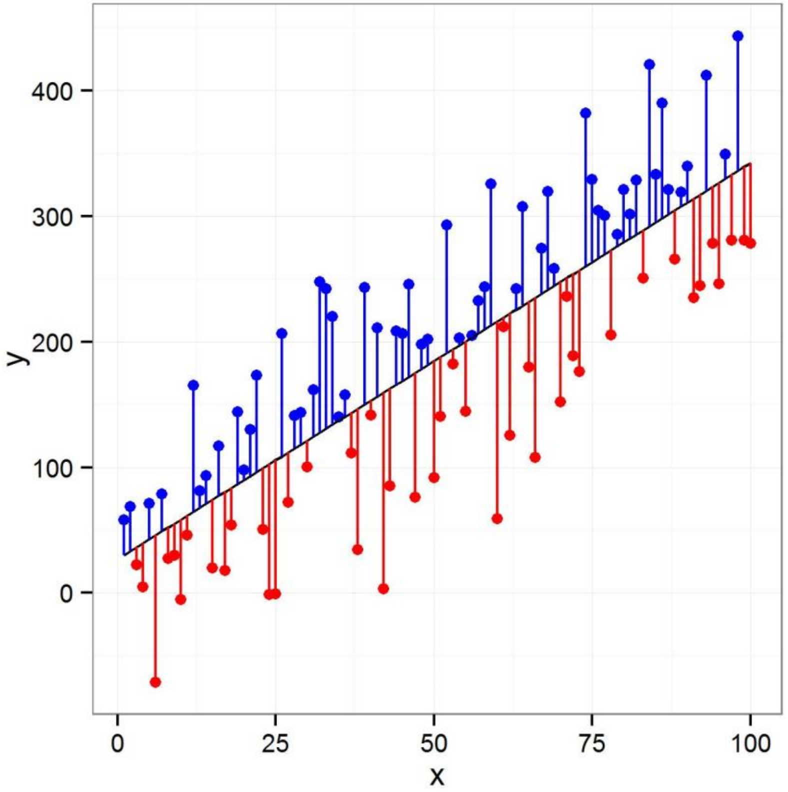
*For bonus points, refer to this as the Moore-Penrose pseudoinverse. Name dropping dead mathematicians makes you sound smart.

Linear Regression – Normal Equation

- To recap:
  - Hypothesis function in linear regression:
    - $y = w_0 + w_1 x_1 + \cdots + w_n x_n$
  - Has a solution that looks like:
    - $w = (X^T X)^{-1} X^T \underline{y}$
    - This is called the **Normal equation**.
  - We now want to prove that the **Normal equation** is a solution to the **linear regression** problem with a **mean square cost function**.
    - $min_w \left(\left\| \underline{y} - Xw \right\|_2^2 \right)$
- We want to minimize the least square cost function:
  - $J(w) = \frac{1}{m} \sum_{i=1}^{m} (y^{(i)} - w^T x^{(i)})^2$

AIMLab.

Mathematical Proof: Using Matrix Calcul



- We want to minimize the least square cost function:
  - $J(w) = \frac{1}{m}\sum_{i=1}^{m}(y^{(i)} - w^{T}x^{(i)})^2$
  - $J(w) = (X\,w - \underline{y})^{T}\,(X\,w - \underline{y})$
    $= (X\,w)^{T}X\,w - (X\,w)^{T}\underline{y} - \underline{y}^{T}(X\,w) + \underline{y}^{T}\underline{y}$
    $= (w^{T}X^{T}\,X\,w - 2(X\,w)^{T}\underline{y} + \underline{y}^{T}\underline{y})$
  - $\frac{\partial J}{\partial w} = 2X^{T}Xw - 2X^{T}\underline{y} = 0$
  - $X^{T}Xw = X^{T}\underline{y}$
  - $w = (X^{T}\,X)^{-1}X^{T}\underline{y}$
- We have shown that minimizing the mean square cost function in linear regression is equivalent to solving the normal equation.

Mathematical Proof: Probabilistic Derivation

- We now want to make this mathematical proof by taking a probabilistic approach.
- Probability: measure of the **likelihood** of an event to happen.
- Target scalar y is given by a deterministic function $f(x, w)$ with an additive zero mean Gaussian noise:
  - $y = f(x, w) + \epsilon$
  - $\epsilon \sim \mathcal{N}(0, \beta^{-1}), \beta = 1/\sigma^2$
    - Thus is a zero mean Gaussian random variable.
  - $p(y|x, w, \beta) = \mathcal{N}(y|f(x, w), \beta^{-1}) = \mathcal{N}(y|w^T x, \beta^{-1})$
- We can write the likelihood function:
  - $p\left(\underline{y}\middle|X, w, \beta\right) = \prod_{i=1}^{m} \mathcal{N}(y^{(i)}|w^T x^{(i)}, \beta^{-1}).$

Mathematical Proof: Probabilistic Derivation

- In supervised learning problems such as regression (and classification) we are not seeking to model the distribution of the input variables. Thus X will always appear in the set of conditional variables and so we can simplify the notation:
  - $p\left(\underline{y}\middle|X,w,\beta\right) \rightarrow p\left(\underline{y}\middle|w,\beta\right)$
- Taking the logarithm of the likelihood function:
  - $ln\left(p\left(\underline{y}\middle|w,\beta\right)\right) = \sum_{i=1}^{m} ln(\mathcal{N}\left(y^{(i)}\middle|w^T x^{(i)},\beta^{-1}\right))$

$$= \frac{m}{2} ln(\beta) - \frac{m}{2} ln(2\pi) - \beta \frac{1}{2} \sum_{i=1}^{m} (y^{(i)} - w^T x^{(i)})^2$$

Sum-of-squares error function

Mathematical Proof: Probabilistic Derivation

- We now take the derivative of the log likelihood:
  - $\nabla\, ln\big(p(y|w,\beta)\big) = \beta \sum_{i=1}^{m} (y^{(i)} - w^T x^{(i)})\, x^{(i)T}$
- Setting the gradient to zero leads to:
  - $\sum_{i=1}^{m} (y^{(i)} - w^T x^{(i)}) x^{(i)T} = 0$
  - $\sum_{i=1}^{m} y^{(i)} x^{(i)T} - w^T \sum_{i=1}^{m} x^{(i)} x^{(i)T} = 0$
  - $w^T = (X^T X)^{-1} X^T \underline{y}$
- We assumed the distribution of the error term to belong to a certain parametric family f_θ of probability distribution.
- We further assumed that $\epsilon \sim \mathcal{N}(0, \beta^{-1})$
- In this particular case we showed that the maximum likelihood estimate is equal to the OLS estimate.

Sequential Learning

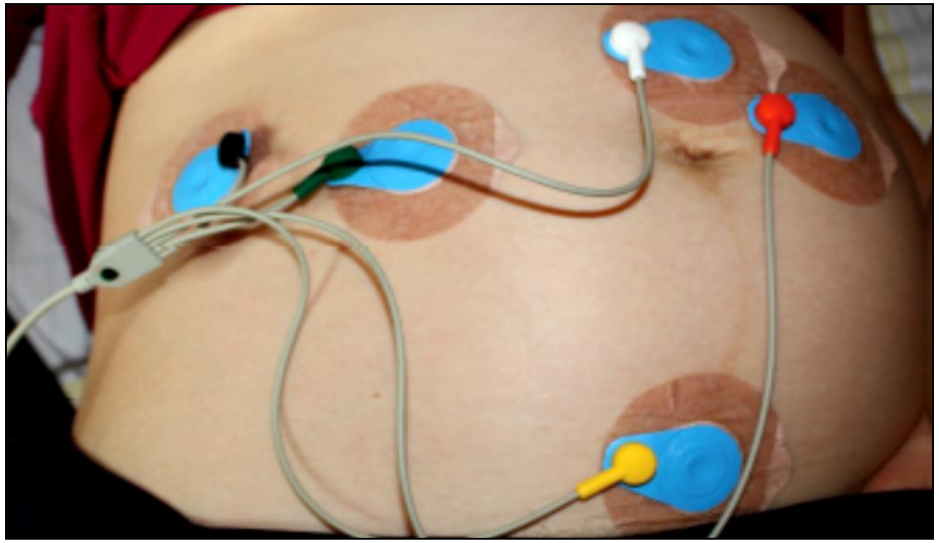
Sequential Learning

- The **normal equation** is a closed form solution. It involves processing the entire training set in one go. This can be computationally costly for large datasets.
- **Sequential algorithm**/on-line algorithm can be useful: data points are considered one at a time and model parameters are updated after each such presentation.
- It is also useful when observations are arriving in a continuous stream and prediction must be made before all prediction are seen.

Sequential Learning

- **Stochastic gradient descent**:
  - $w(n+1) = w(n) + \eta \cdot \nabla J(n)$
- Assuming a sum of squared error:
  - $w(n+1) = w(n) + \eta \cdot \left(y(n) - w^T(n) \cdot x(n)\right)x(n)$
  - This is known as the **least mean square (LMS) algorithm**.
  - η is the learning rate - must be chosen carefully to ensure convergence.
  - w is initialized to some starting values
  - $J(n)$ the error of the nth incoming data point.

Sequential Learning - Example



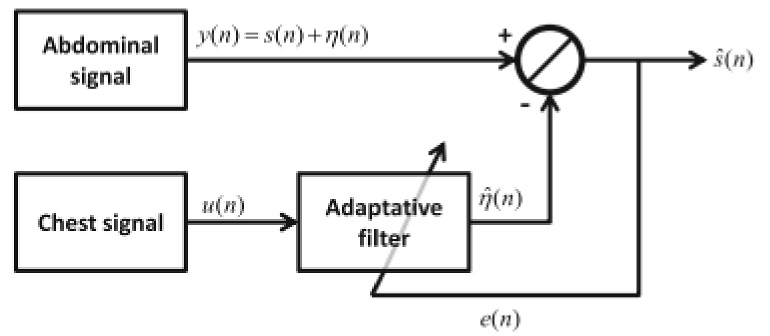
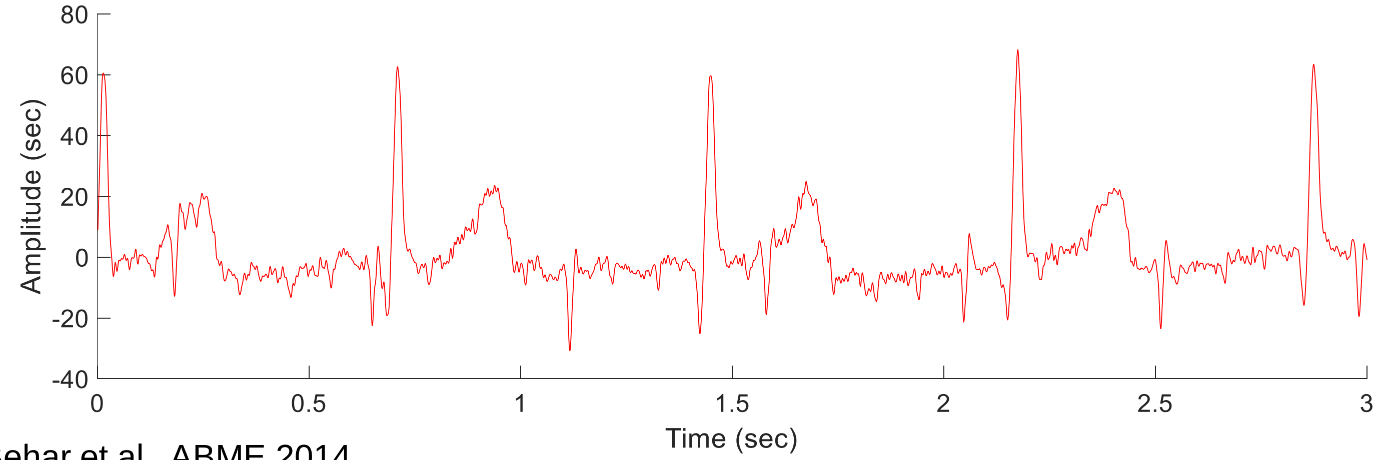


FIGURE 2. Adaptive noise canceling block diagram in the case of one reference input $u(n)$. On the diagram : the FECG $s(n)$, the noise $\eta(n)$, the abdominal ECG $y(n) = s(n) + \eta(n)$, the chest signal $u(n)$, the estimated noise $\hat{\eta}(n)$, the estimation error $e(n)$ and the output signal $\hat{s}(n)$. n corresponds to a time index.



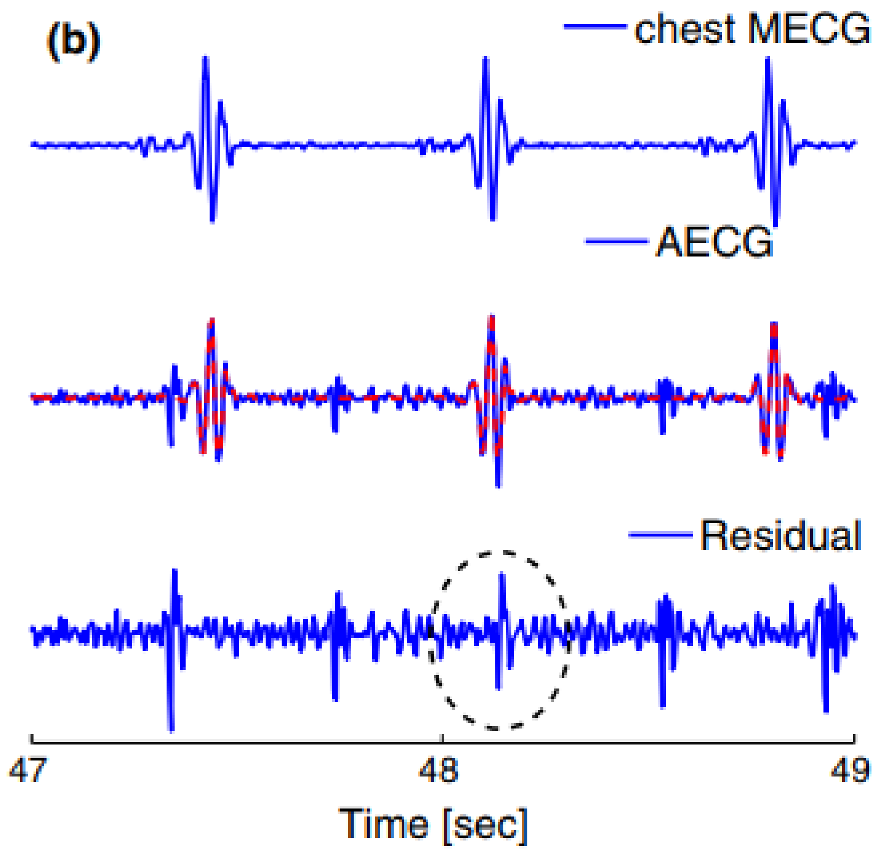
$$\hat{\eta}(n) = \underline{\mathbf{w}}^T(n-1)\underline{\mathbf{u}}(n) \qquad (1)$$

$$e(n) = y(n) - \hat{\eta}(n) \qquad (2)$$

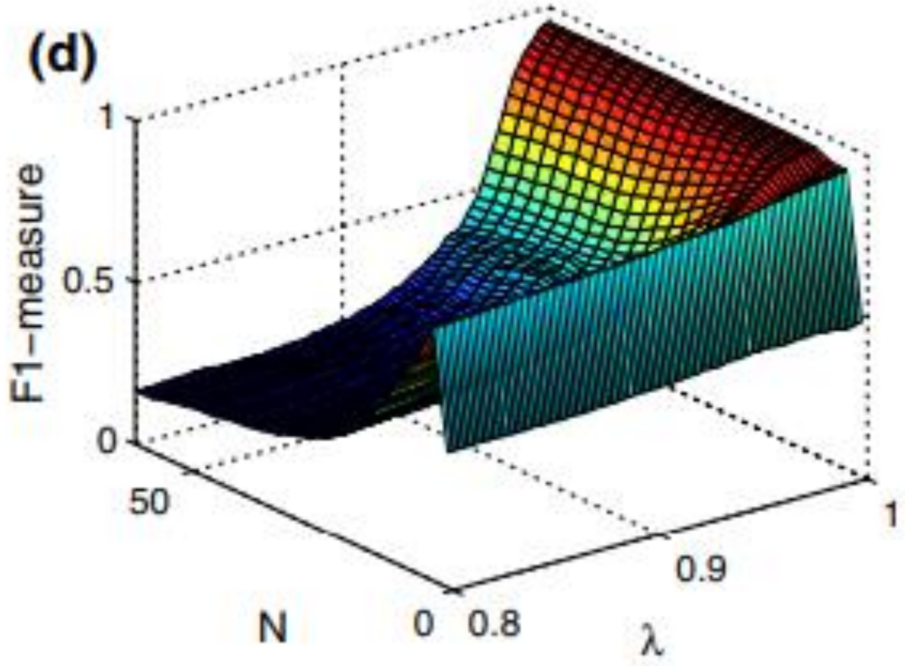
$$\underline{\mathbf{w}}(n) = \underline{\mathbf{w}}(n-1) + \mu e(n)\underline{\mathbf{u}}(n) \qquad (3)$$

Behar et al., ABME 2014

Sequential Learning - Example



- Dataset 1 for training and dataset 2 for test.



Behar et al., ABME 2014

Take Home

- **Linear regression**: predict an independent variable from one or more dependent variables.
- **Algebraic** and **Probabilistic derivation** of the solution.
  - Differences in assumptions and approach to the same problem.
  - **Normal equation** - closed form solution.
  - Probabilistic derivation - also provides an estimate of the noise distribution.
- **Stochastic gradient descent** - sequential learning.

Next Lecture

- Regression or Classification?
- The approach you take depends on the question you ask:
  - How long will this patient stay in ICU? ➔ regression.
  - Will this patient survive from his ICU stay? ➔ classification.
- In the next lecture we will talk about **Linear Models for Classification**.
- Important note: defining your question i.e. whether you are dealing with a regression or classification problem is critical before starting any development!

References

[1] Oxford, CDT course 2015
[2] Pattern recognition and Machine Learning. Christopher M. Bishop. 2006 Springer Science.
[3] https://eli.thegreenplace.net/2014/derivation-of-the-normal-equation-for-linear-regression/