Supervised Learning : Linear Regression and Logistic Regression

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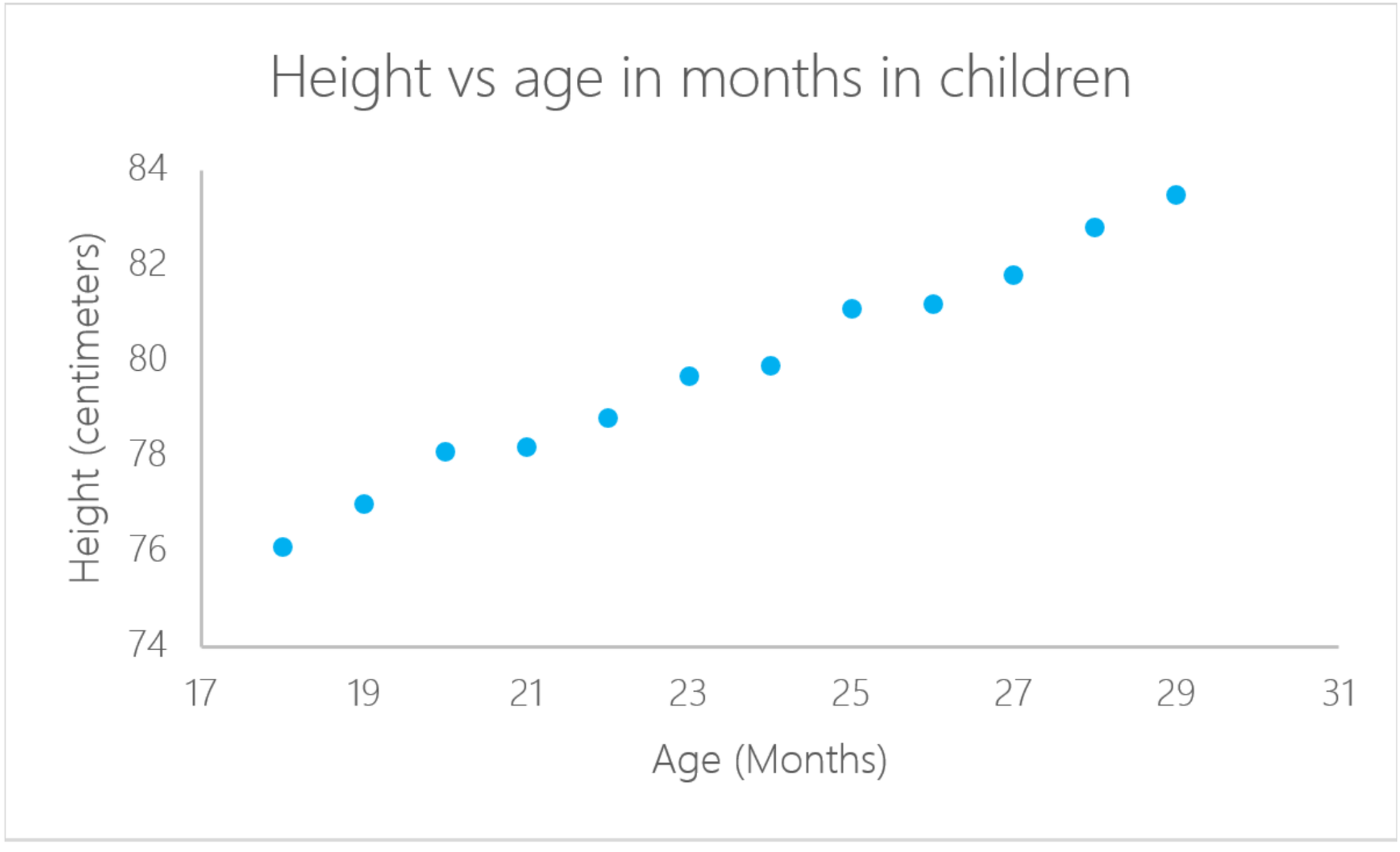
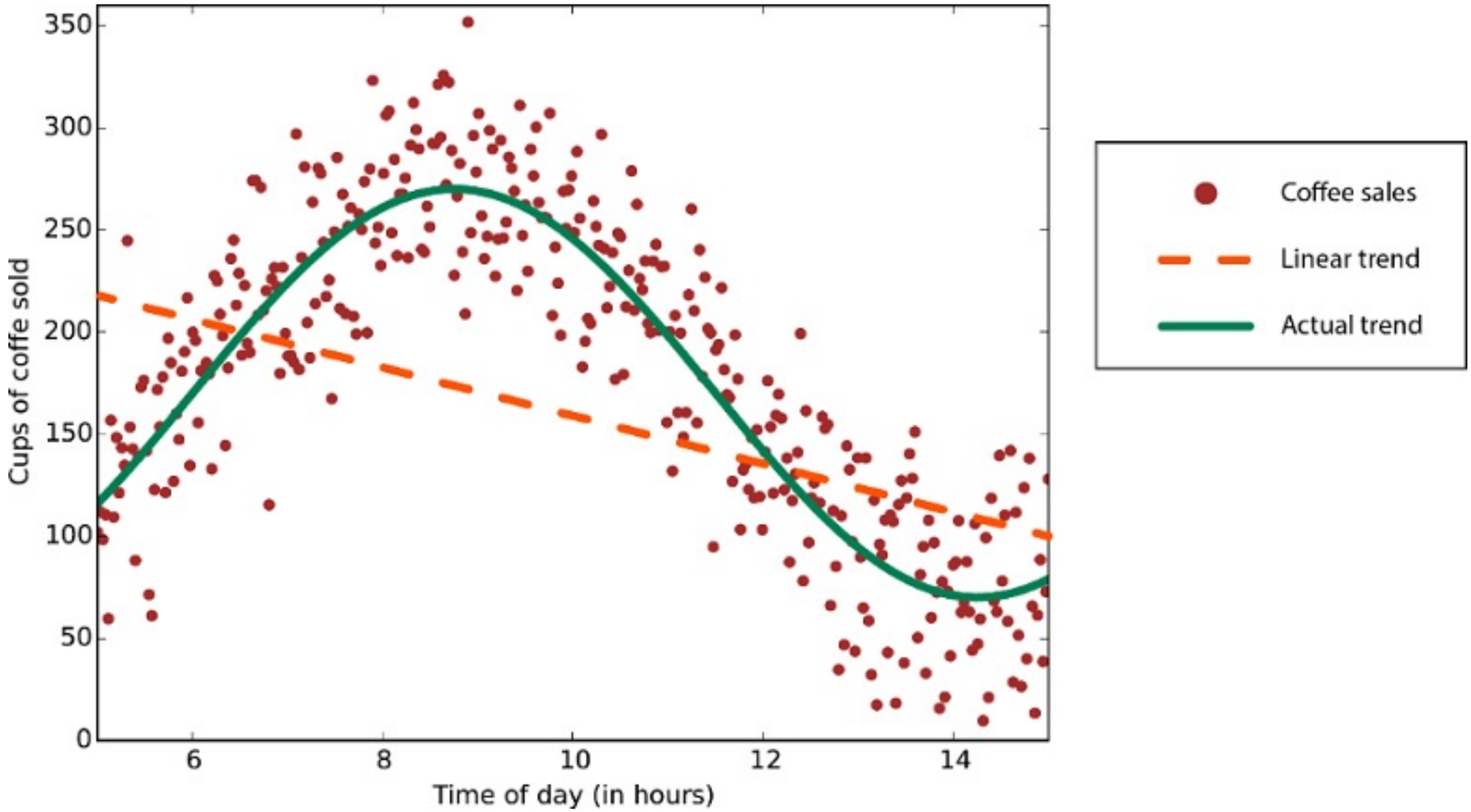
Supervised learning



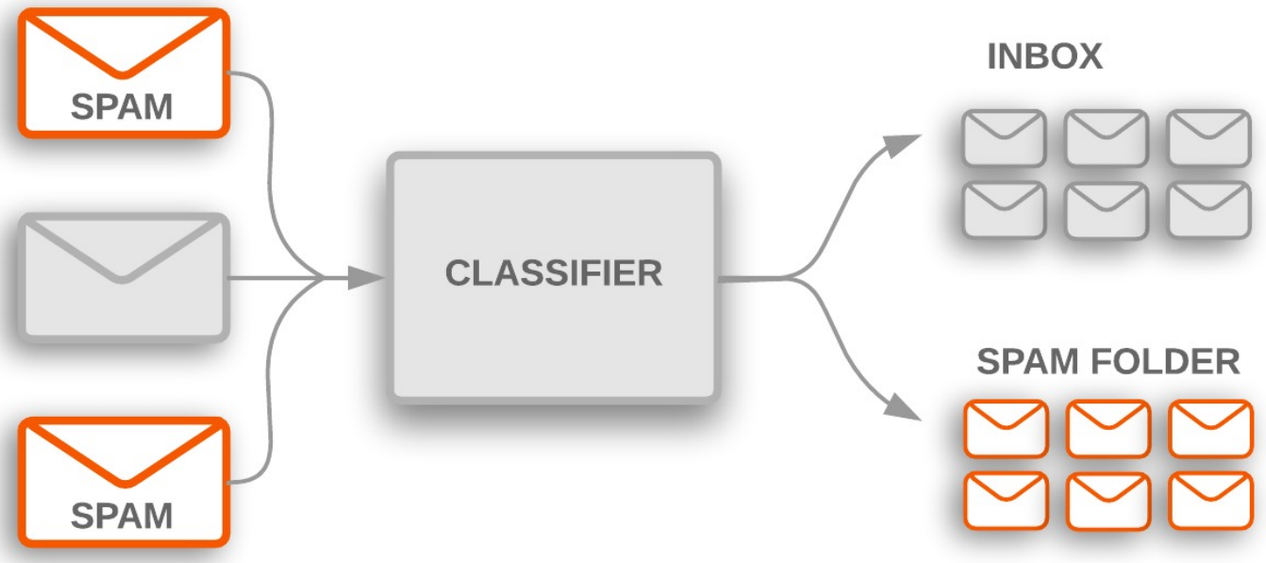
https://www.datacamp.com/community/tutorials/linear-regression-R

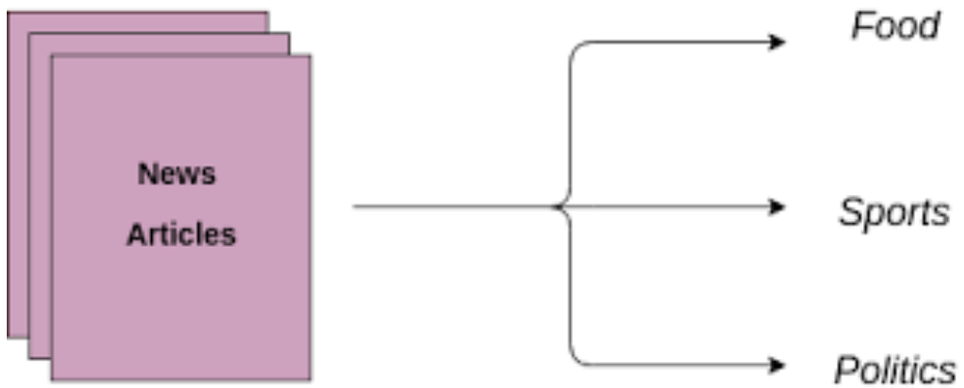
Supervised learning



https://medium.com/@heyozramos/regression-vs-classification-86d73c281c5e

Supervised Learning





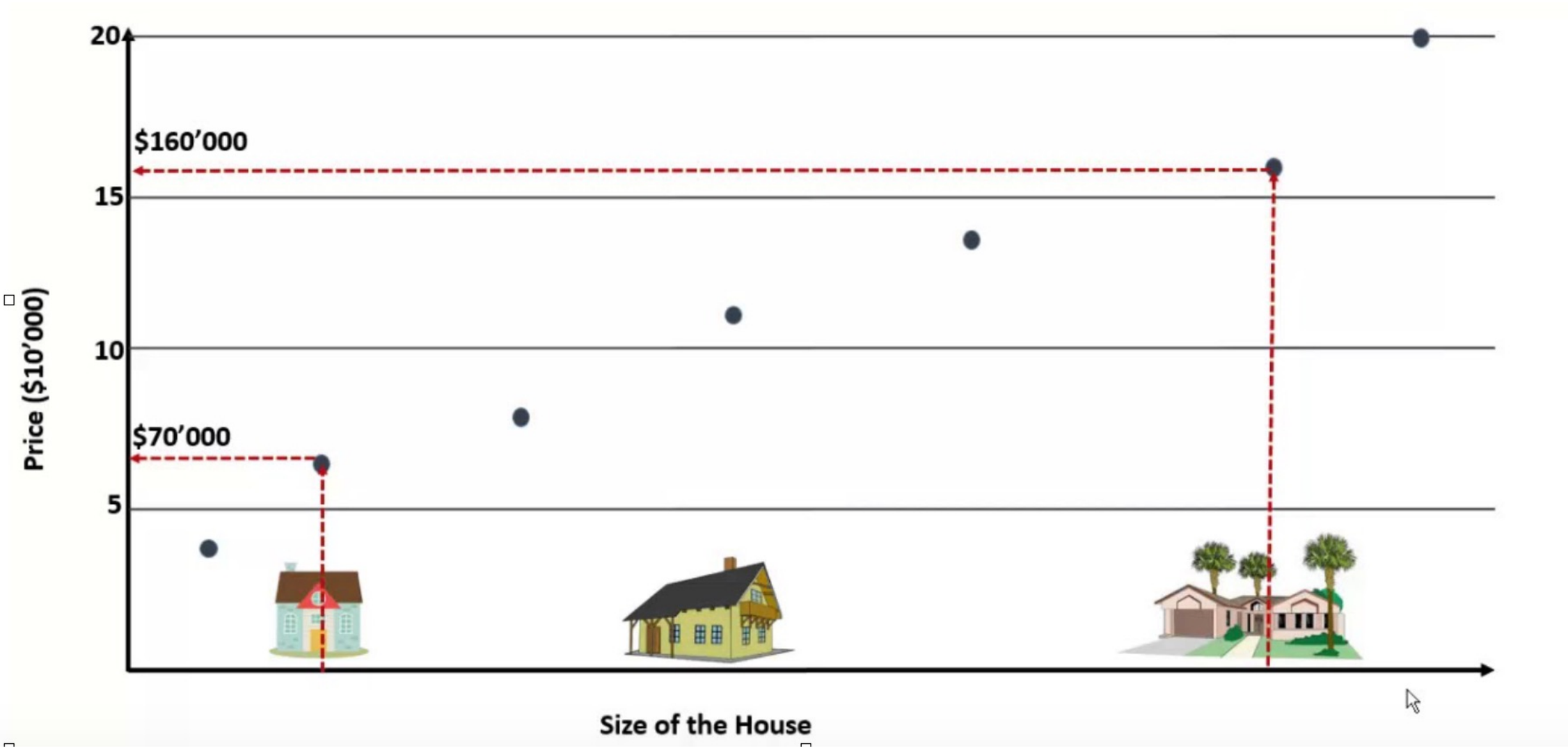
"I love this movie.
I've seen it many times
and it's still awesome."

"This movie is bad.
I don't like it it all.
It's terrible."

Outline

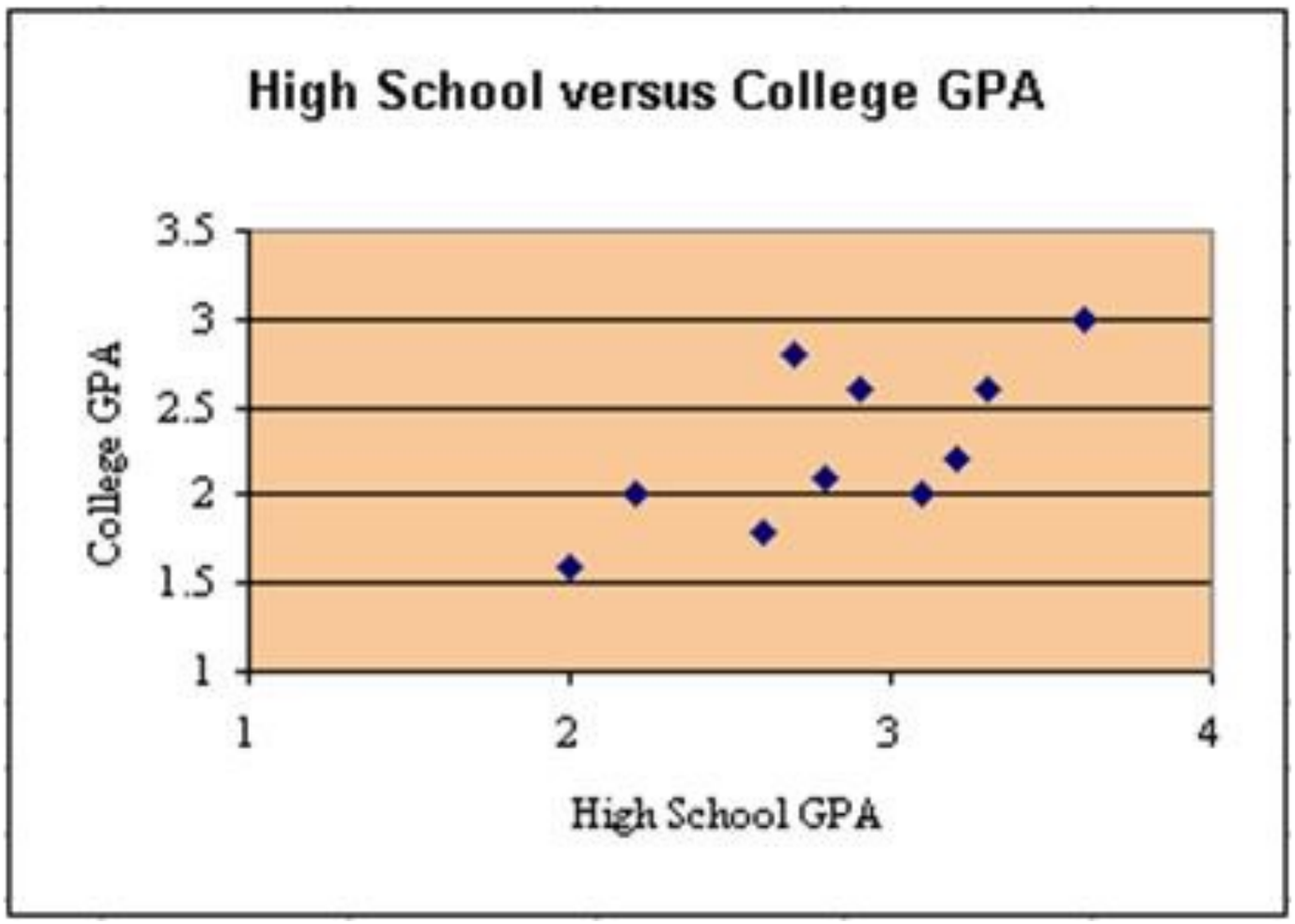
- Supervised Learning
- Regression
- Classification
- Linear Regression
- Logistic Regression
- Poisson Regression

Supervised learning : Regression

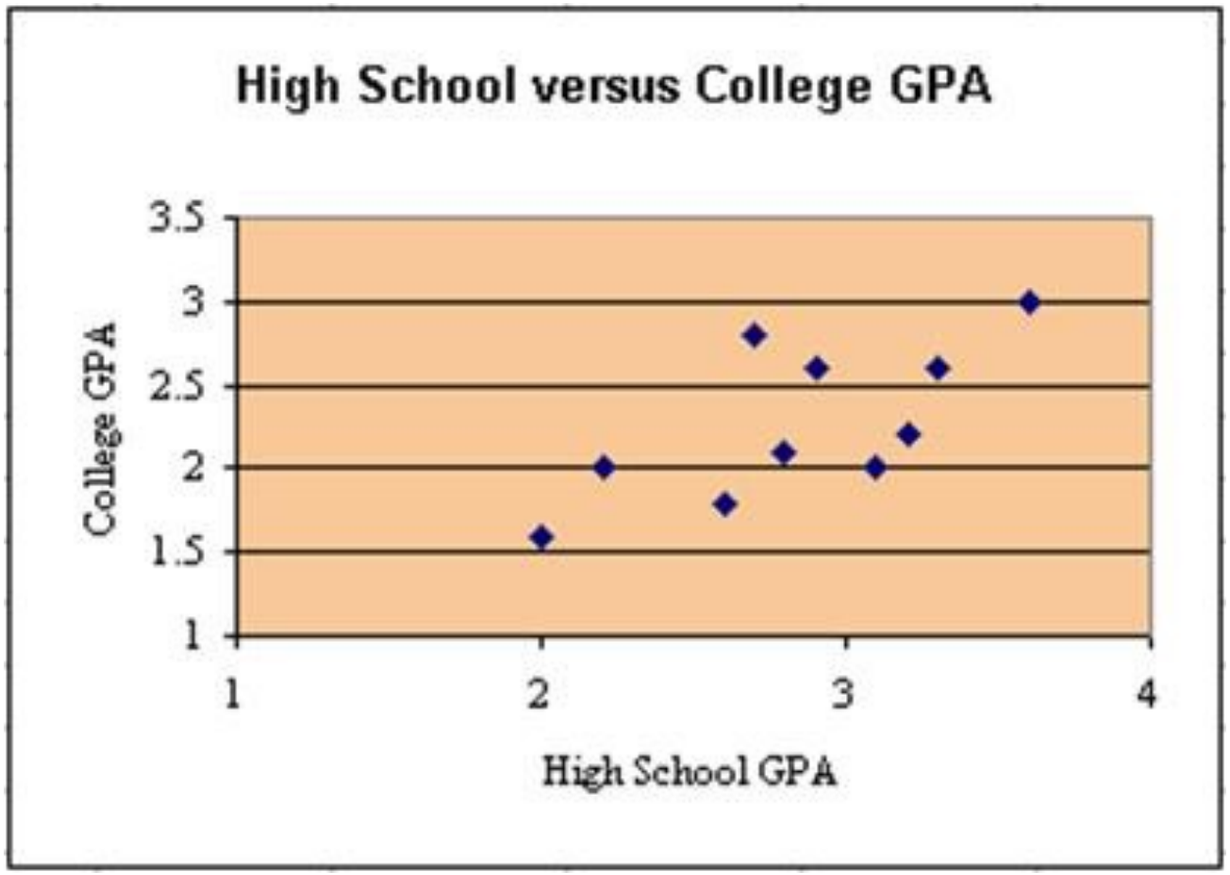


https://www.youtube.com/watch?v=dnKETo-gWbc

Supervised learning : Regression



Supervised learning : Regression



Real valued targets (outputs)

Generalization performance

Goal is to learn a function which maps inputs to outputs so that it will predict well on future data points

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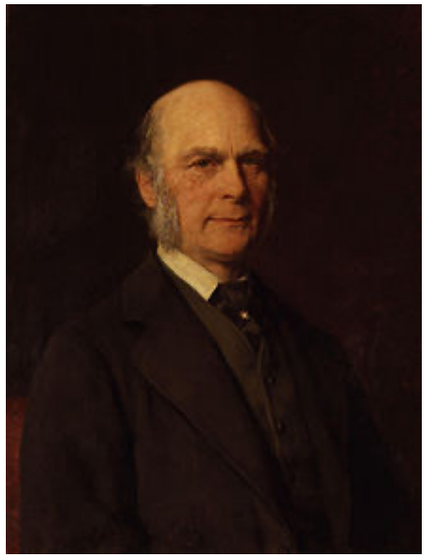
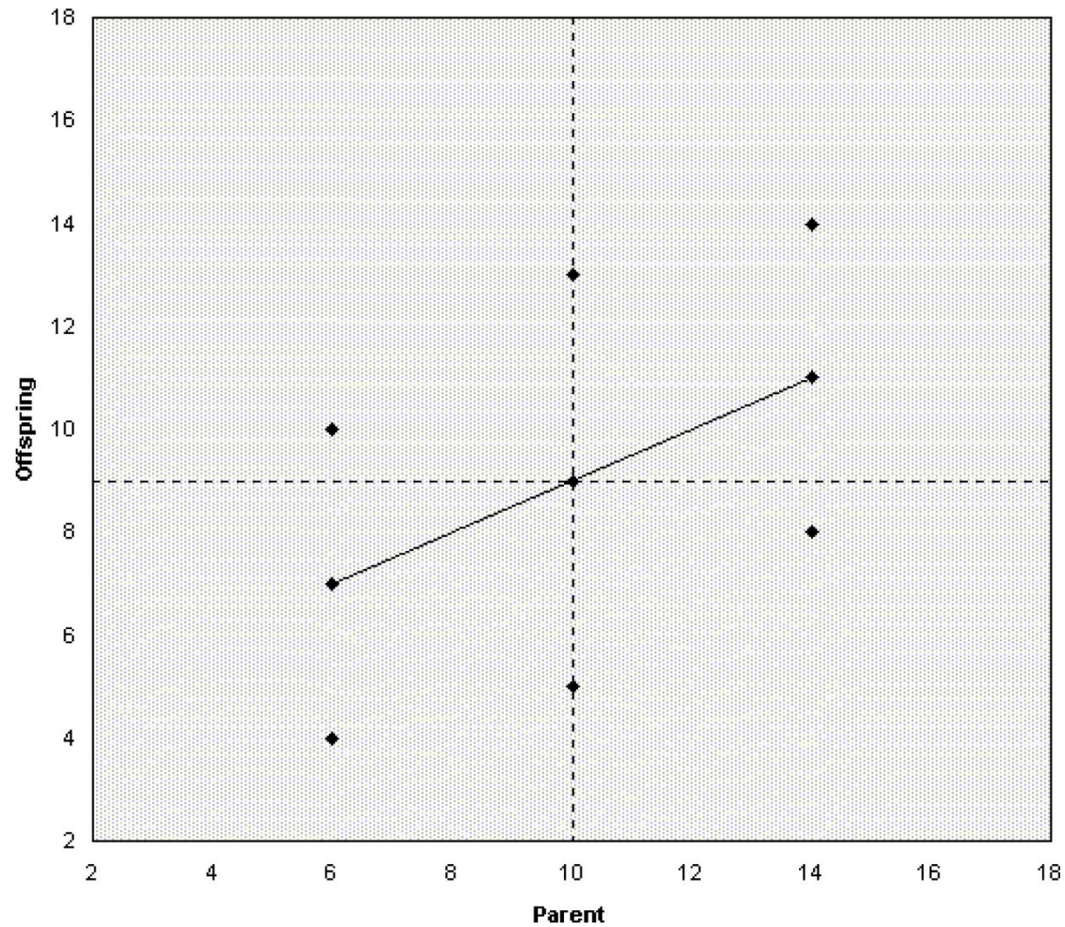
A historical look at regression

Genetics : parent sweet pea size on the *X*-axis and the offspring sweet pea size on the *Y*-axis (1900s)



Sir Francis Galton



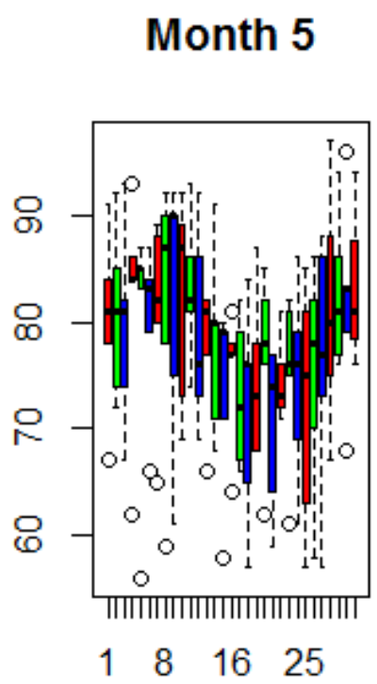
{(6, 4), (6, 7), (6, 10), (10, 5), (10, 9), (10, 13), (14, 8), (14, 11), (14, 14)}

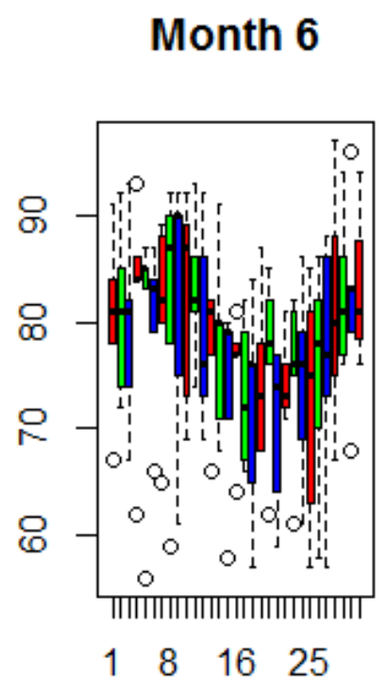
Airquality data.

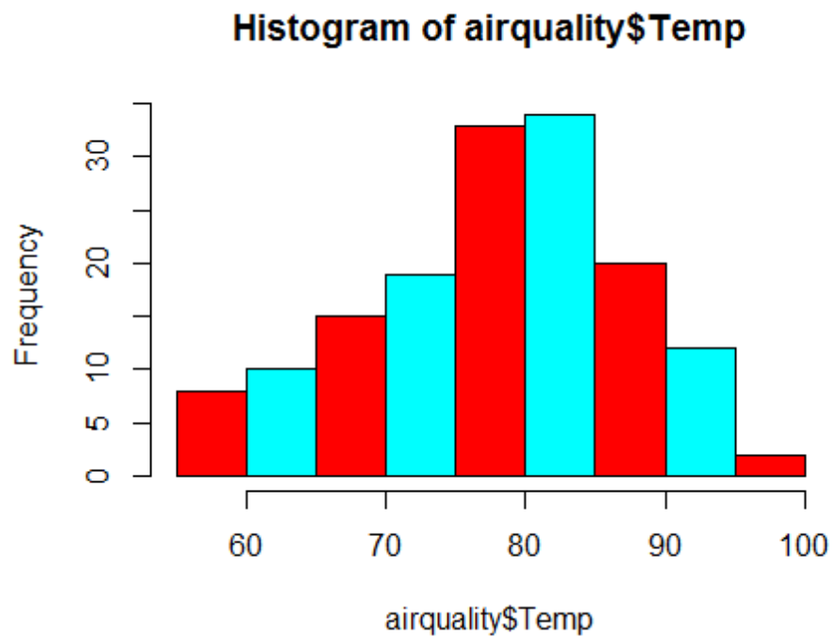
- Data set has various air quality parameters in New York city.
- These are the parameters in the data set:
- Daily temperature from May to August
- Solar radiation data
- Ozone data
- Wind data
- Goal : predict the temperature for a particular month in New York using solar radiation, ozone and wind data.

Airquality data

```
##    Ozone Solar.R Wind Temp Month Day
## 1     41     190  7.4   67     5   1
## 2     36     118  8.0   72     5   2
## 3     12     149 12.6   74     5   3
## 4     18     313 11.5   62     5   4
## 5     NA      NA 14.3   56     5   5
## 6     28      NA 14.9   66     5   6
## 7     23     299  8.6   65     5   7
## 8     19      99 13.8   59     5   8
## 9      8      19 20.1   61     5   9
## 10    NA     194  8.6   69     5  10
```

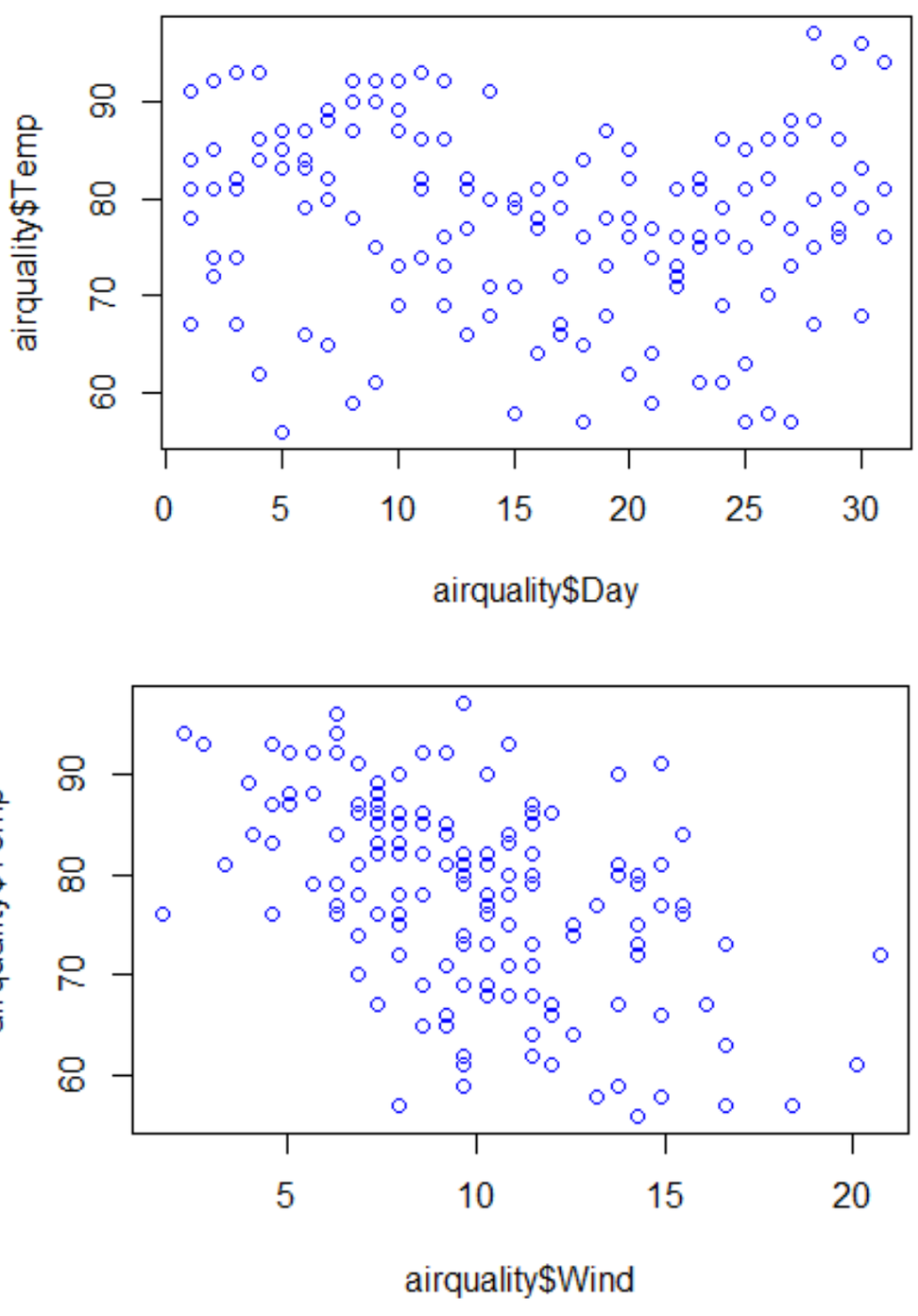


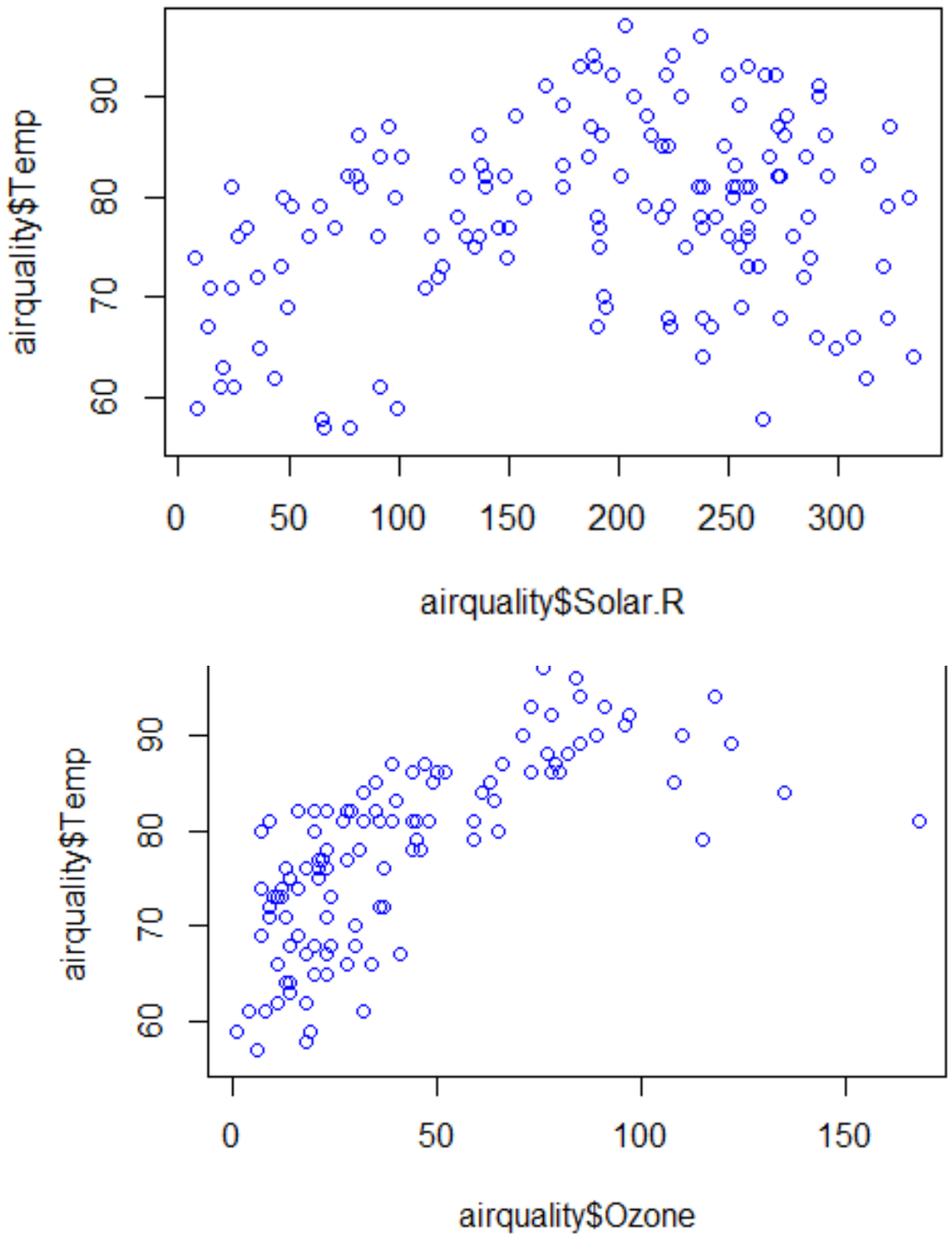




https://www.edvancer.in/step-step-guide-to-execute-linear-regression-r/

Airquality data





Linear regression

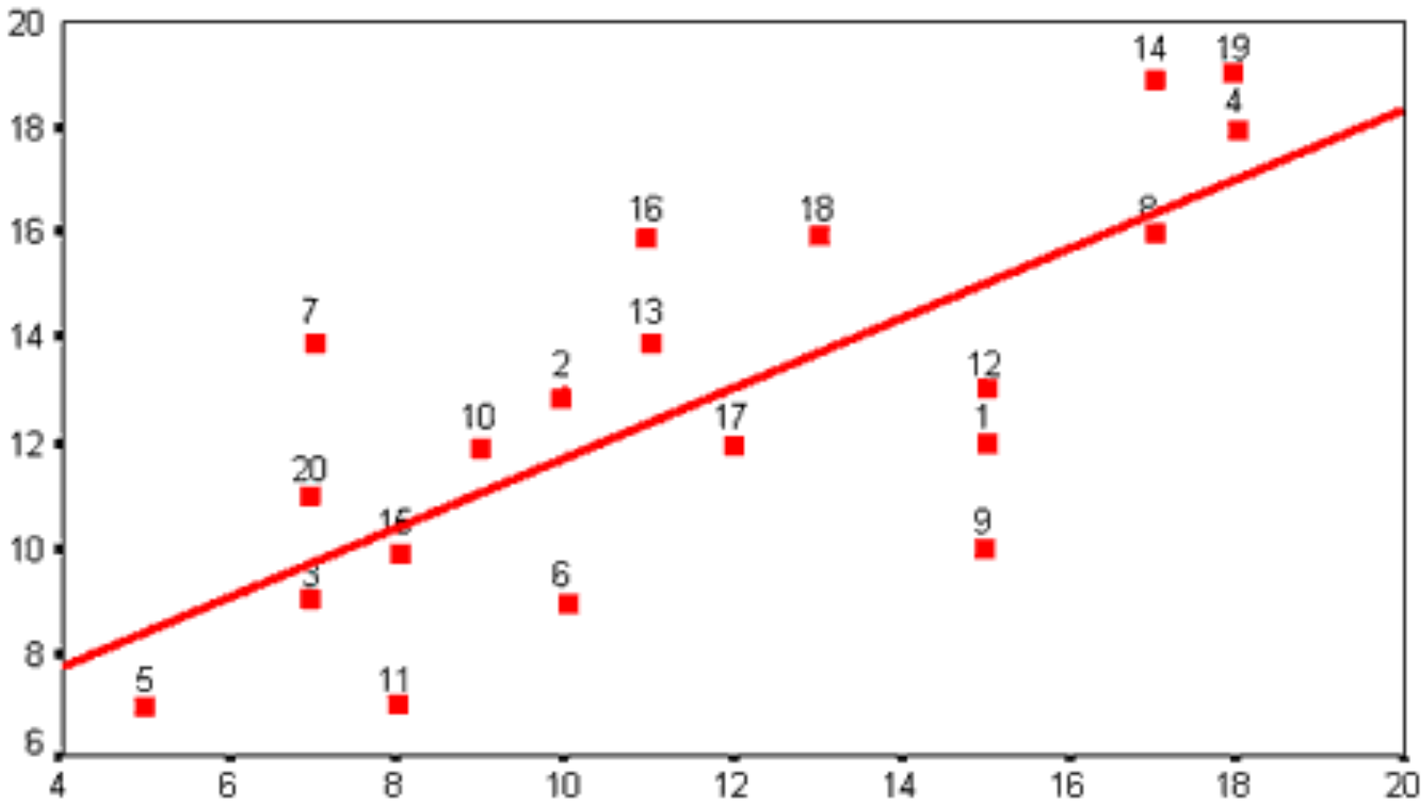
- Temp=w1.Solar.R +w2.Ozone + w3.Wind + error.

- Temperature of house depends on ozone, wind and solar radiations

- linear regression helps to discover relation between dependent and independent variables

Linear Regression

- Observations need not lie on a line
  - Observations are not generated by a linear line
  - Observations are noisy, due to measurement errors



Linear regression

- Learn a function which maps input to output f : X -> Y

Regression Output is real and scalar, $y \in \mathbb{R}$

- Consider a Linear function

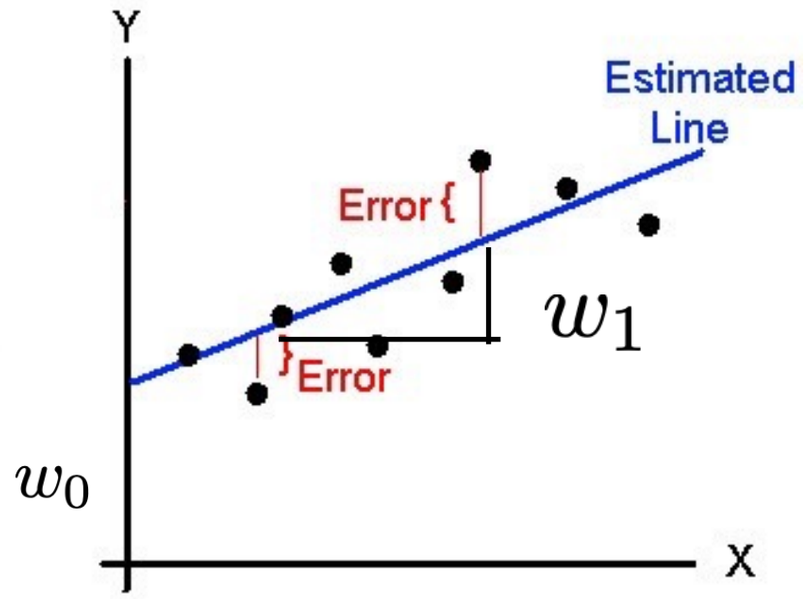
Estimated (or predicted) Y value for observation i

Estimate of the regression intercept

Estimate of the regression slope

Value of X for observation i

$$\hat{Y}_i = w_0 + w_1 X_i$$



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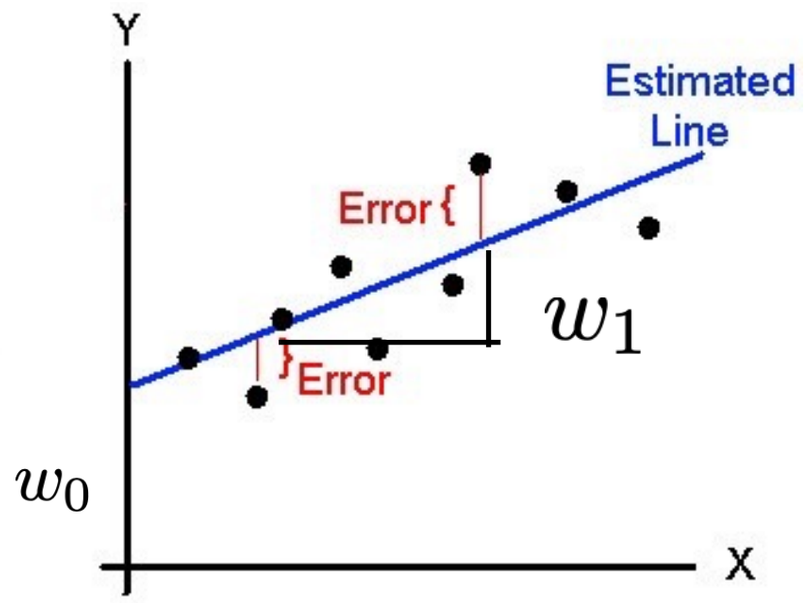
$$\hat{Y}_i = w_0 + w_1 X_i$$

$$= X_i^\top w$$



1 dim input $X_i = [1, X_i]^T$ $w = [w_0, w_1]^T$

D dim input $X_i = [1, X_{i1}, \ldots, X_{iD}]^T$ $w = [w_0, w_1, \ldots, w_D]^T$

Linear Regression - Learning Parameters

- Learn the function which passes through as many points as possible : Minimize the **Least Squares Error**

$$E(w) = \frac{1}{2}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

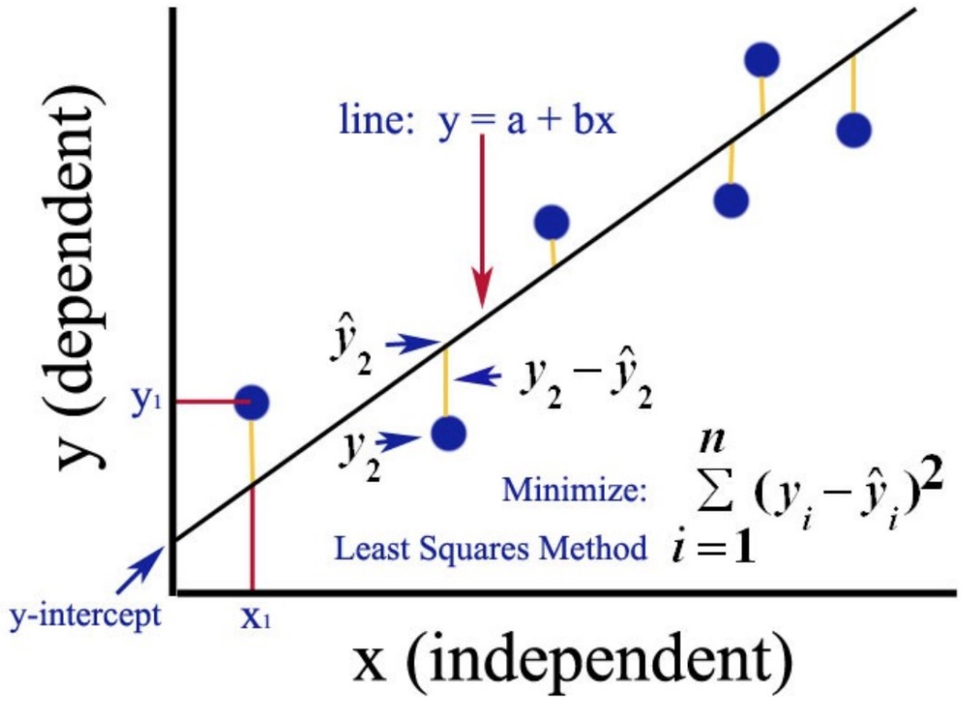
$$= \frac{1}{2}\sum_{i=1}^{N}(y_i - X_i^\top w)^2$$

$$\frac{1}{2}\|(y - X^\top w)\|^2$$

$$X_i = [1, X_{i1}, \ldots, X_{iD}]^T$$

Design matrix

$$X = \begin{pmatrix} X_1, X_2, \ldots X_N \end{pmatrix}_{(D+1) \times N}$$



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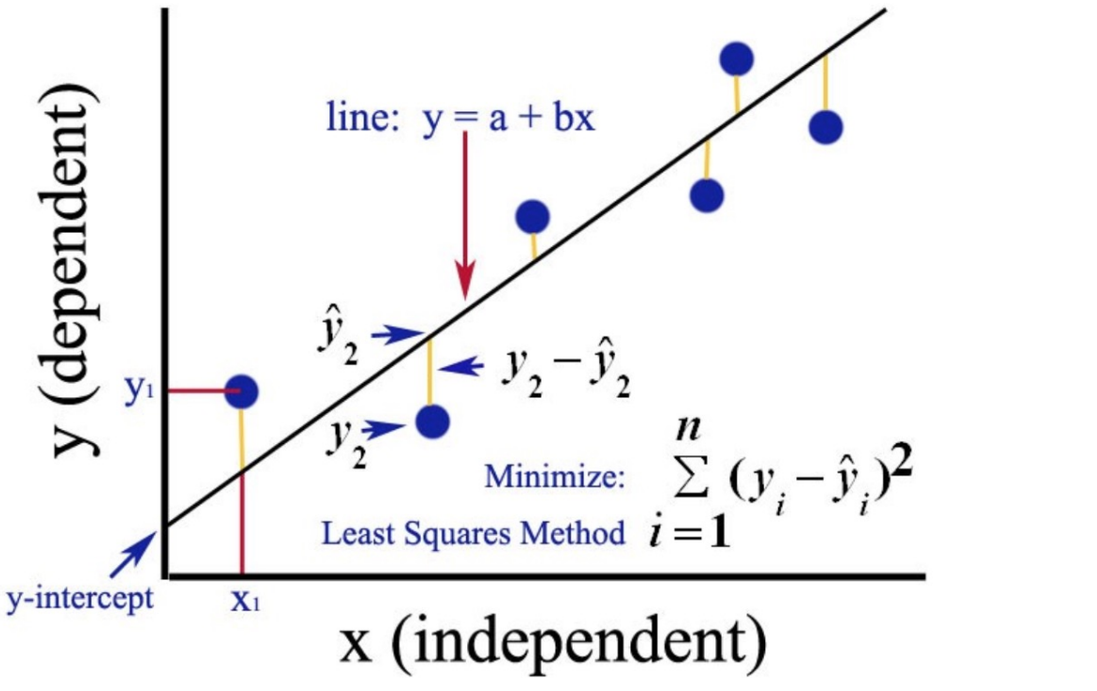


$$\nabla E(w) = Xy - XX^\top w = 0$$

$$w_{ML} = (XX^\top)^{-1}Xy$$

$$\frac{\partial}{\partial s}(x - As)^\top W(x - As) = -2(x - As)^\top WA$$

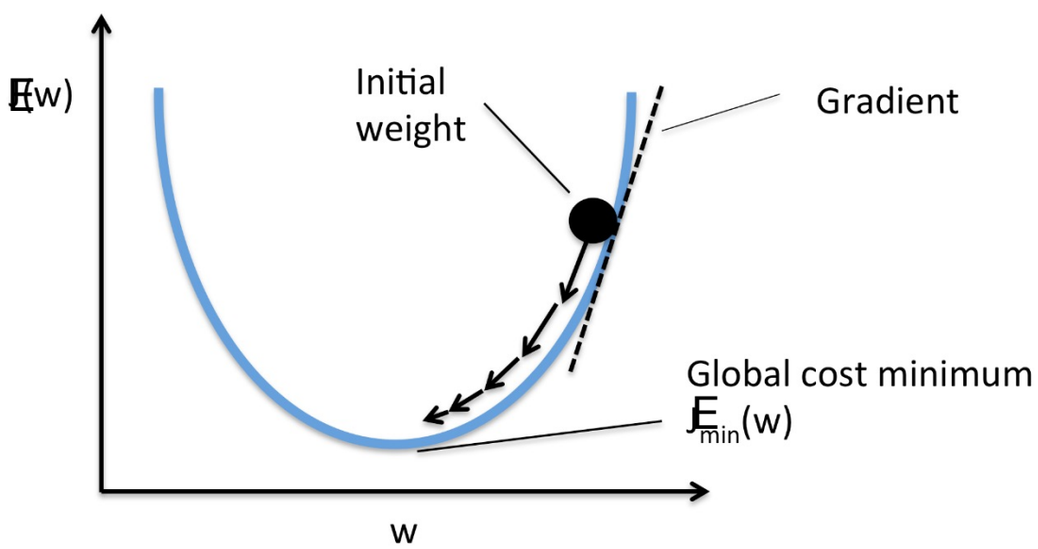
Linear Regression - Learning Parameters

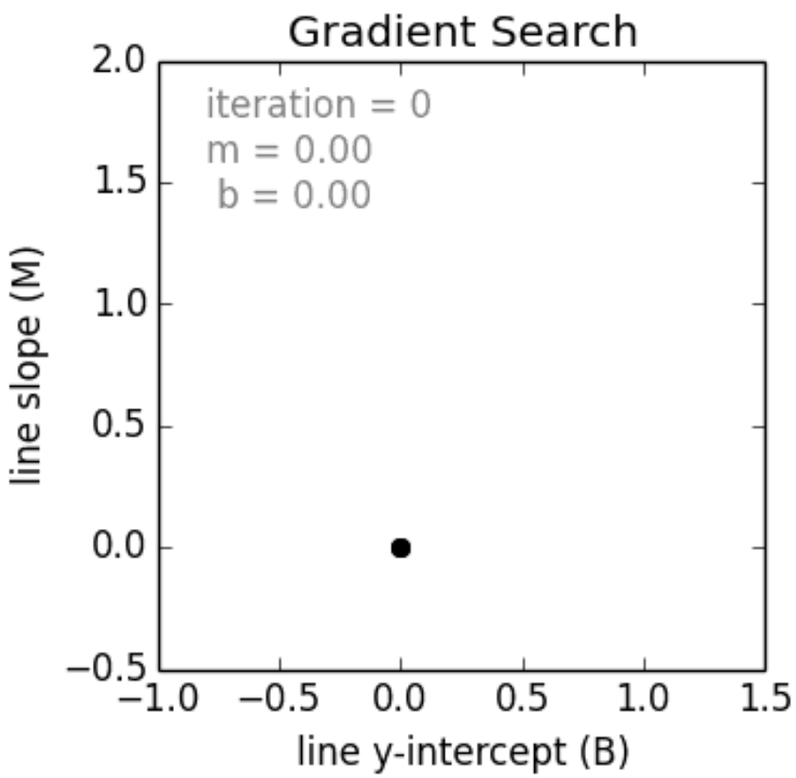
- Learn the function which passes through as many points as possible
  : Minimize the **least squares error** using **gradient descent**

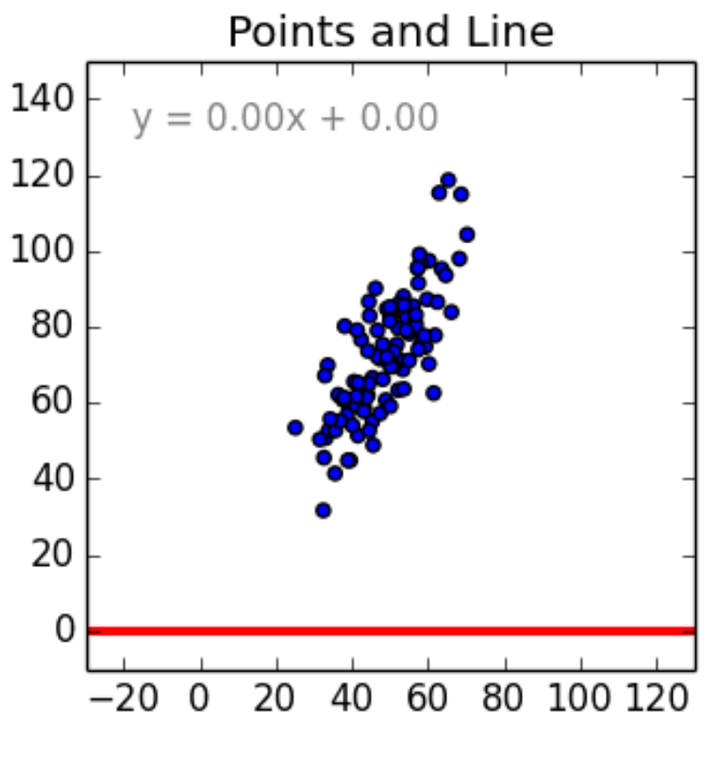
$$\nabla E(w) = Xy - XX^{\top}w$$

$$Error_{(m,c)} = \frac{1}{N}\sum_{i=1}^{N}(y_i - (mx_i + c))^2$$

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta \nabla E_n$$







Question

- write down three equations for the line **y = mx+c** to go through **y = 7** at **x = -1**, **y = 7** at **x = 1** and **y = 21** at **x = 2**. Find the least squares solution **(c,m)**?

- Implement In python least squares solution to linear regression
  - Analytical approach
  - Gradient descent approach

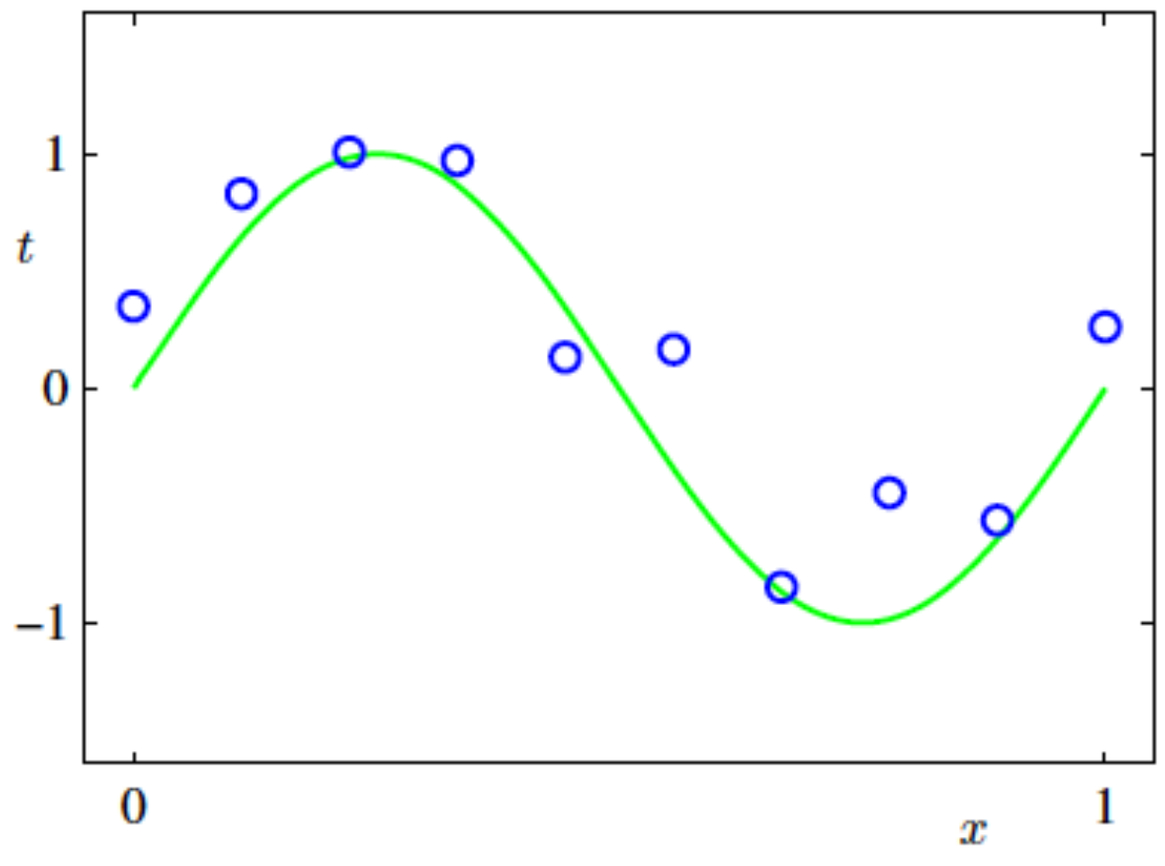
Question

- write down three equations for the line $y = mx+c$ to go through $y = 7$ at $x = -1$, $y = 7$ at $x = 1$ and $y = 21$ at $x = 2$. Find the least squares solution (c,m)?

- Answer : (9,4)

Regression - curve fitting

- Remember high school maths !
- Real-valued target variable t.
- Training set comprising N observations

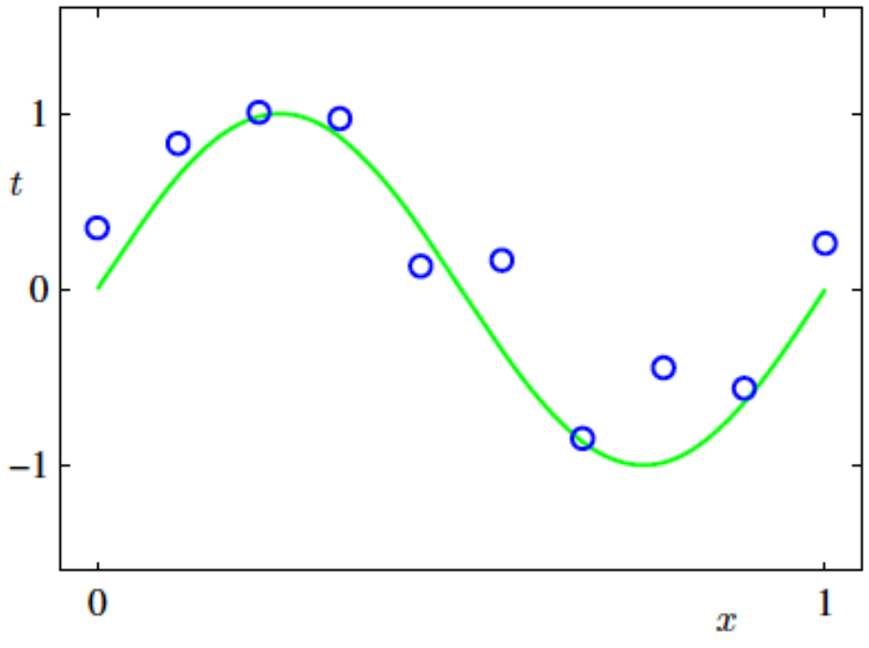


Polynomial Regression - curve fitting

- M is the order of the polynomial, y(x,w) is a nonlinear function of x, it is a linear function of the coefficients w.

- Functions, such as the polynomial, which are linear in the unknown parameters have important properties and are called **linear models**

$$y(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M = \sum_{j=0}^{M} w_j x^j$$



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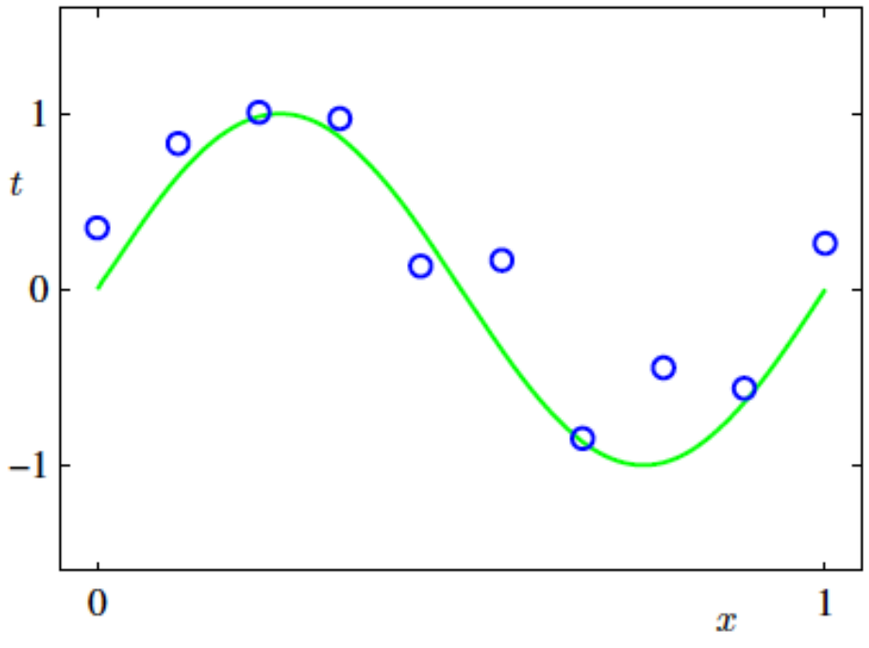
Linear regression



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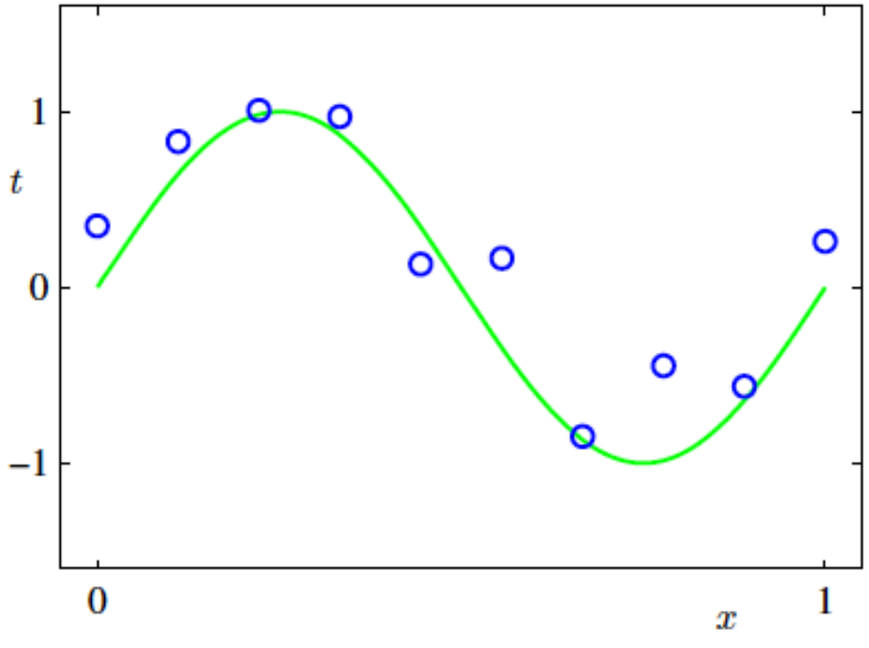


Non-Linear regression

$$y_i = \frac{e^{\beta_0 + \beta_1 x_i}}{1 + e^{\beta_0 + \beta_1 x_i}}$$

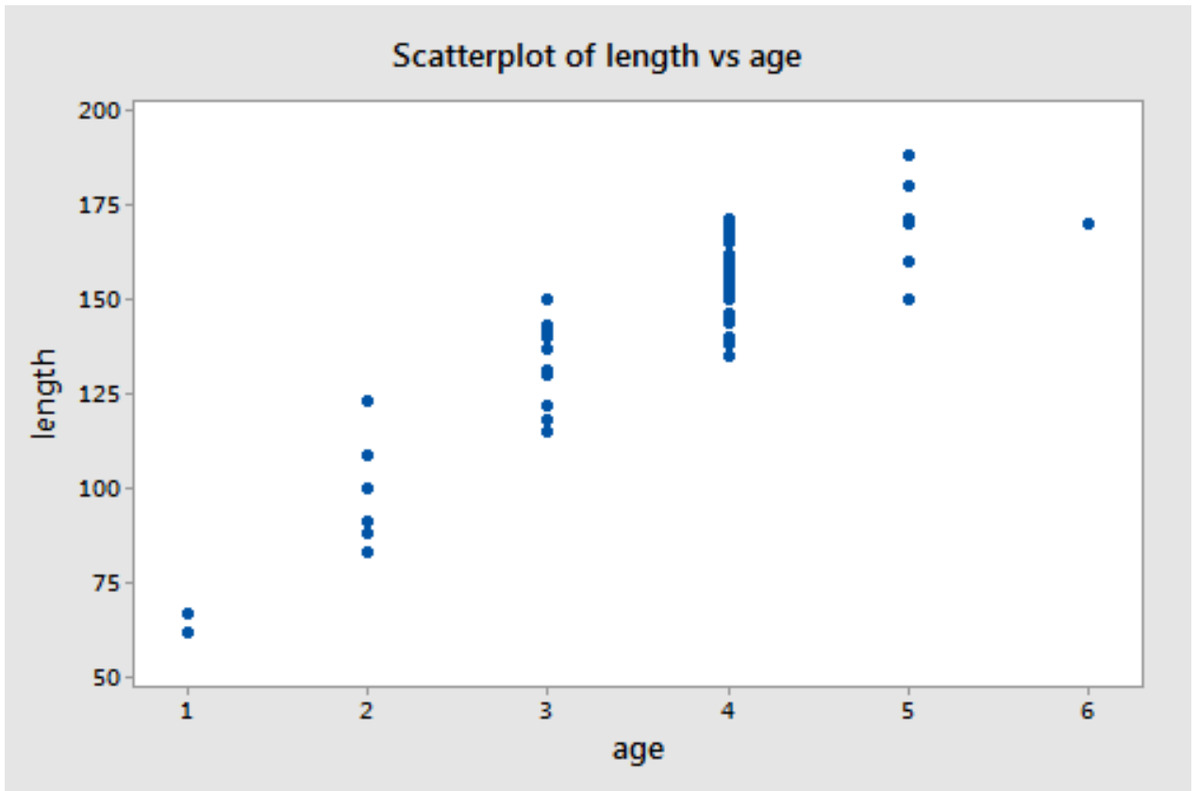
$$y_i = \frac{\beta_0 + \beta_1 x_i}{1 + \beta_2 e^{\beta_3 x_i}} \qquad Y = \frac{\beta_0 X}{\beta_1 + X}$$

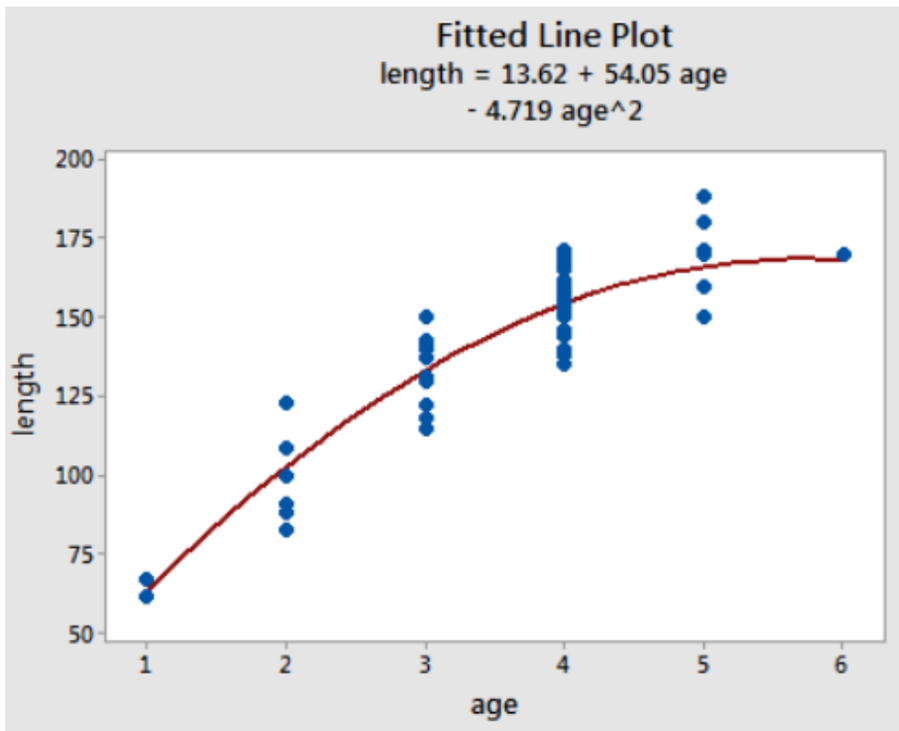
Polynomial Regression - Example

- Some researchers are interested in learning how the length of a bluegill fish is related to its age. To study this, some bluegill fishes were randomly sampled from a Lake and recorded the following data
  Response (y): length (in mm) of the fish
  Input (x): age (in years) of the fish

- Positive trend but not linear : **Second-order polynomial model**

$$y_i = (\beta_0 + \beta_1 x_i + \beta_{11} x_i^2)$$



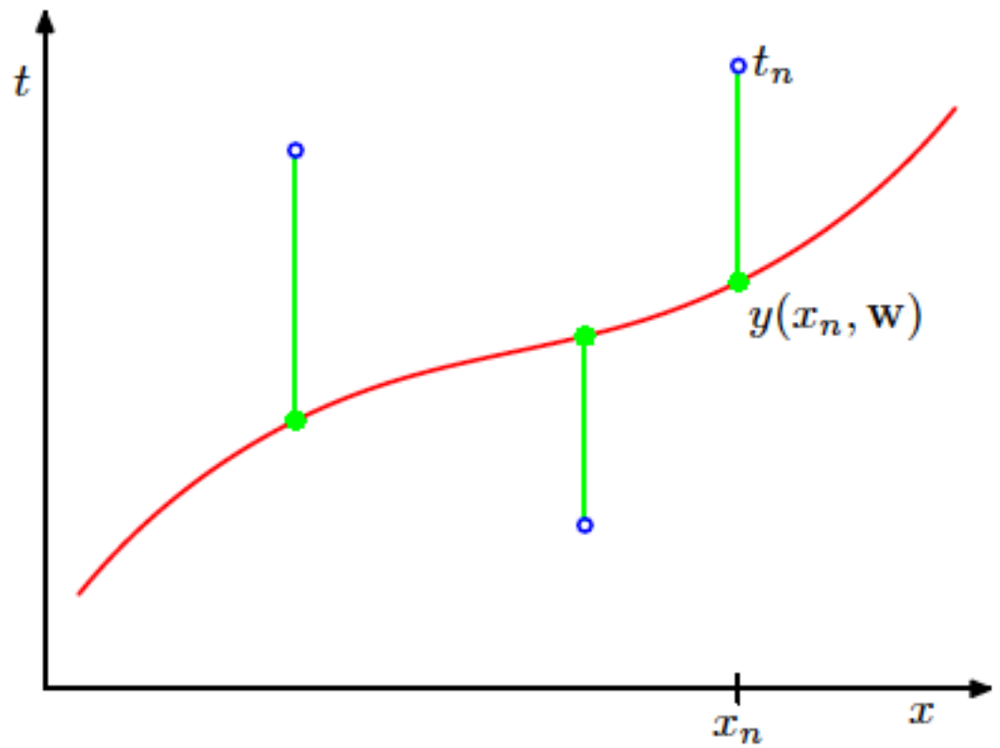


Polynomial Regression - Parameter estimation

$$y(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M = \sum_{j=0}^{M} w_j x^j$$

- Coefficients will be determined by fitting the polynomial to the training data. This can be done by minimizing an error function

$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} \{y(x_n, \mathbf{w}) - t_n\}^2$$



Polynomial Regression - Parameter estimation

$$y(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \ldots + w_{M-1} x^{M-1} = \sum_{j=0}^{M-1} w_j x^j$$

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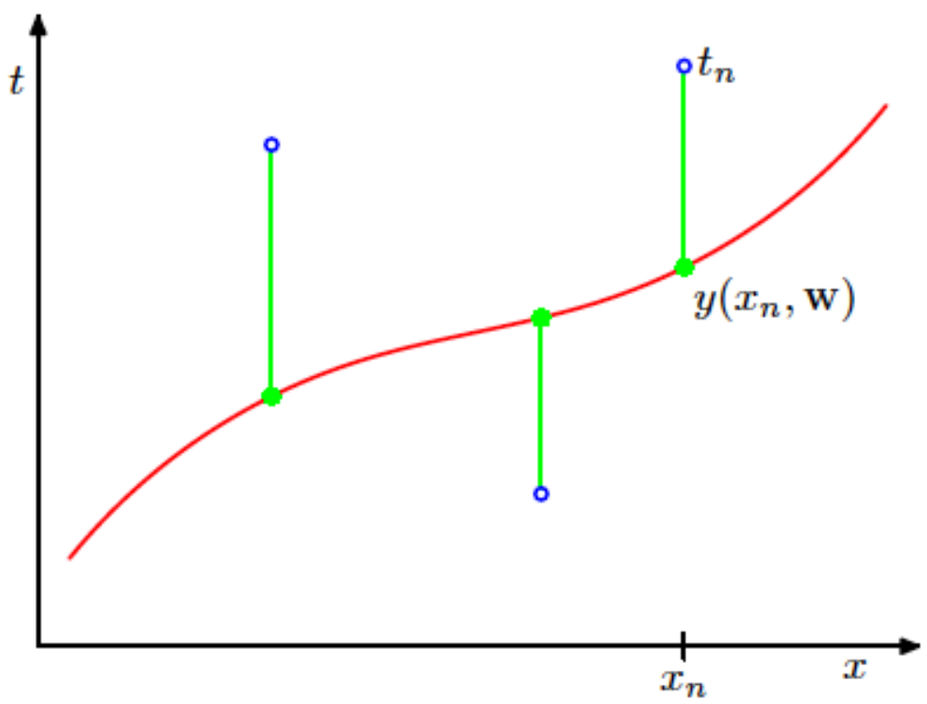


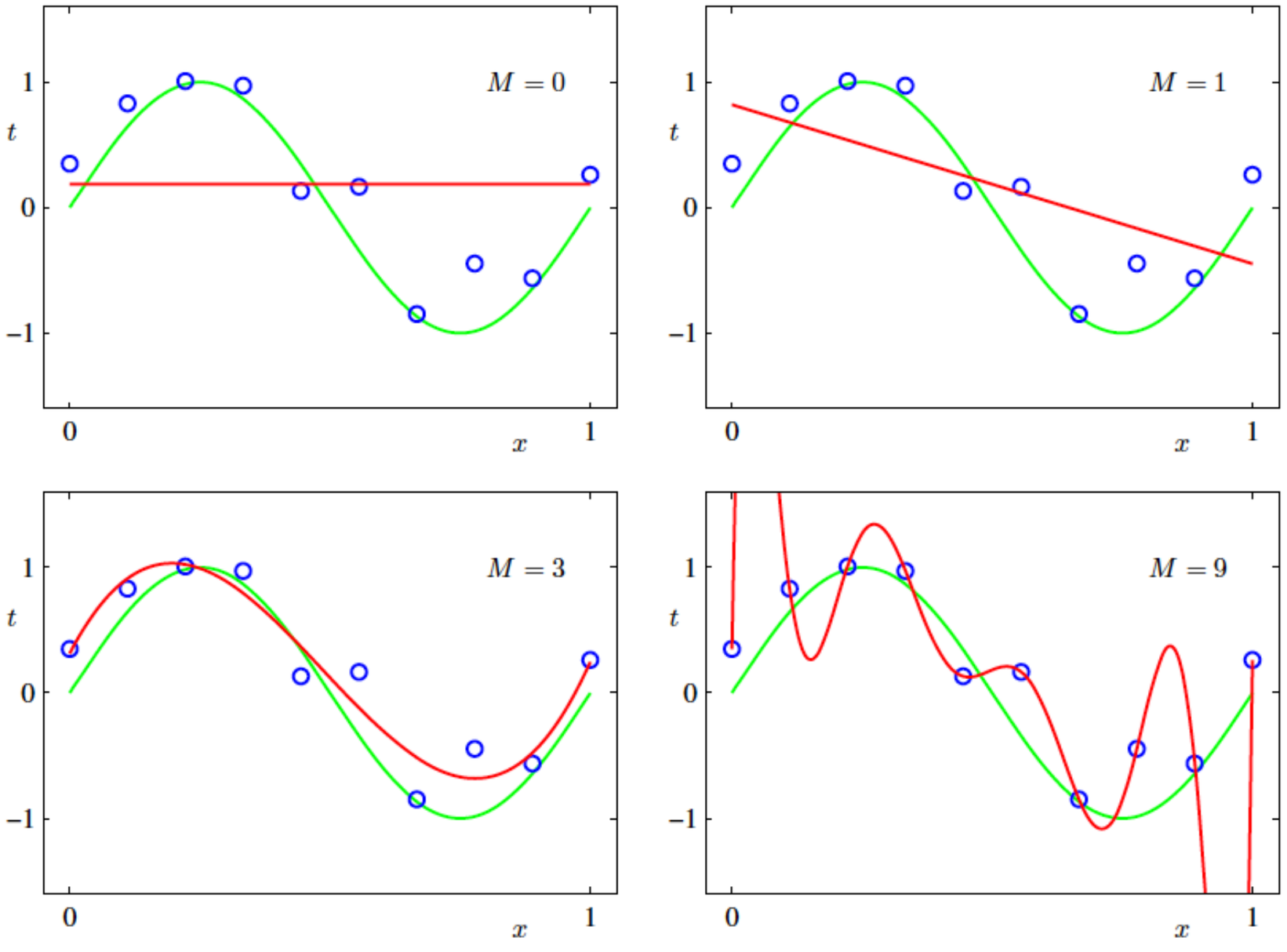
$$\mathbf{\Phi} = \begin{pmatrix} \phi_0(\mathbf{x}_1) & \phi_1(\mathbf{x}_1) & \cdots & \phi_{M-1}(\mathbf{x}_1) \\ \phi_0(\mathbf{x}_2) & \phi_1(\mathbf{x}_2) & \cdots & \phi_{M-1}(\mathbf{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_0(\mathbf{x}_N) & \phi_1(\mathbf{x}_N) & \cdots & \phi_{M-1}(\mathbf{x}_N) \end{pmatrix}$$

N × M

$$\mathbf{w} = (\mathbf{\Phi}^\top \mathbf{\Phi})^{-1} \mathbf{\Phi}^\top \mathbf{t}$$

Polynomial regression – Model Selection

- Model selection (choosing M) : higher order polynomial (M = 9), provide excellent fit to the training data but gives a very poor representation of the function



Polynomial regression
Overfitting

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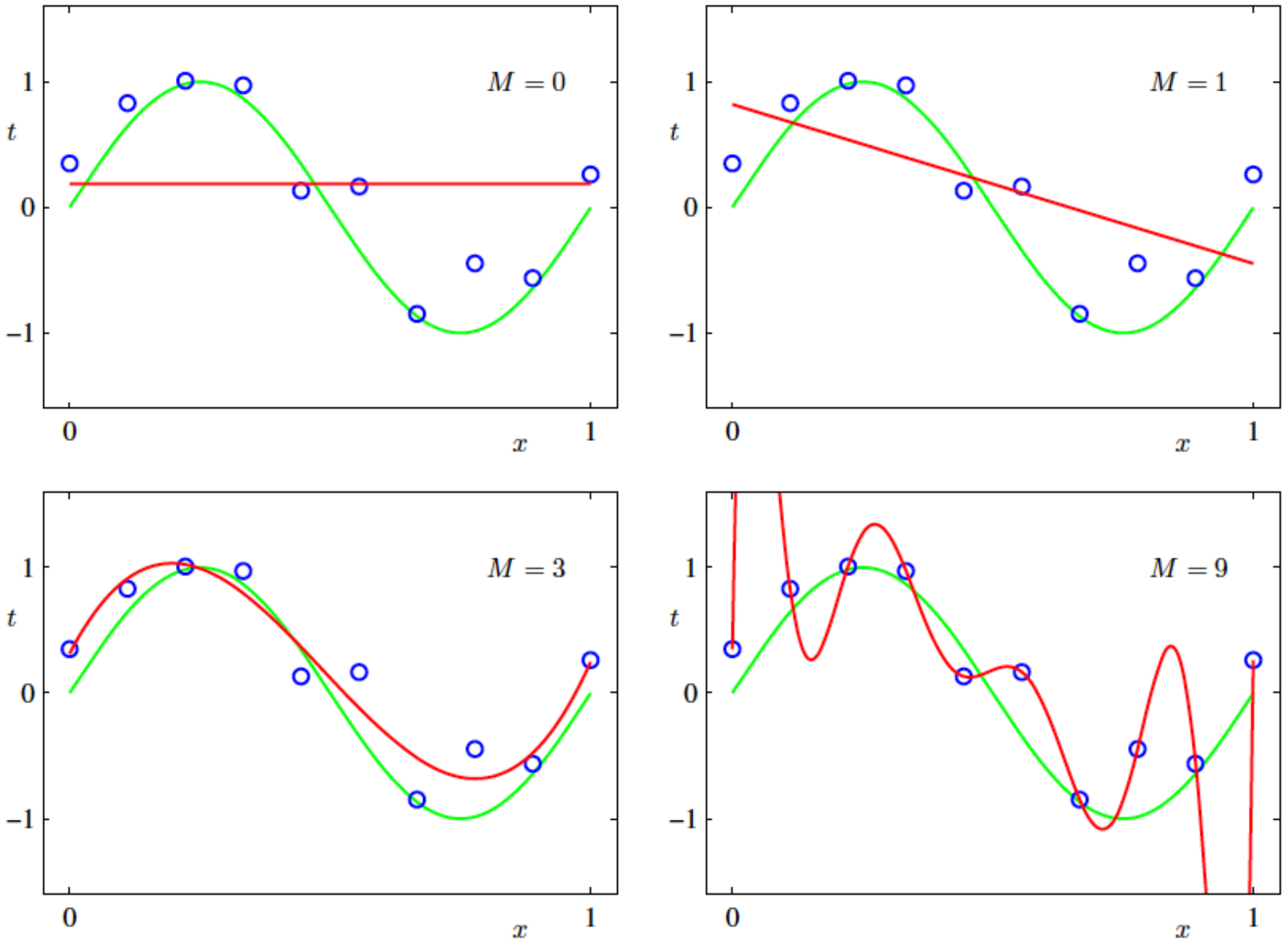


model that is too flexible with respect to the number of data

Polynomial regression - Model Selection

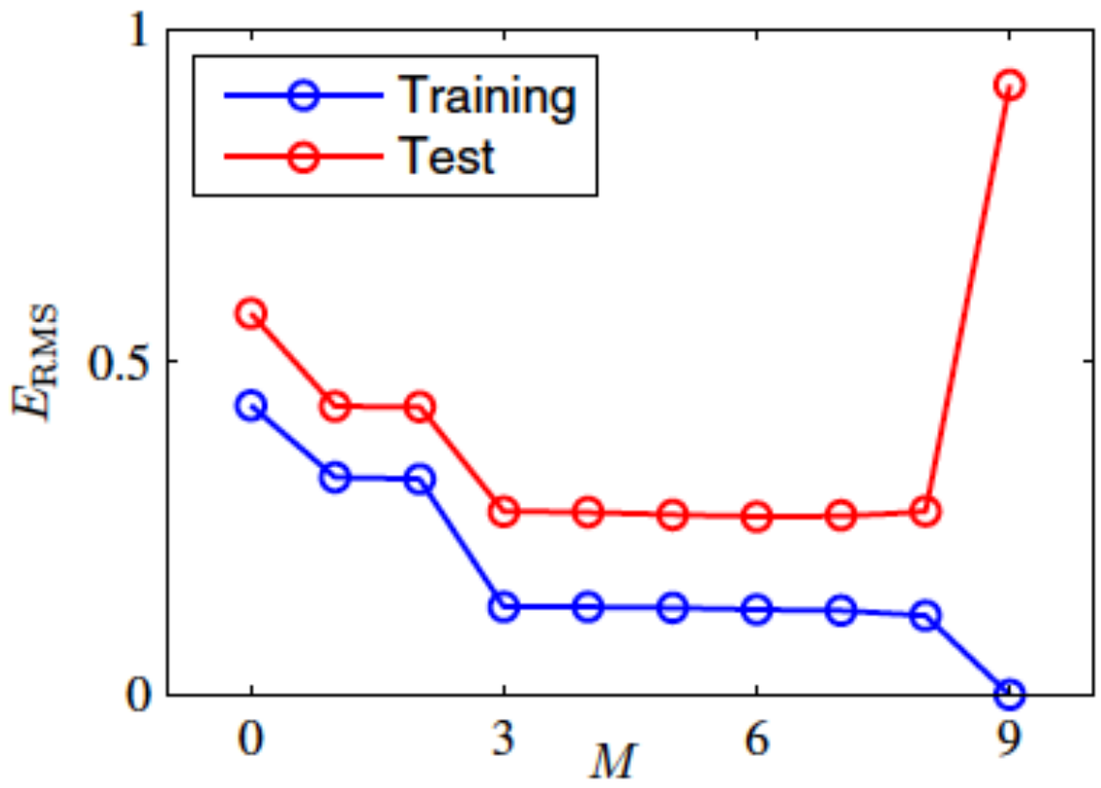
- Generalization performance : root mean square error on test data

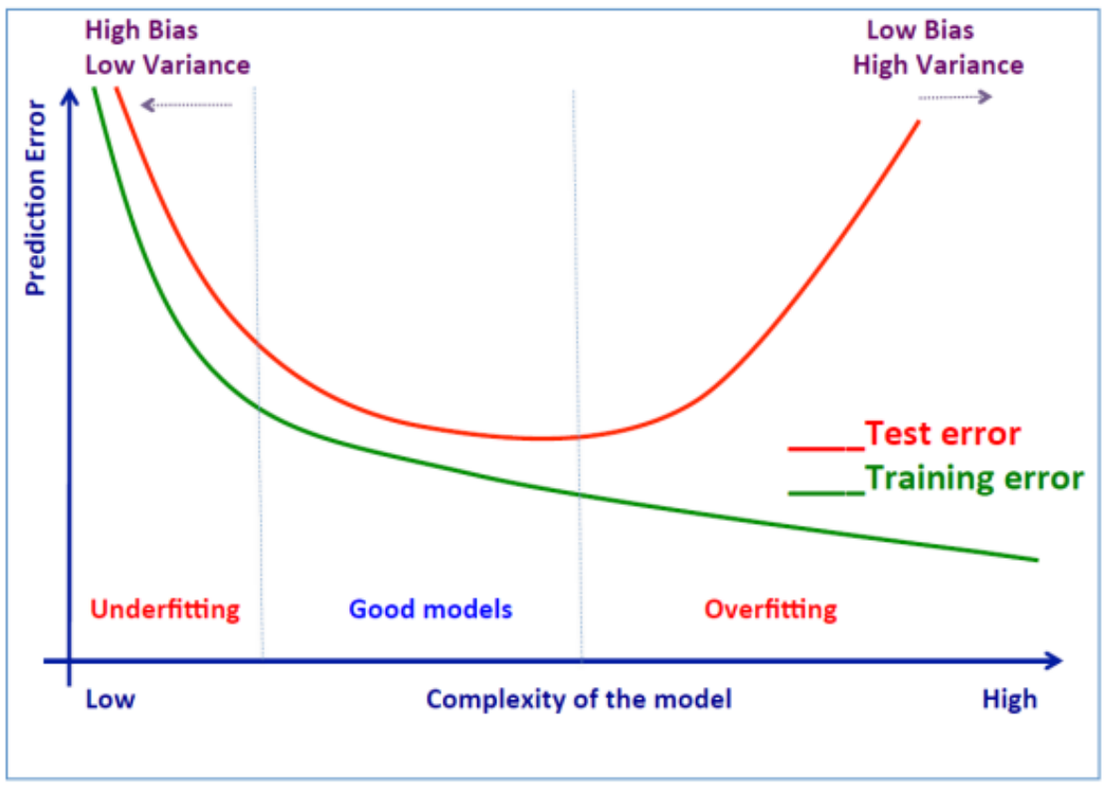
- Weights coefficients for M=9 is extremely large !

$$E_{\mathrm{RMS}} = \sqrt{2E(\mathbf{w}^\star)/N}$$

$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n, \mathbf{w}) - t_n\}^2$$

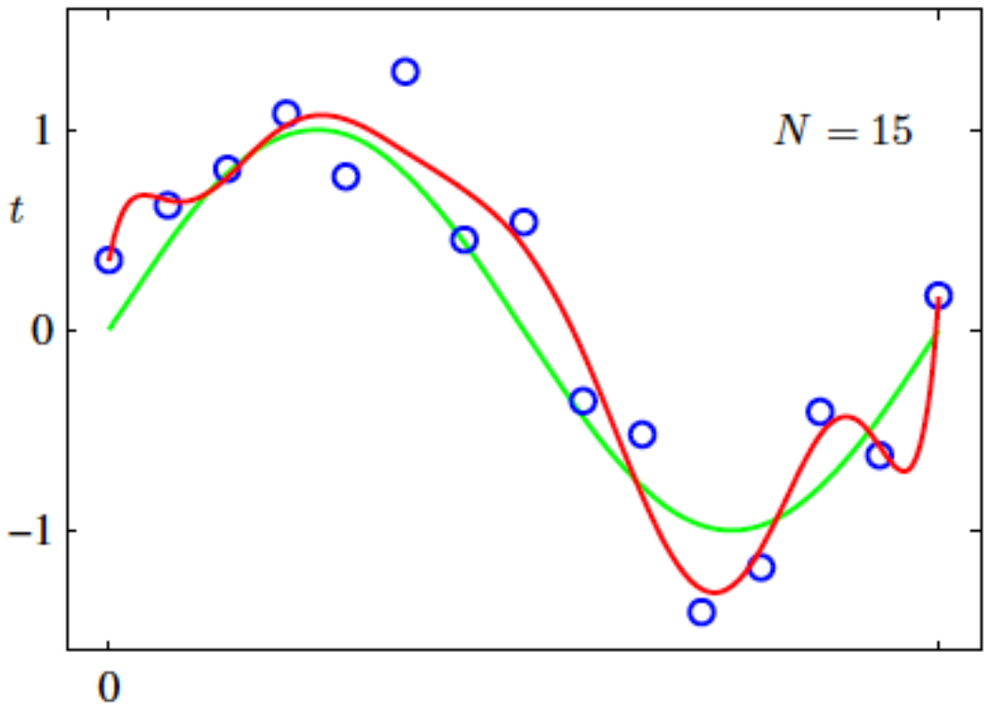
	$M=0$	$M=1$	$M=6$	$M=9$
$w_0^\star$	0.19	0.82	0.31	0.35
$w_1^\star$		-1.27	7.99	232.37
$w_2^\star$			-25.43	-5321.83
$w_3^\star$			17.37	48568.31
$w_4^\star$				-231639.30
$w_5^\star$				640042.26
$w_6^\star$				-1061800.52
$w_7^\star$				1042400.18
$w_8^\star$				-557682.99
$w_9^\star$				125201.43

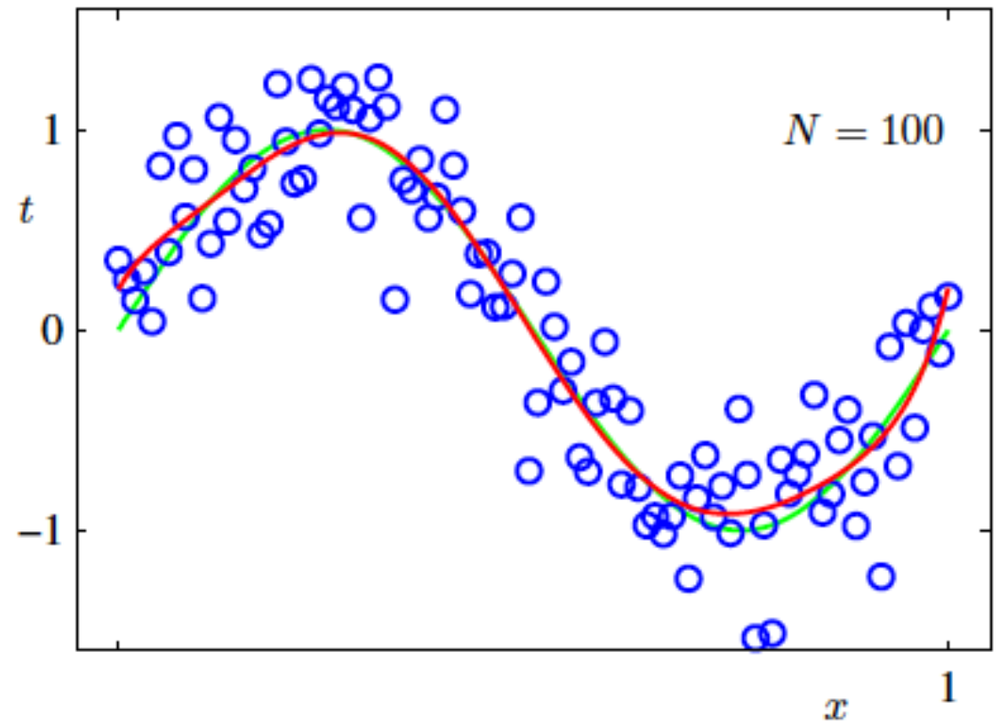


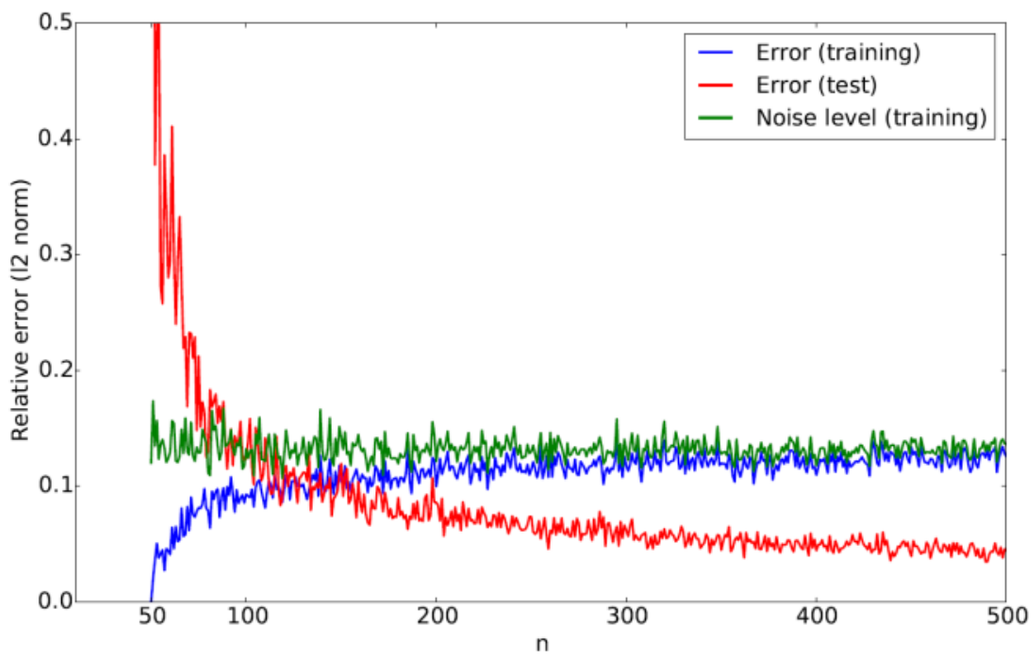


Polynomial regression - Model Selection

- Given model complexity, the over-fitting problem become less severe as the size of the data set increases.







Polynomial regression - regularization

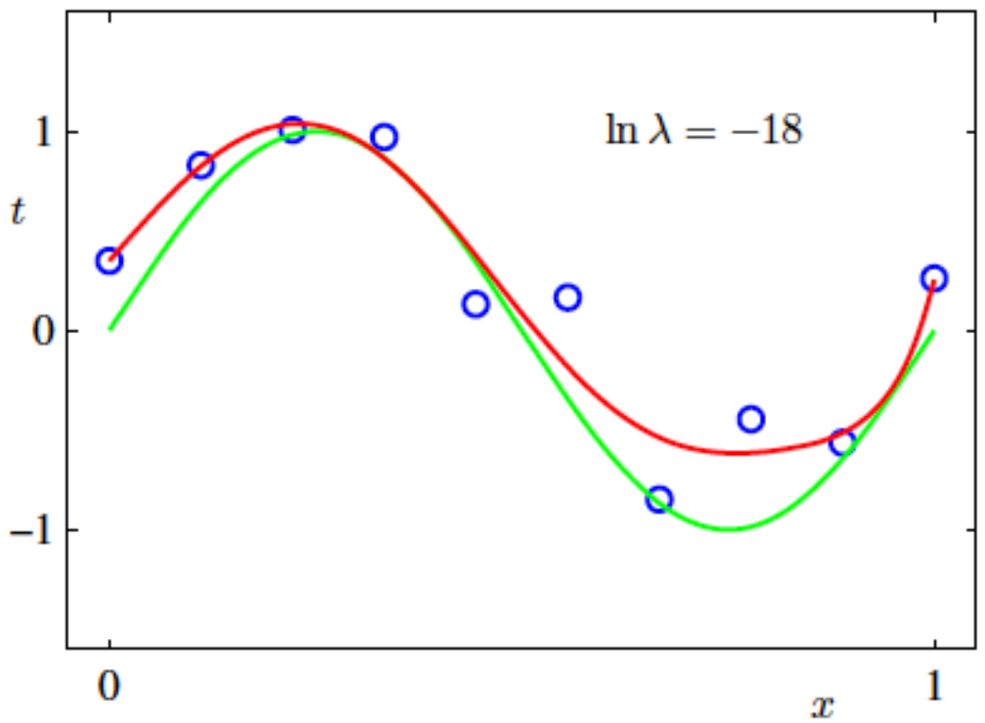
- Add a penalty term to the error function (1.2) in order to discourage the coefficients from reaching large values

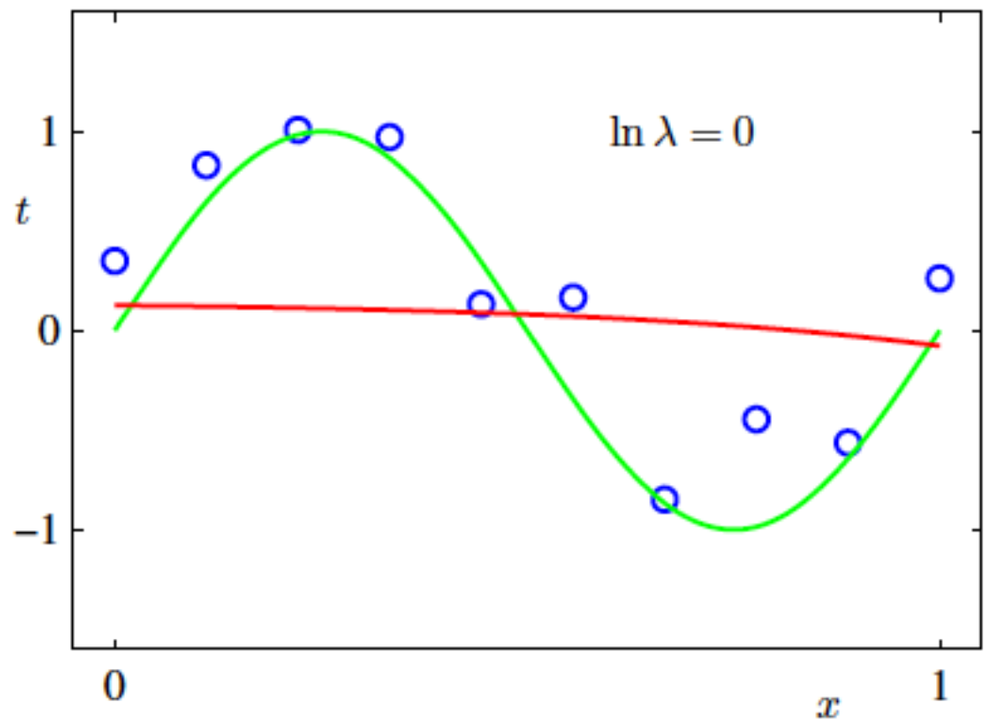
$$\widetilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n, \mathbf{w}) - t_n\}^2 + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

- Ridge regression : L2 norm

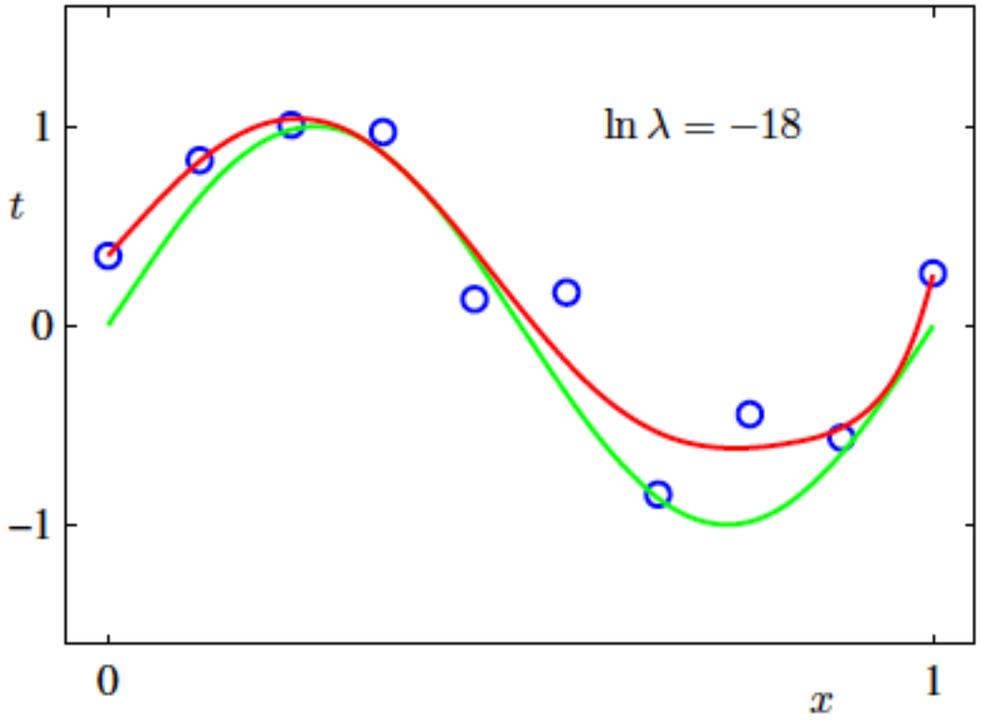
$$\|\mathbf{w}\|^2 \equiv \mathbf{w}^{\mathrm{T}}\mathbf{w} = w_0^2 + w_1^2 + \ldots + w_M^2$$

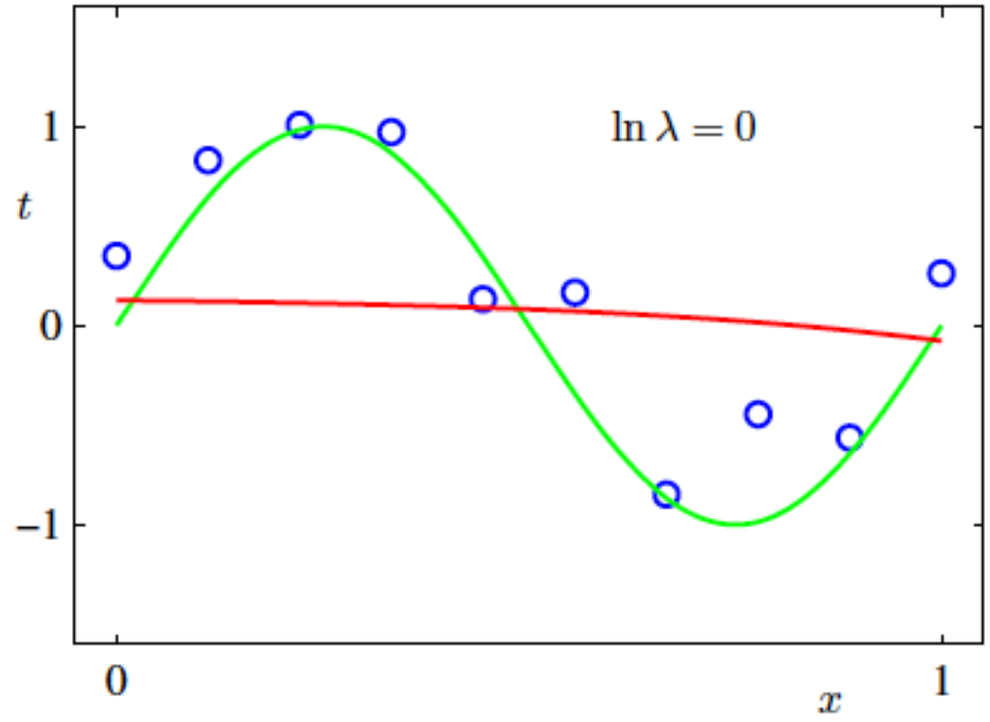
Regularization constant

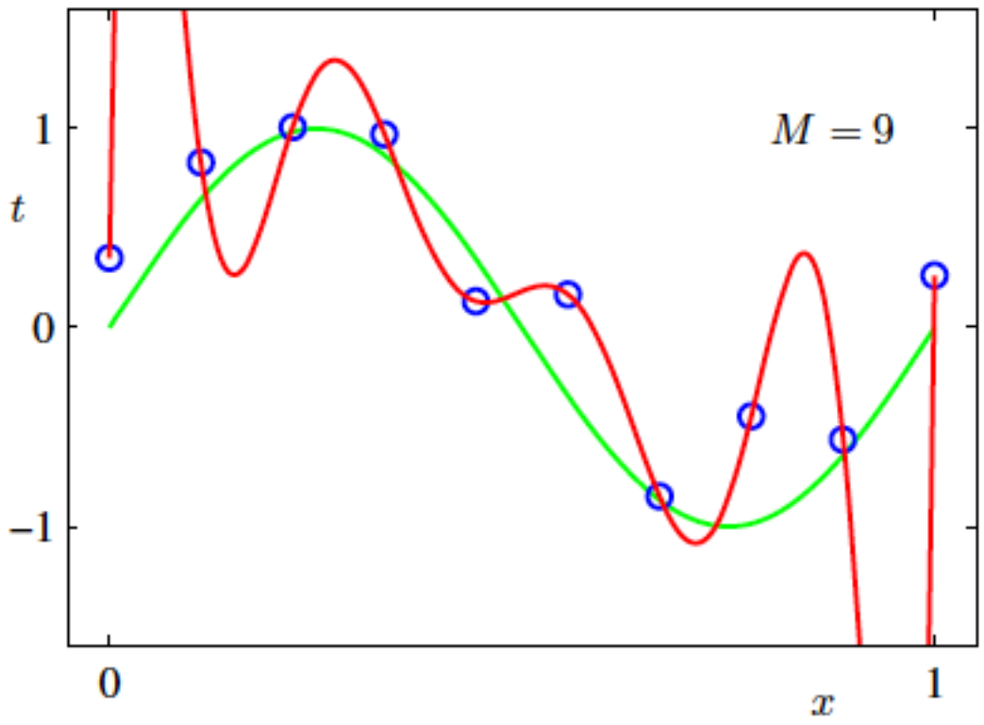




Polynomial regression - regularization







	$\ln \lambda = -\infty$	$\ln \lambda = -18$	$\ln \lambda = 0$
$w_0^\star$	0.35	0.35	0.13
$w_1^\star$	232.37	4.74	-0.05
$w_2^\star$	-5321.83	-0.77	-0.06
$w_3^\star$	48568.31	-31.97	-0.05
$w_4^\star$	-231639.30	-3.89	-0.03
$w_5^\star$	640042.26	55.28	-0.02
$w_6^\star$	-1061800.52	41.32	-0.01
$w_7^\star$	1042400.18	-45.95	-0.00
$w_8^\star$	-557682.99	-91.53	0.00
$w_9^\star$	125201.43	72.68	0.01

Regularized Least Squares

- Parameter shrinkage, weight decay

- **Ridge regression** q=2

$$\frac{\lambda}{2}\sum_{j=1}^{M} w_j^2$$

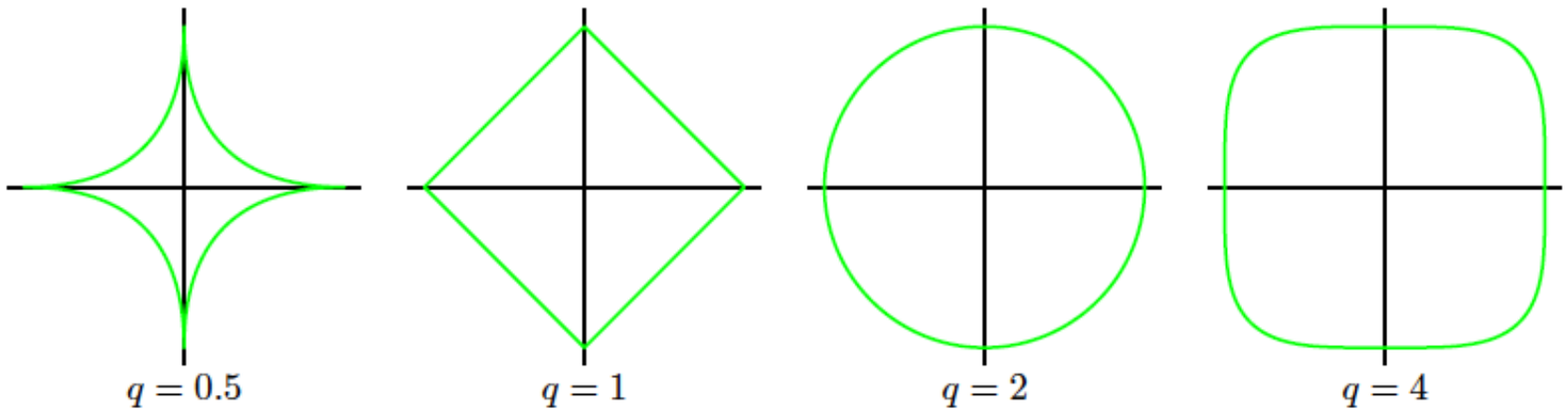
- **Lasso regression** q=1, if λ is sufficiently large, some of the coefficients are driven to zero

$$\frac{1}{2}\sum_{n=1}^{N}\{t_n - \mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n)\}^2 + \frac{\lambda}{2}\sum_{j=1}^{M}|w_j|^q$$

$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{t_n - \mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n)\}^2 + \frac{\lambda}{2}\sum_{j=1}^{M}|w_j|$$

- Elastic net regularization

$$\frac{1}{n}\|Y - \mathrm{X}\,w\|_2^2 + \lambda_1\sum_{j=1}^{d}|w_j| + \lambda_2\sum_{j=1}^{d}|w_j|^2$$



Regularized Least Squares

- Parameter shrinkage, weight decay
- **Ridge regression** q=2 $\frac{\lambda}{2}\sum_{j=1}^{M} w_j^2$
- **Lasso regression** q=1, if λ is sufficiently large, some of the coefficients are driven to zero

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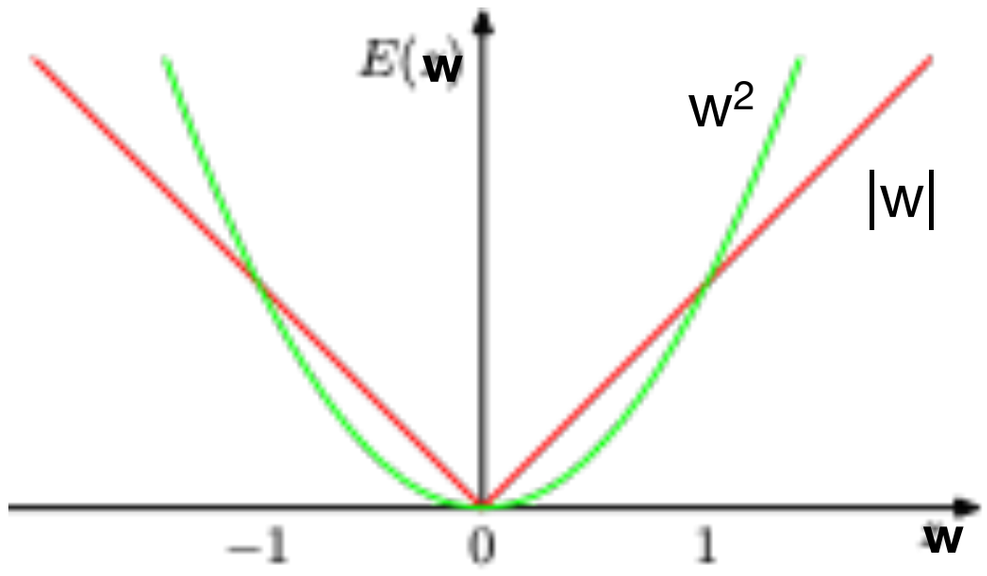
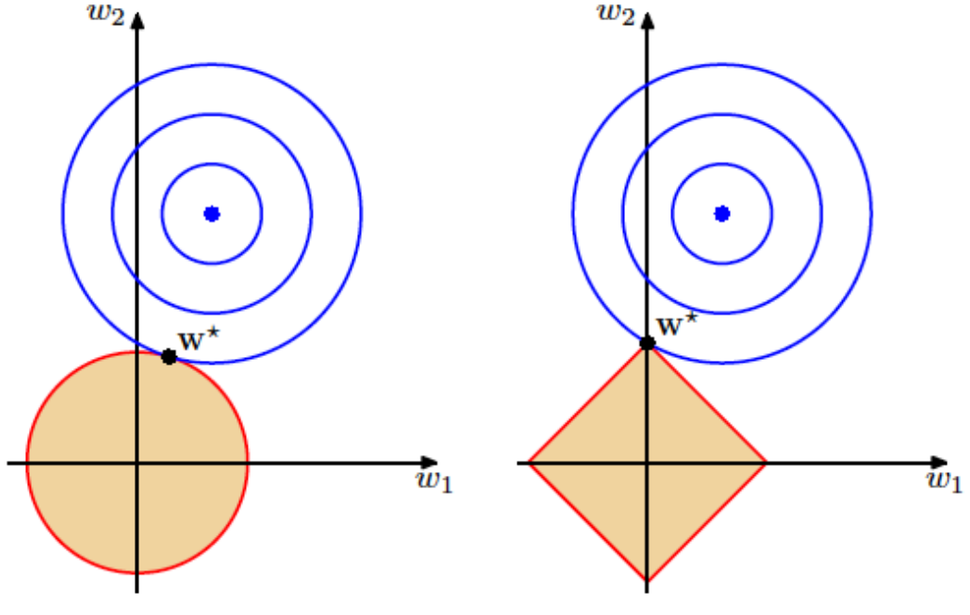




Ridge Regression

- Regularized Least Squares

$$\frac{1}{2}\sum_{n=1}^{N}\{t_n - \mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n)\}^2 + \frac{\lambda}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w}.$$

$$\boldsymbol{\Phi} = \begin{pmatrix} \phi_0(\mathbf{x}_1) & \phi_1(\mathbf{x}_1) & \cdots & \phi_{M-1}(\mathbf{x}_1) \\ \phi_0(\mathbf{x}_2) & \phi_1(\mathbf{x}_2) & \cdots & \phi_{M-1}(\mathbf{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_0(\mathbf{x}_N) & \phi_1(\mathbf{x}_N) & \cdots & \phi_{M-1}(\mathbf{x}_N) \end{pmatrix}$$

N × M

- Show that the regularized least squares solution is

$$\mathbf{w} = \left(\lambda\mathbf{I} + \boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi}\right)^{-1}\boldsymbol{\Phi}^{\mathrm{T}}\mathbf{t}.$$

Stable and unique solution

Least Squares Geometric Interpretation

$$\boldsymbol{\Phi} = \begin{pmatrix} \phi_0(\mathbf{x}_1) & \phi_1(\mathbf{x}_1) & \cdots & \phi_{M-1}(\mathbf{x}_1) \\ \phi_0(\mathbf{x}_2) & \phi_1(\mathbf{x}_2) & \cdots & \phi_{M-1}(\mathbf{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_0(\mathbf{x}_N) & \phi_1(\mathbf{x}_N) & \cdots & \phi_{M-1}(\mathbf{x}_N) \end{pmatrix}$$

φ_j

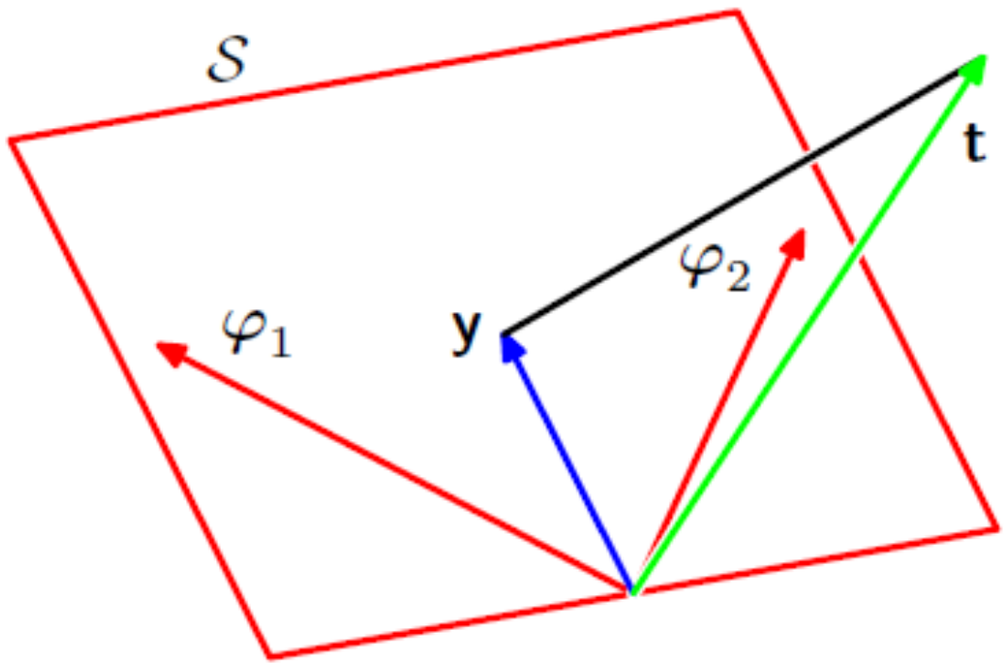
N × M

$$\mathbf{w} = (\boldsymbol{\Phi}^\top \boldsymbol{\Phi})^{-1} \boldsymbol{\Phi}^\top \mathbf{t}$$

$$\Phi\mathbf{w} = \Phi(\Phi^\top \Phi)^{-1} \Phi^\top \mathbf{t}$$

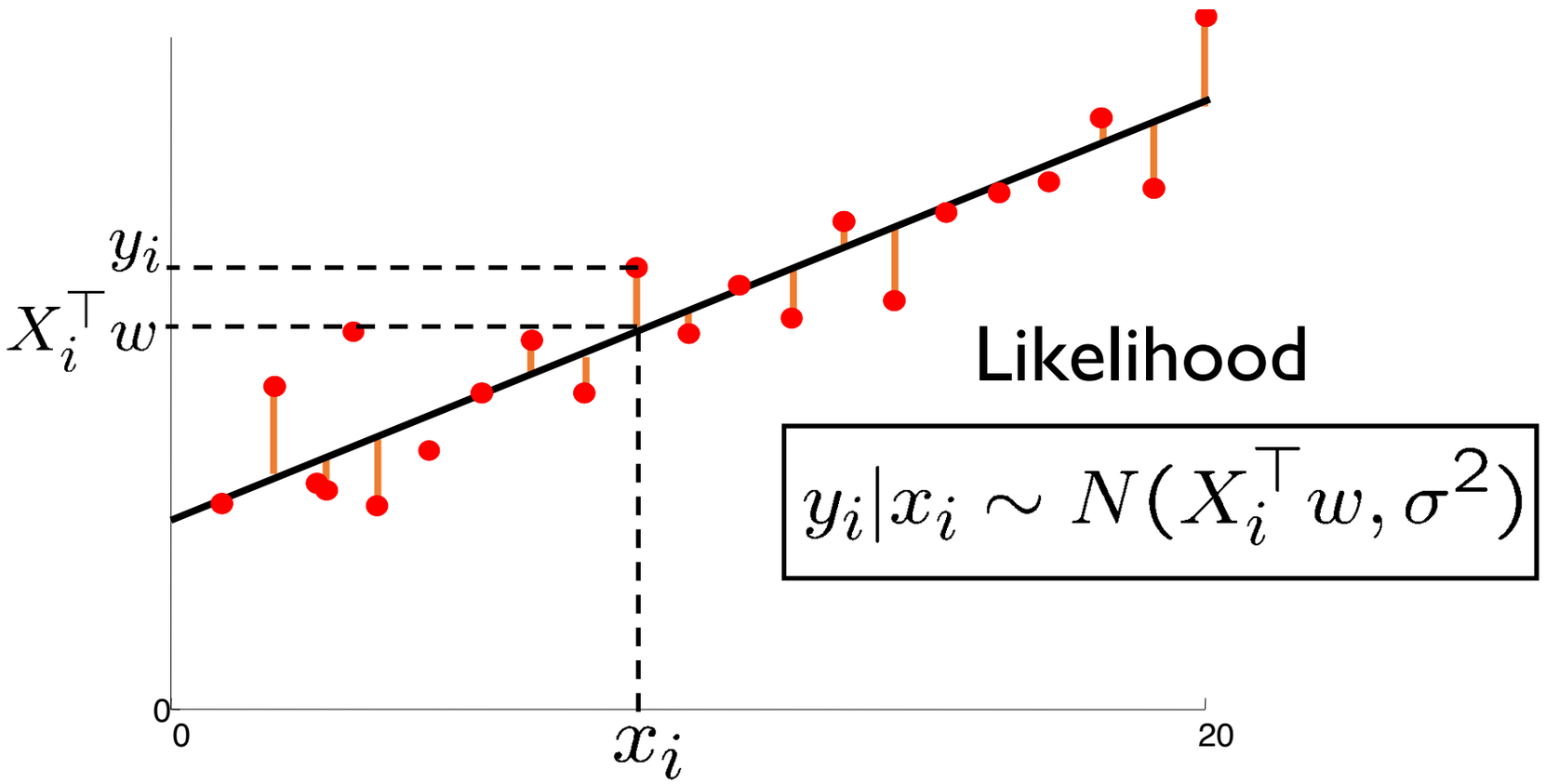
Orthogonal Projection

Geometrical interpretation of the least-squares solution, in an N-dimensional space whose axes are the values of $t_1, \ldots, t_N$. The least-squares regression function is obtained by finding the orthogonal projection of the data vector **t** onto the subspace spanned by the basis functions $\phi_j(\mathbf{x})$ in which each basis function is viewed as a vector φ_j of length N with elements $\phi_j(\mathbf{x}_n)$.



Probabilistic Interpretation : Least Squares = Maximum likelihood estimation

$$y_i \sim w \cdot x_i + N(0, \sigma^2) = N(w \cdot x_i, \sigma^2)$$



$$L = \prod_i \exp -\frac{1}{2\sigma^2}(X_i^\top w - y_i)^2 = \exp -\frac{1}{2\sigma^2}\sum_i (X_i^\top w - y_i)^2$$

$$\underset{w}{\text{argmax}}\, L = \underset{w}{\text{argmin}}\, E$$

- Similarly Regularized least squares is same as maximum aposteriori estimate assuming p(w) to be a Gaussian : argmax p(yi |w, xi) p(w)

Slide Credits : Vineeth Balasubramanian, Applied Machine Learning, IITH

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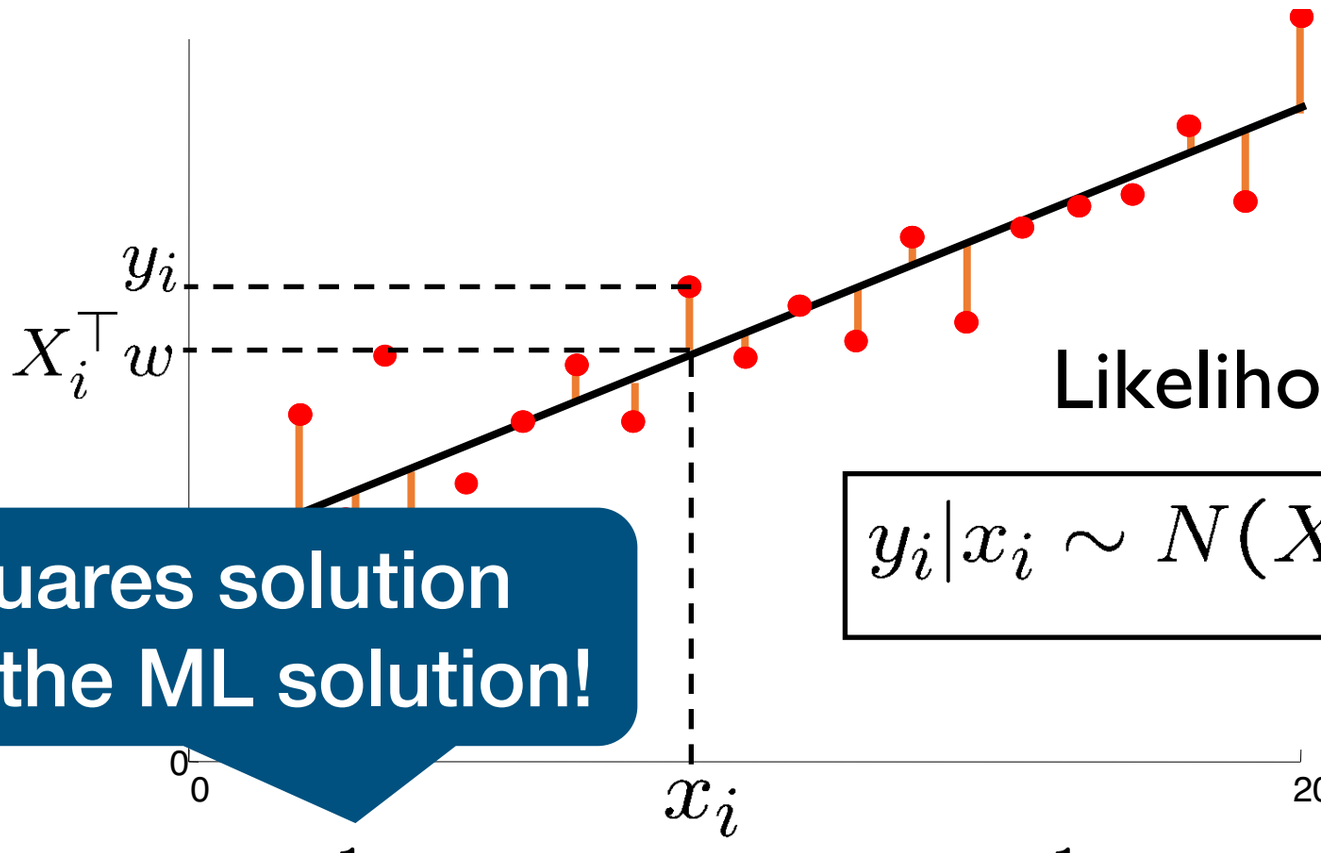

Likelihood

$$y_i | x_i \sim N(X_i^\top w, \sigma^2)$$

Least squares solution overfit like the ML solution!

$$L = \prod_i \exp -\frac{1}{2\sigma^2}(X_i^\top w - y_i)^2 = \exp -\frac{1}{2\sigma^2} \sum_i (X_i^\top w - y_i)^2$$

$$\underset{w}{\text{argmax}}\, L = \underset{w}{\text{argmin}}\, E$$

- Similarly Regularized least squares is same as maximum aposteriori estimate assuming p(w) to be a Gaussian : argmax p(yi |w, xi) p(w)

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Regularized least squares regression = Maximum Aposteriori Estimate

- Ridge Regression $$\widetilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n,\mathbf{w}) - t_n\}^2 + \frac{\lambda}{2}\|\mathbf{w}\|^2$$
- Compute Maximum aposteriori (MAP) estimate
- Prior over parameters $$p(\mathbf{w}|\alpha) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}) = \left(\frac{\alpha}{2\pi}\right)^{(M+1)/2}\exp\left\{-\frac{\alpha}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w}\right\}$$
- Posterior $$p(\mathbf{w}|\mathbf{x},\mathbf{t},\alpha,\beta) \propto p(\mathbf{t}|\mathbf{x},\mathbf{w},\beta)p(\mathbf{w}|\alpha).$$
- MAP estimate $$\frac{\beta}{2}\sum_{n=1}^{N}\{y(x_n,\mathbf{w}) - t_n\}^2 + \frac{\alpha}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w}.$$

Unique Solution

$$\mathbf{w} = \left(\lambda\mathbf{I} + \mathbf{\Phi}^{\mathrm{T}}\mathbf{\Phi}\right)^{-1}\mathbf{\Phi}^{\mathrm{T}}\mathbf{t}. \qquad \lambda = \alpha/\beta.$$

Model Selection

- Limiting the number of basis functions in order to avoid over-fitting has the side effect of limiting the flexibility of the model to capture interesting and important trends in the data.
- Regularization allows complex models to be trained on data sets of limited size without severe over-fitting, essentially by limiting the effective model complexity.
- Model Selection : determining a suitable value of the hyper-parameter which is the regularization coefficient λ.

- What happens when you minimizes the regularized error function with respect to weight vector w and regularization coefficient λ ?

Regularized Least Squares : Cross Validation

How to choose λ ?
Use validation data!

$$\frac{1}{2}\sum_{n=1}^{N}\{t_n - \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n)\}^2 + \frac{\lambda}{2}\sum_{j=1}^{M}|w_j|^q$$

1. Training set is a set of examples used for learning a model parameters (e.g., weight vector w in linear regression

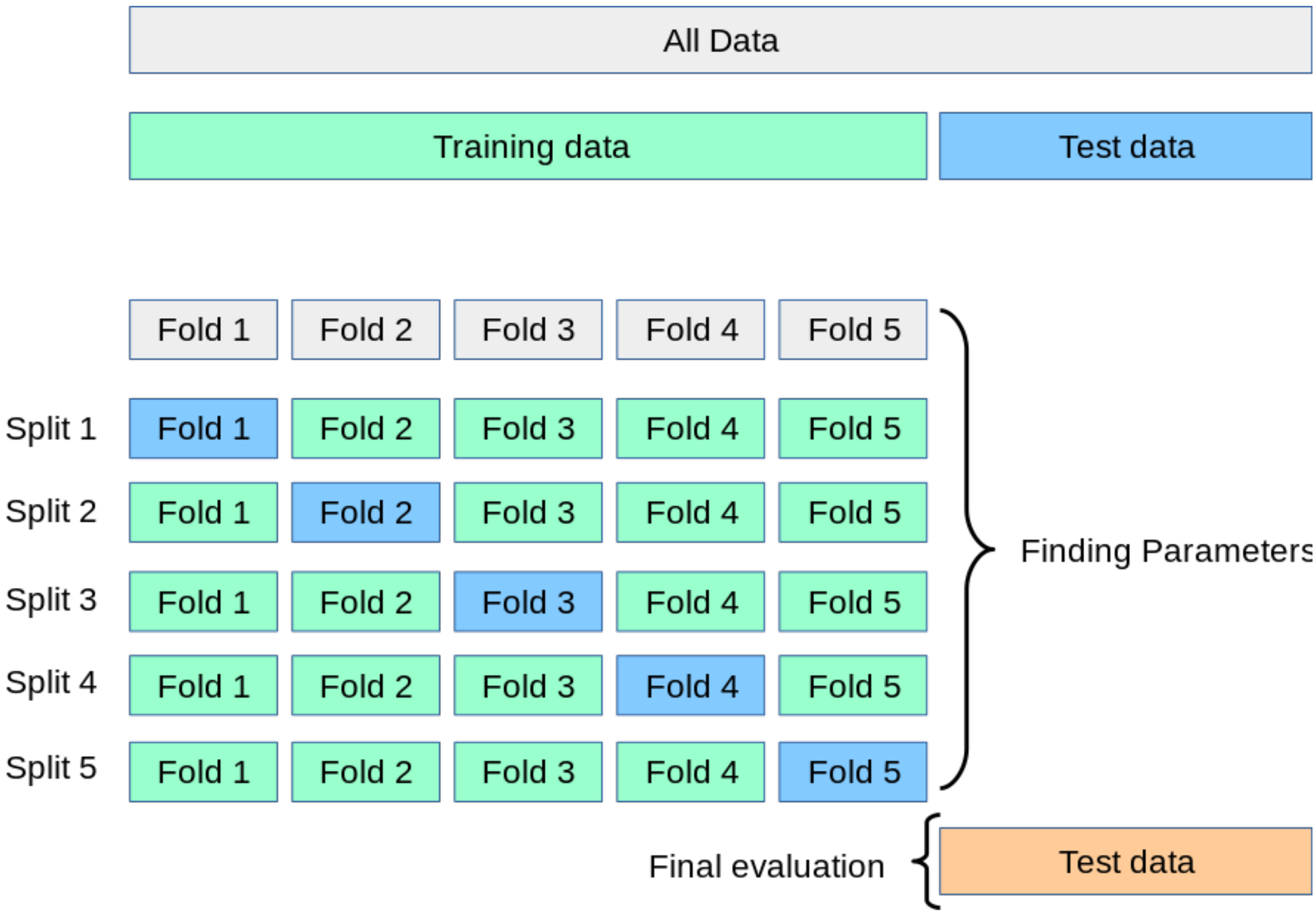
2. Validation set is a set of examples that cannot be used for learning the model parameter but can help tune model hyper-parameters e.g Regularization constant in LR. Validation helps control overfitting.

3. Test set is used to assess the performance of the final model and provide an estimation of the test error.

Example: Split the data randomly into 60% for training, 20% for validation and 20% for testing.

Note: Dont use the test set to further tune the parameters or revise the model.

Cross Validation



https://scikit-learn.org/stable/modules/cross_validation.html

Linear Regression

- Parameter Estimation
  - Maximum Likelihood
  - Maximum Aposteriori
- Hyper-parameter Estimation
  - Cross-validation
- Evaluation : Root mean square error, absolute error

$$RMSE = \sqrt{\sum_{i=1}^{n} \frac{(\hat{y}_i - y_i)^2}{n}}$$

Training vs Generalization Error

- Training Error
  - Not very useful
  - Relatively easy to obtain low error

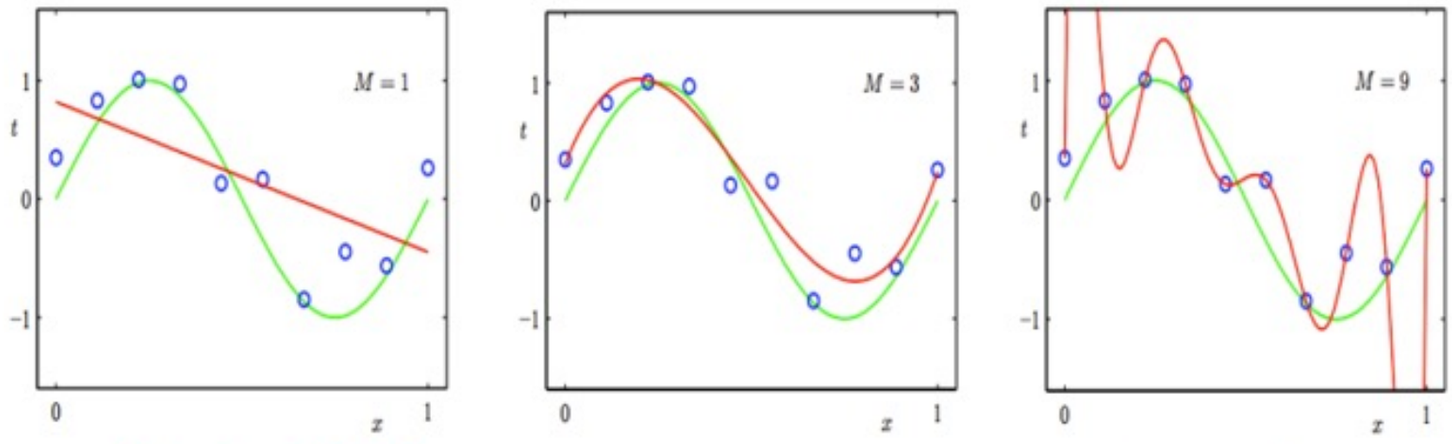
$$E_{train} = \frac{1}{n} \sum_{i=1}^{n} \overbrace{error}^{\text{same? different by how much?}}(\underbrace{f_D(\mathbf{x}_i)}_{\text{value we predicted}}, \underbrace{y_i}_{\text{true value}})$$

training examples

- Generalization Error
  - How well we do on future data

How to compute generalization error?

Regression



predictor too inflexible: cannot capture pattern

predictor too flexible: fits noise in the data

Estimating Generalization Error

- Testing Error
  - Set aside part of training data (testing set)
  - Learn a predictor without using any of this test data
  - Predict values for testing set, compute error
  - This is an estimate of generalization error

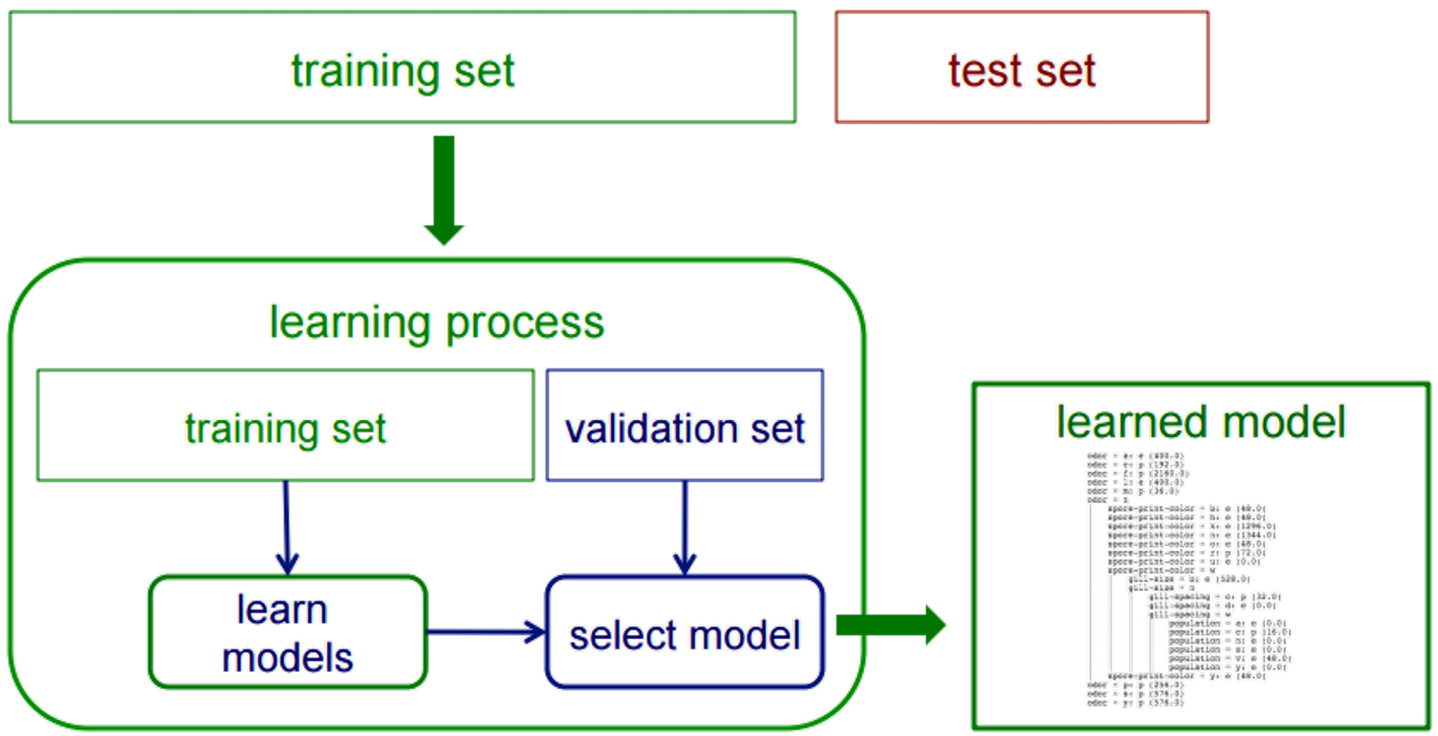
$$E_{test} = \frac{1}{n} \sum_{i=1}^{n} error(f_D(\mathbf{x}_i), y_i)$$

over testing set

$$RMSE = \sqrt{\sum_{i=1}^{n} \frac{(\hat{y}_i - y_i)^2}{n}}$$

Use of Validation and Test Sets

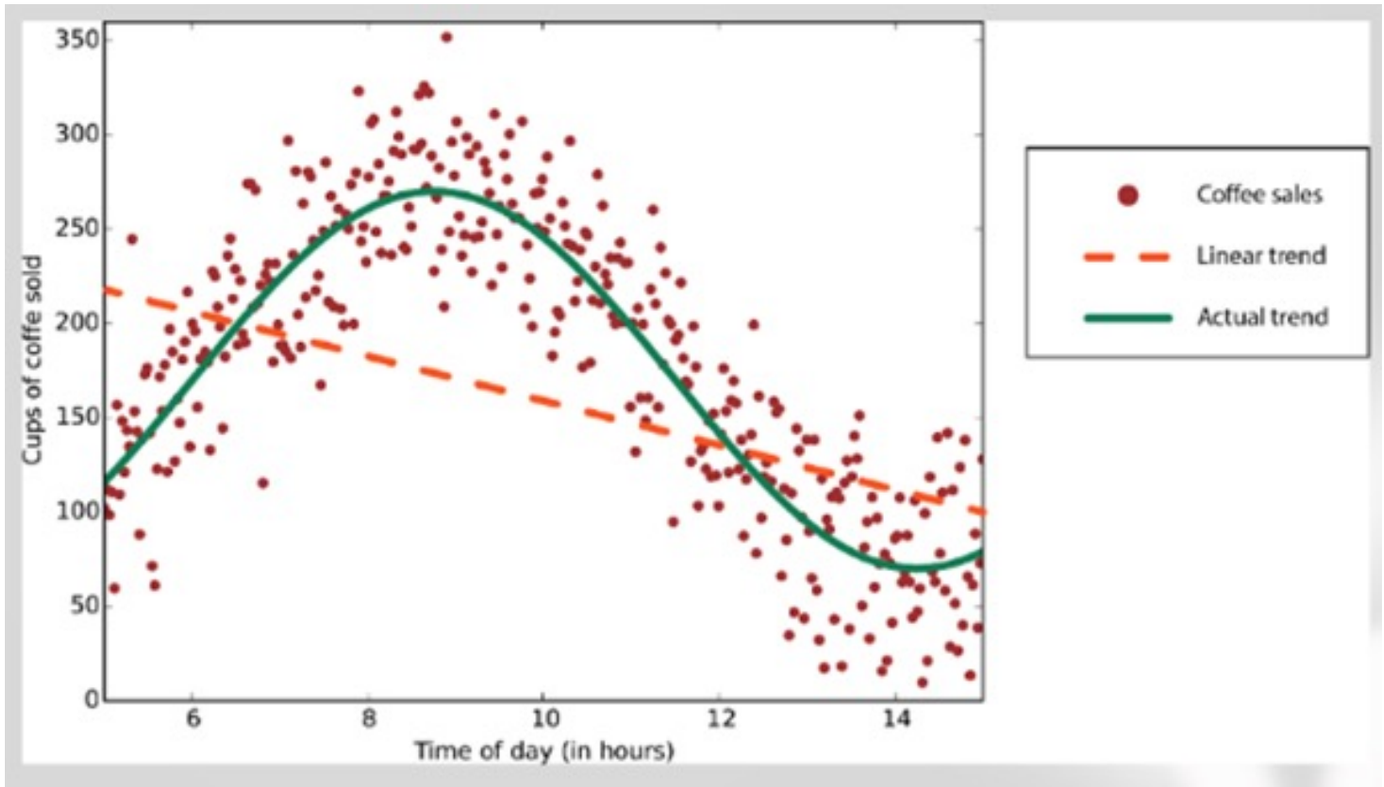
- If we want unbiased estimates of accuracy during the learning process:



Linear Regression

- Parameter Estimation
  - Maximum Likelihood
  - Maximum Aposteriori
- Hyper-parameter Estimation
  - Cross-validation
- Prediction $$p(t|\mathbf{x}, \mathbf{w}, \beta) = \mathcal{N}(t|y(\mathbf{x}, \mathbf{w}), \beta^{-1}).$$

Supervised learning : Regression



Number of vehicles passing a junction

p(y|x)?

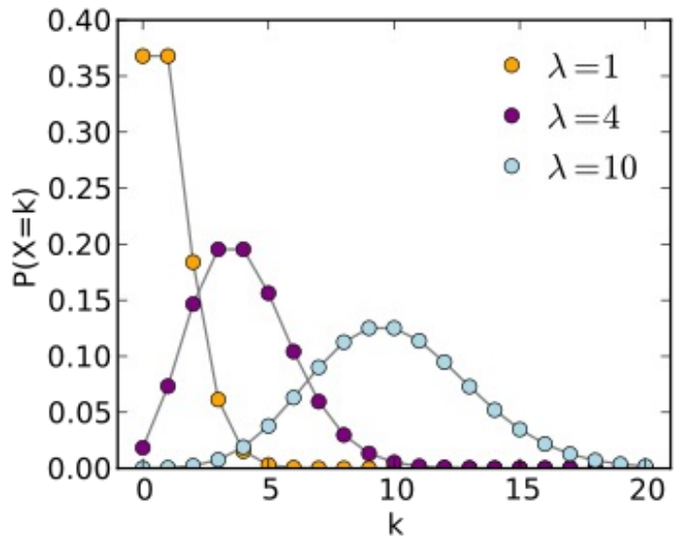
Y take values 0,1,2,3,….. but not 2.1, 3.4, 5.55……

https://medium.com/@heyozramos/regression-vs-classification-86d73c281c5e

Poisson Regression

- Poisson distribution : Model number of events occurring in a fixed interval of time/space

$$P(k \text{ events in interval}) = e^{-\lambda} \frac{\lambda^k}{k!}$$



- λ is the average (mean) number of events

- Y has a Poisson distribution, and assumes the logarithm of its expected value can be modeled by a linear combination of unknown parameters.

$$\lambda := \mathrm{E}(Y \mid x) = e^{\theta' x}$$

$$p(y \mid x; \theta) = \frac{\lambda^y}{y!} e^{-\lambda} = \frac{e^{y\theta' x} e^{-e^{\theta' x}}}{y!}$$

Poisson Regression : Learning parameters

- Likelihood

$$p(y_1, \ldots, y_m \mid x_1, \ldots, x_m; \theta) = \prod_{i=1}^{m} \frac{e^{y_i \theta' x_i} e^{-e^{\theta' x_i}}}{y_i!}.$$

- Estimate parameters by maximum likelihood estimation

$$\ell(\theta \mid X, Y) = \log L(\theta \mid X, Y) = \sum_{i=1}^{m} \left(y_i \theta' x_i - e^{\theta' x_i} - \log(y_i!) \right).$$

- Use gradient descent to find the optimal value of θ.

Bias Variance Decomposition

Given the actual conditional distribution $p(t|\mathbf{x})$, **and** $p(\mathbf{x},t) = p(t|x)\,p(x)$, let the optimal function one can learn is given by $h(\mathbf{x})$

For any given data set D, we can run our learning algorithm and obtain a prediction function $y(\mathbf{x};D)$.

Expected squared difference between $y(\mathbf{x};D)$ and the regression function $h(\mathbf{x})$, averaged across multiple data sets

$$\mathbb{E}_{\mathcal{D}}\left[\{y(\mathbf{x};\mathcal{D}) - h(\mathbf{x})\}^2\right]$$
$$= \underbrace{\{\mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})] - h(\mathbf{x})\}^2}_{(\text{bias})^2} + \underbrace{\mathbb{E}_{\mathcal{D}}\left[\{y(\mathbf{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})]\}^2\right]}_{\text{variance}}.$$

$$\{y(\mathbf{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})] + \mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})] - h(\mathbf{x})\}^2$$
$$= \{y(\mathbf{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})]\}^2 + \{\mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})] - h(\mathbf{x})\}^2$$
$$+2\{y(\mathbf{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})]\}\{\mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})] - h(\mathbf{x})\}.$$

Bias- Variance Decomposition

- Bias Error
  - Bias are the simplifying assumptions made by a model to make the target function easier to learn.
  - **Low Bias:** Suggests less assumptions about the form of the target function.
  - **High-Bias**: Suggests more assumptions about the form of the target function.

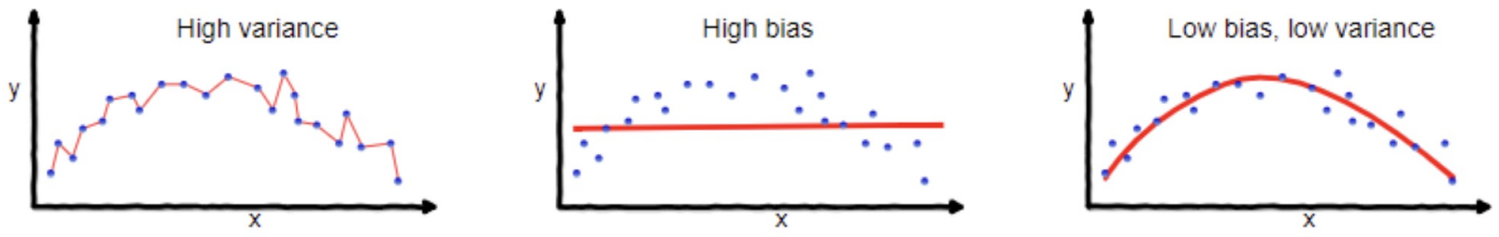
$$\mathbb{E}_{\mathcal{D}}\left[\{y(\mathbf{x};\mathcal{D}) - h(\mathbf{x})\}^2\right]$$
$$= \underbrace{\{\mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})] - h(\mathbf{x})\}^2}_{(\text{bias})^2} + \underbrace{\mathbb{E}_{\mathcal{D}}\left[\{y(\mathbf{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})]\}^2\right]}_{\text{variance}}.$$

There is a trade-off between bias and variance, with very flexible models having low bias and high variance, and relatively rigid models having high bias and low variance.

Bias- Variance Decomposition

- **Variance Error**
  - Variance is the amount that the estimate of the target function will change if different training data was used.
  - **Low Variance**: Suggests small changes to the estimate of the target function with changes to the training dataset.
  - **High Variance**: Suggests large changes to the estimate of the target function with changes to the training dataset.

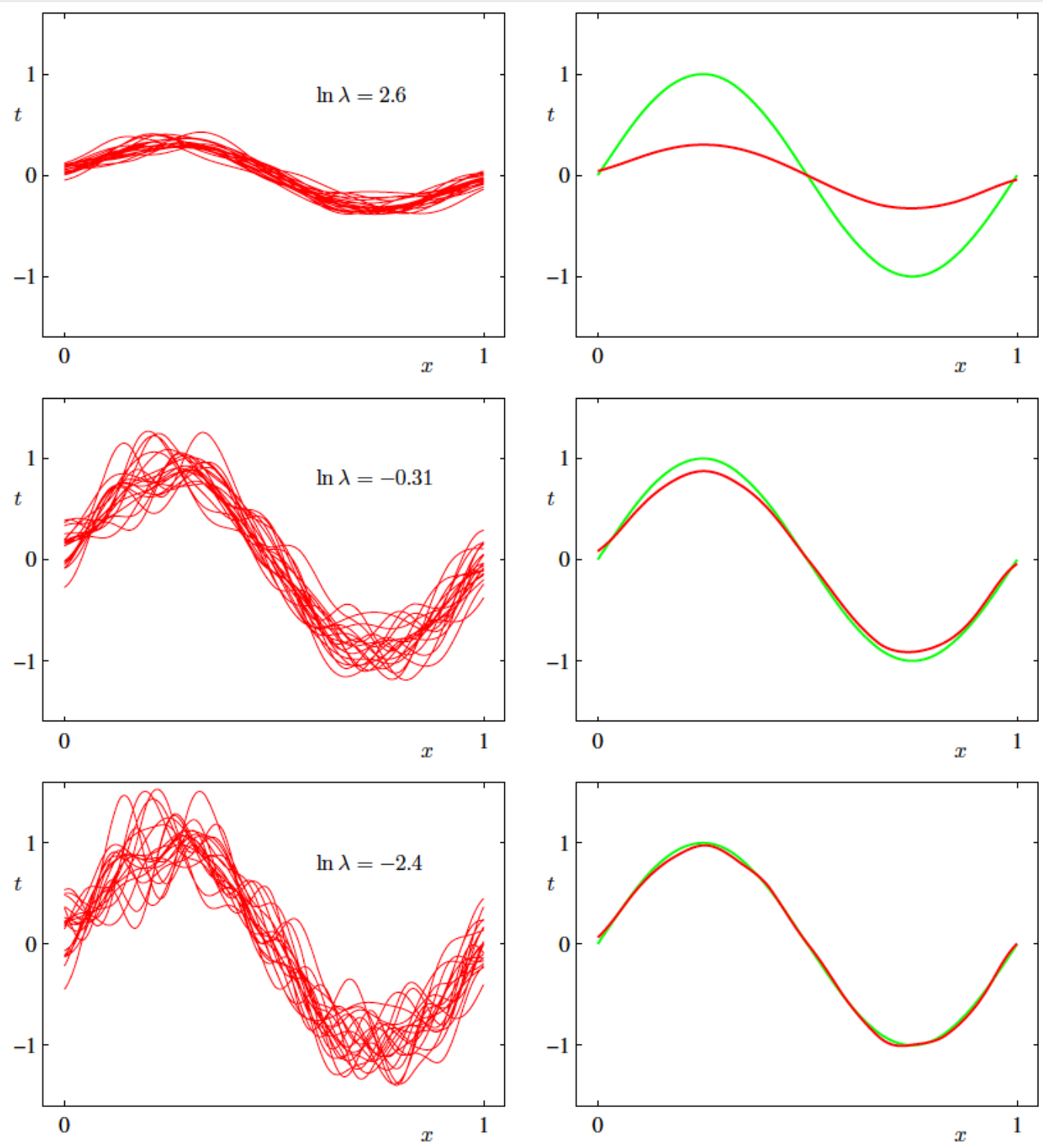
$$\mathbb{E}_{\mathcal{D}}\left[\{y(\mathbf{x};\mathcal{D}) - h(\mathbf{x})\}^2\right]$$
$$= \underbrace{\{\mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})] - h(\mathbf{x})\}^2}_{(\text{bias})^2} + \underbrace{\mathbb{E}_{\mathcal{D}}\left[\{y(\mathbf{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})]\}^2\right]}_{\text{variance}}.$$



overfitting **underfitting** **Good balance**

- **Linear** machine learning algorithms often have a high bias but a low variance.
- **Nonlinear** machine learning algorithms often have a low bias but a high variance.

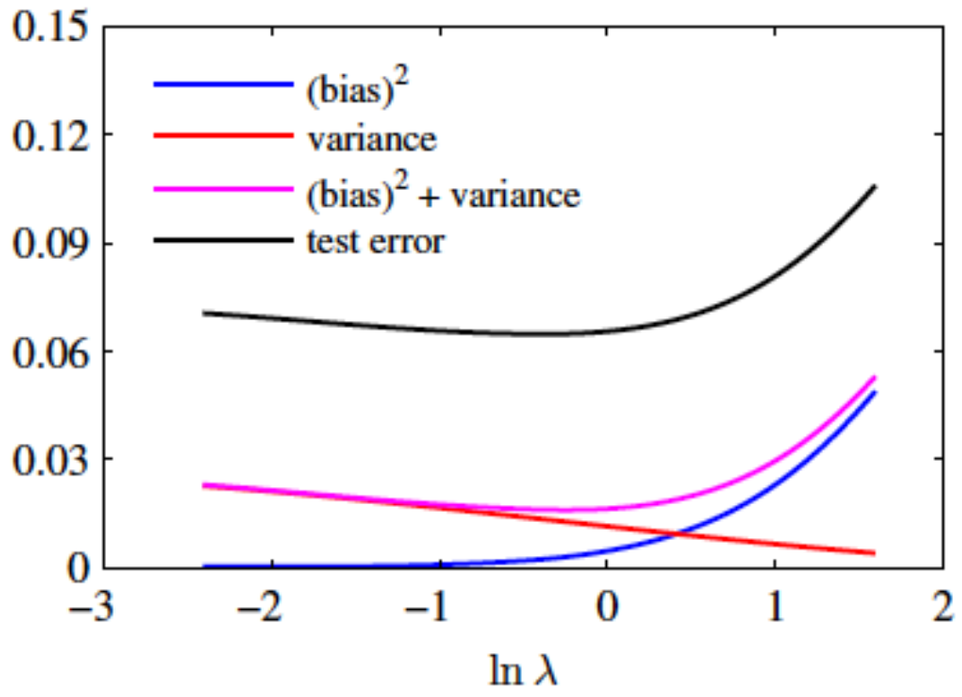
Bias Variance Decomposition



$$h(x) = \sin(2\pi x). \quad \overline{y}(x) = \frac{1}{L}\sum_{l=1}^{L} y^{(l)}(x)$$

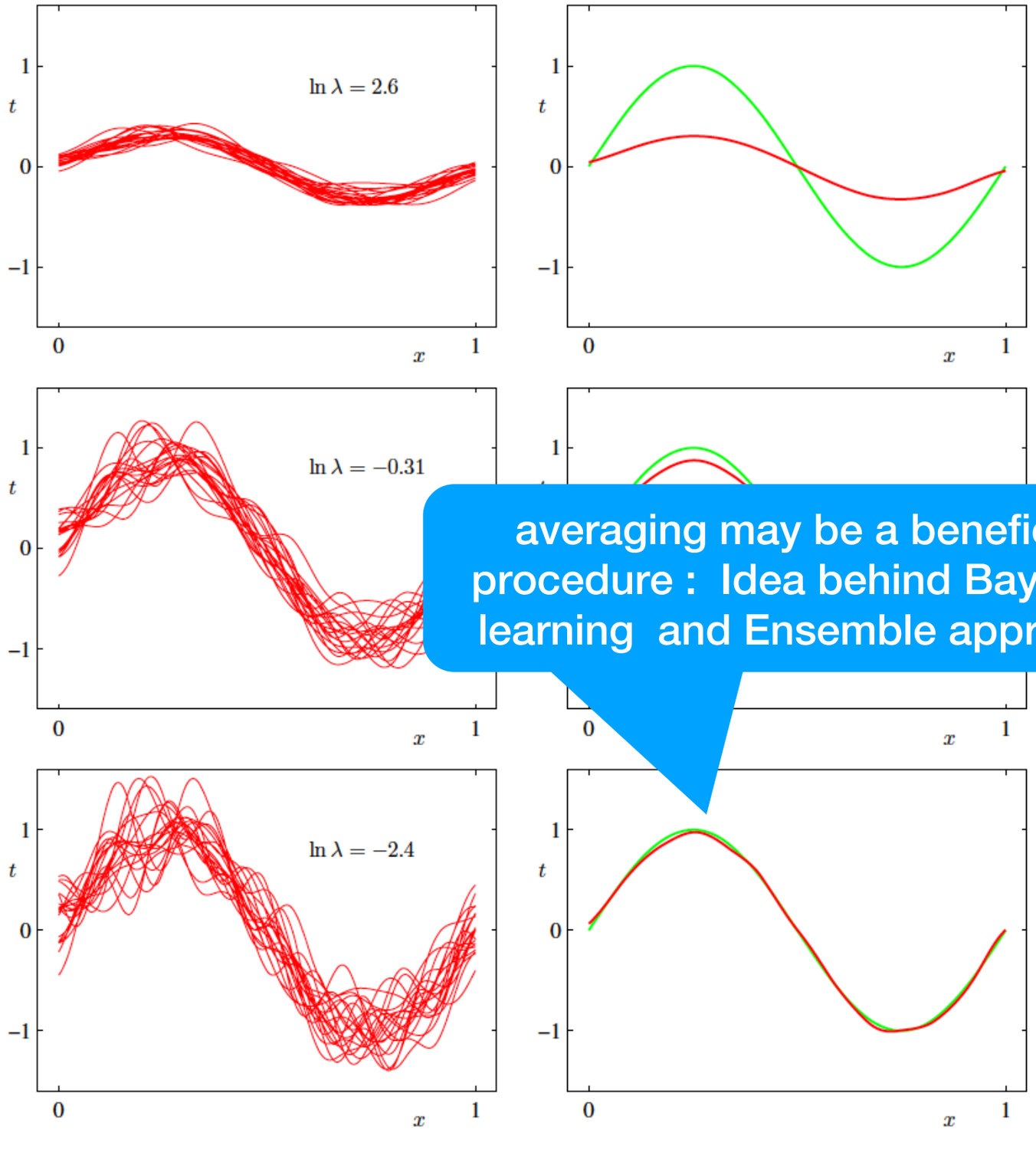
$$(\text{bias})^2 = \frac{1}{N}\sum_{n=1}^{N}\{\overline{y}(x_n) - h(x_n)\}^2$$

$$\text{variance} = \frac{1}{N}\sum_{n=1}^{N}\frac{1}{L}\sum_{l=1}^{L}\left\{y^{(l)}(x_n) - \overline{y}(x_n)\right\}^2$$



L = 100 data sets, each having *N* = 25 data points,

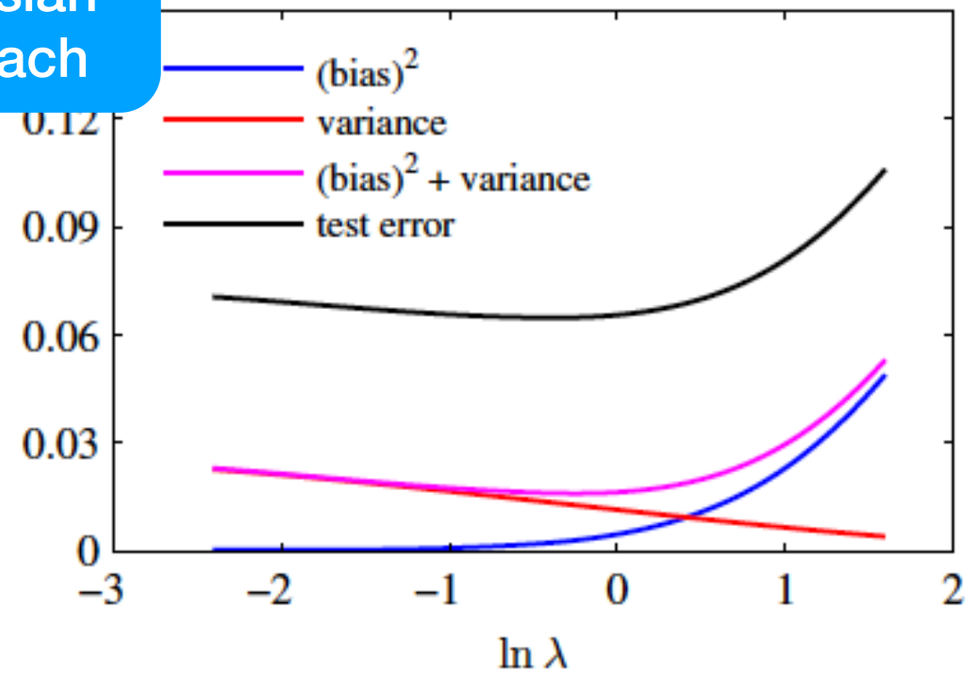
Bias Variance Decomposition



$$h(x) = \sin(2\pi x).$$

L = 100 data sets,
each having *N* = 25
data points,

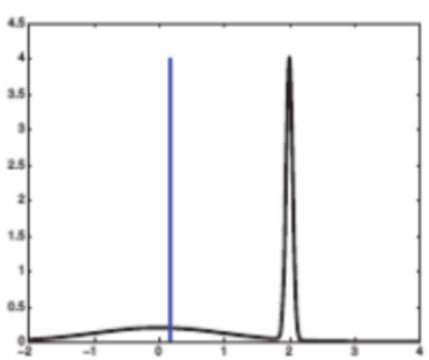
averaging may be a beneficial procedure : Idea behind Bayesian learning and Ensemble approach



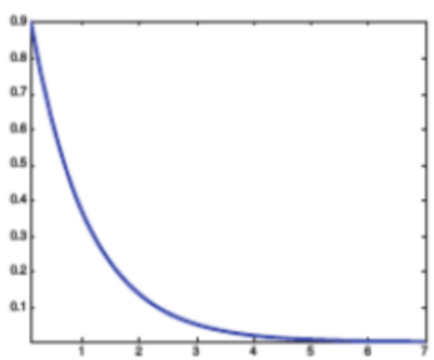
Bayesian Linear Regression

$$Prediction : p(y_*|x_*) = \int p(y_*|x_*, w)p(w|D)dw$$

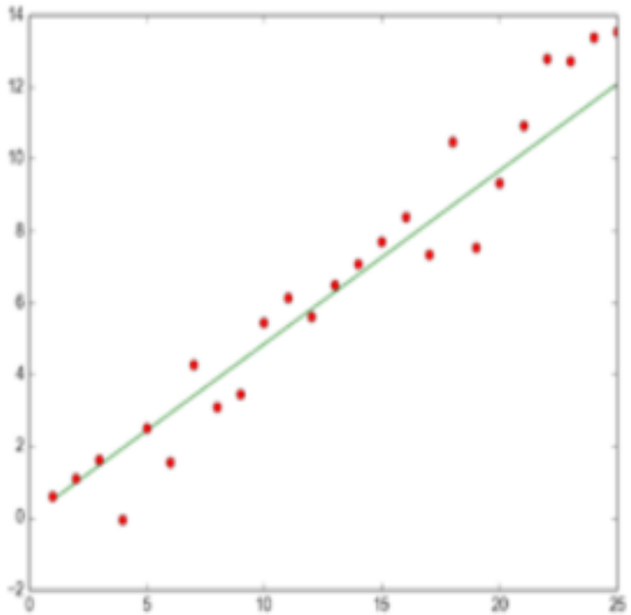
$$\begin{array}{lll} p(w|D) & \propto & p(D|w) \quad p(w) \\ \text{Posterior} & \propto & \text{Likelihood} \quad \text{Prior} \end{array}$$

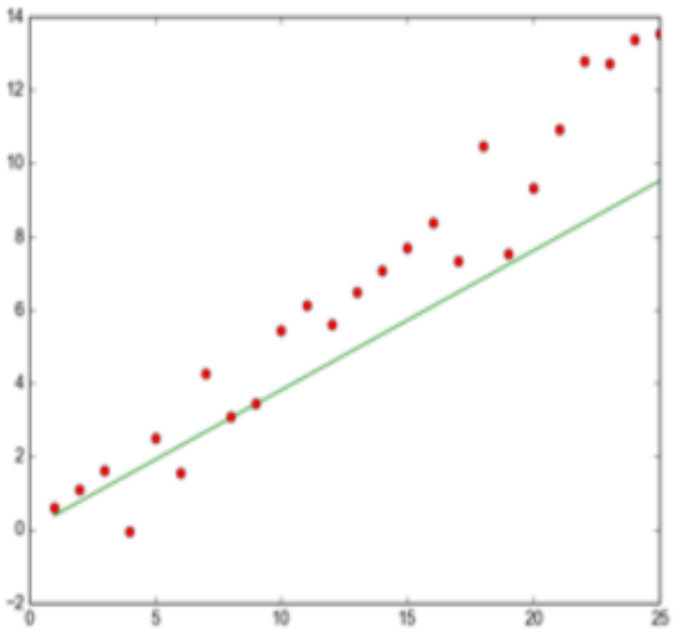


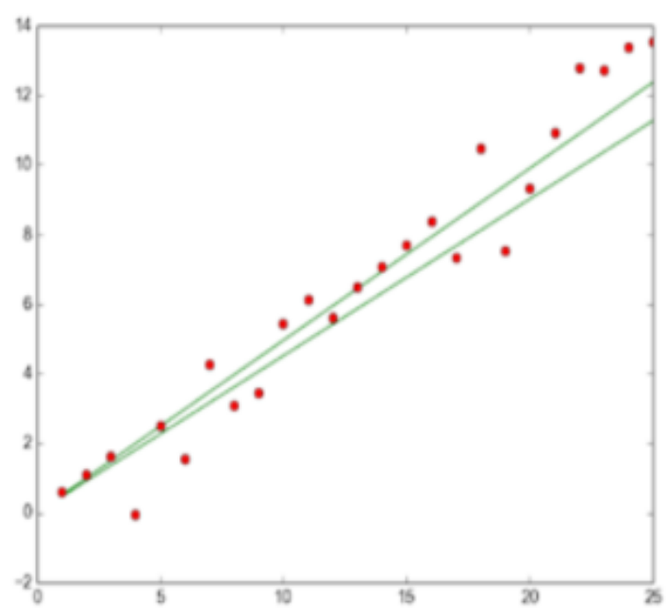
(a)

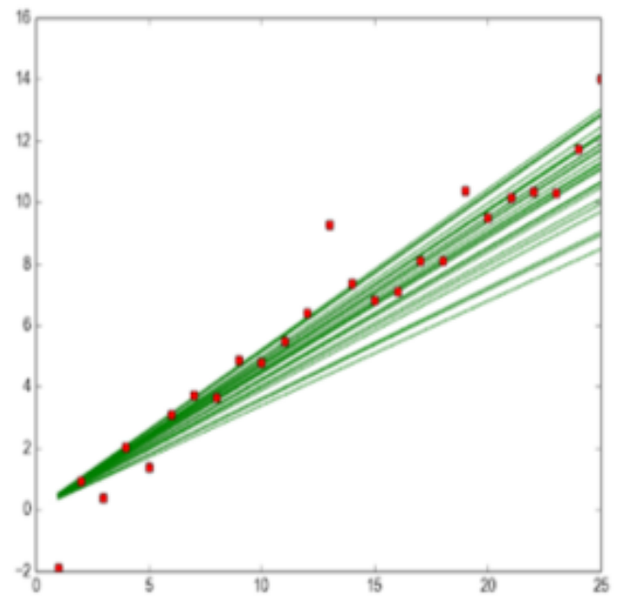


(b)







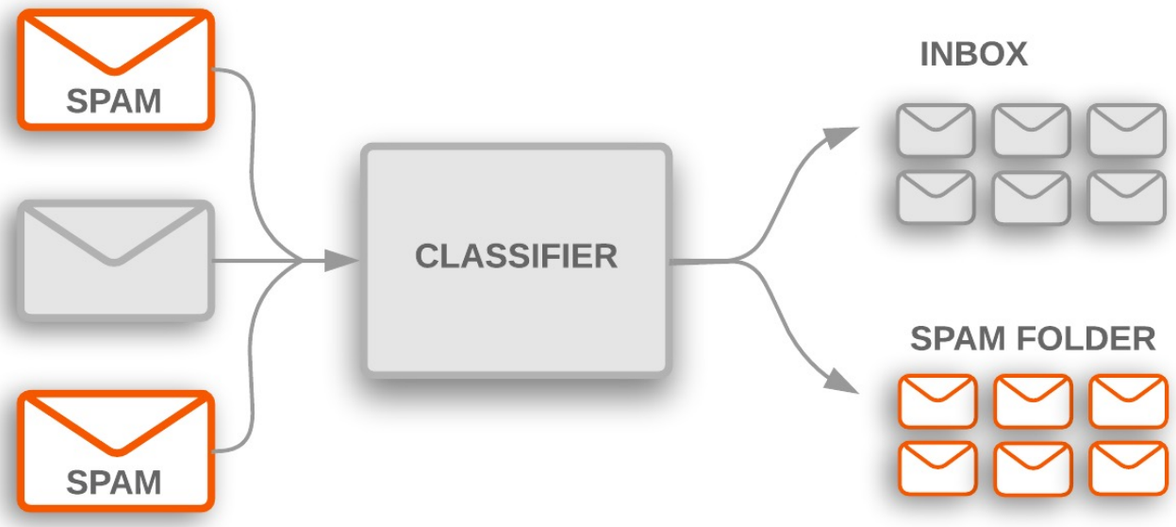


Bias Variance Tradeoff

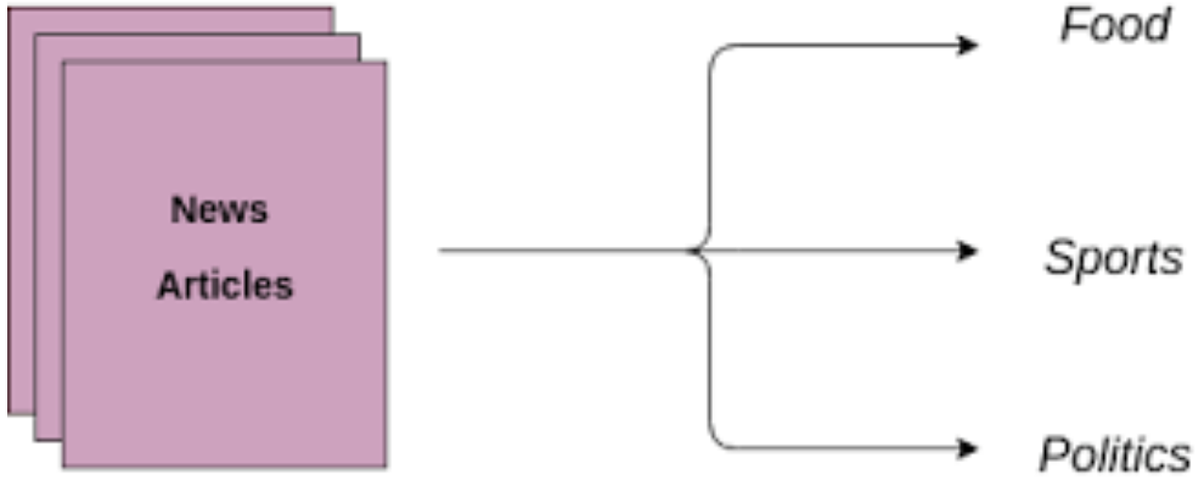
- Dimensionality reduction and feature selection can decrease variance by simplifying models.
- Similarly, a larger training set tends to decrease variance.
- Adding features (predictors) tends to decrease bias, at the expense of introducing additional variance.
- linear and Generalized linear models can be regularized to decrease their variance at the cost of increasing their bias

Supervised Learning : Classification

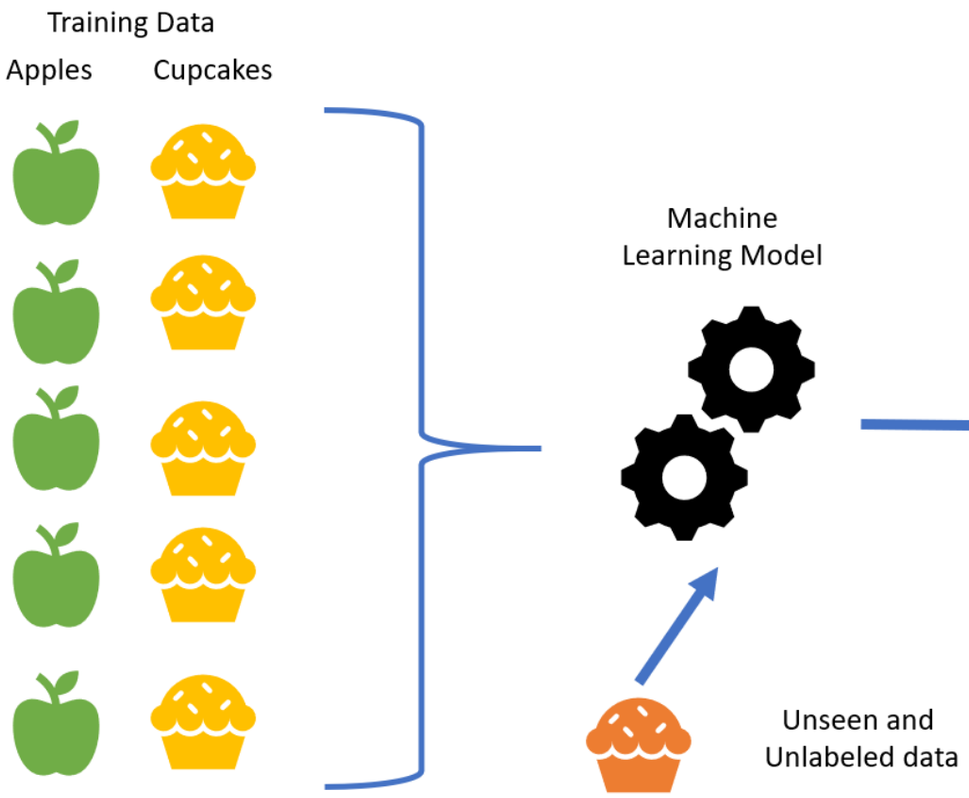
- Binary classification : y = {0,1}
- Multiclass classification : y = {1,2,…K}

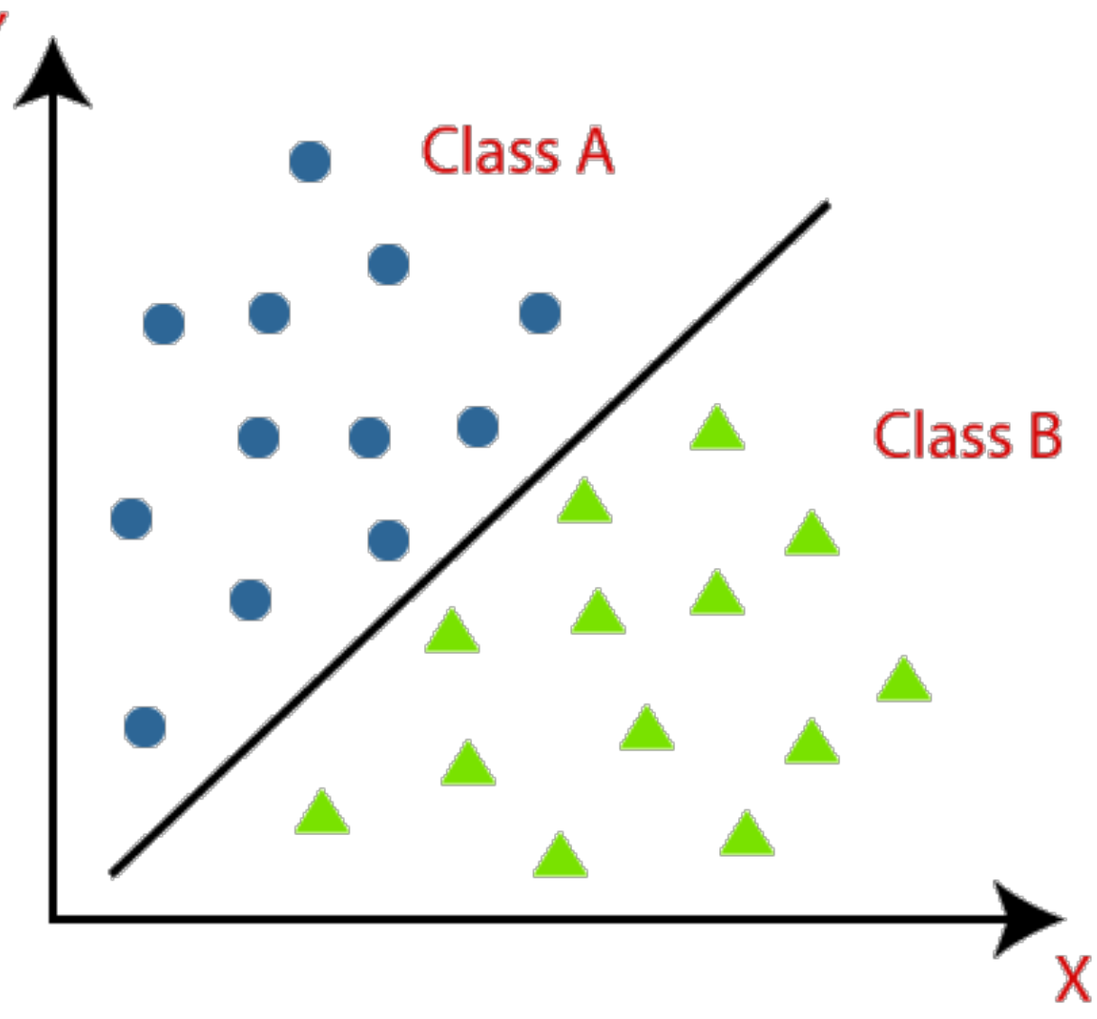


p(y|x)?



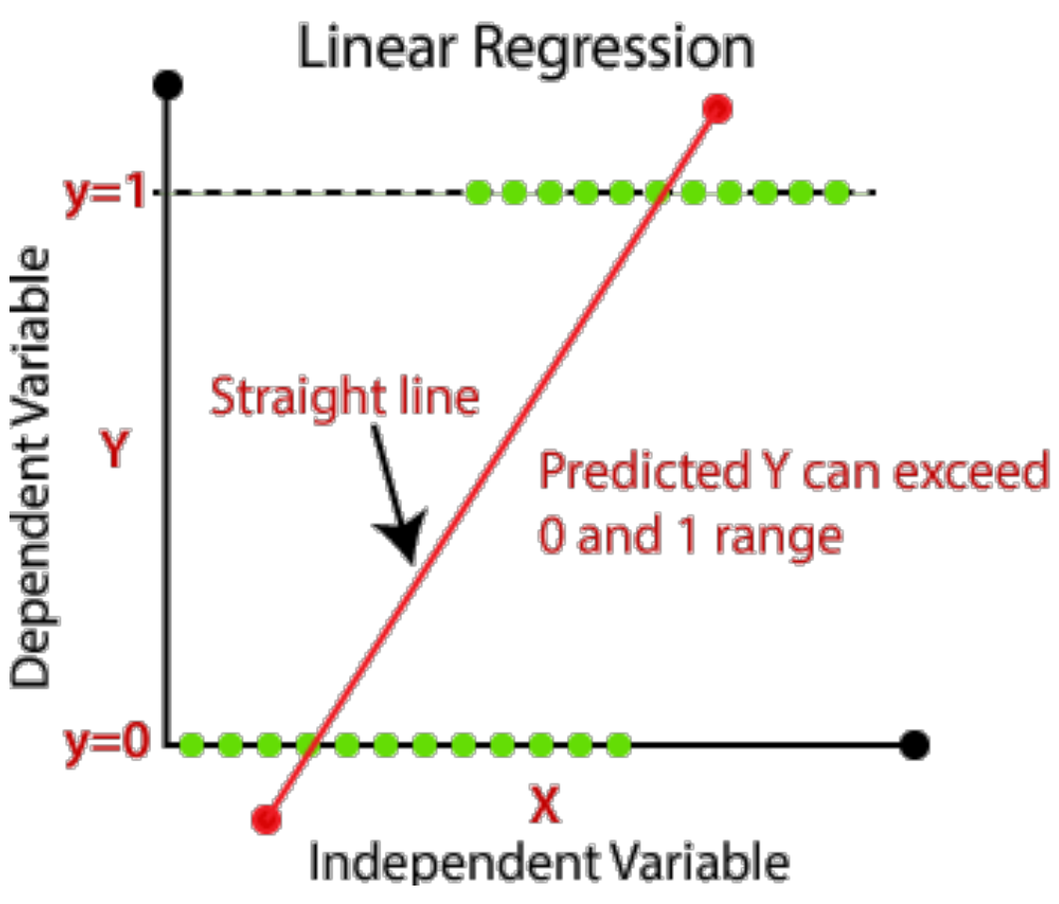
Classification : Linear Models

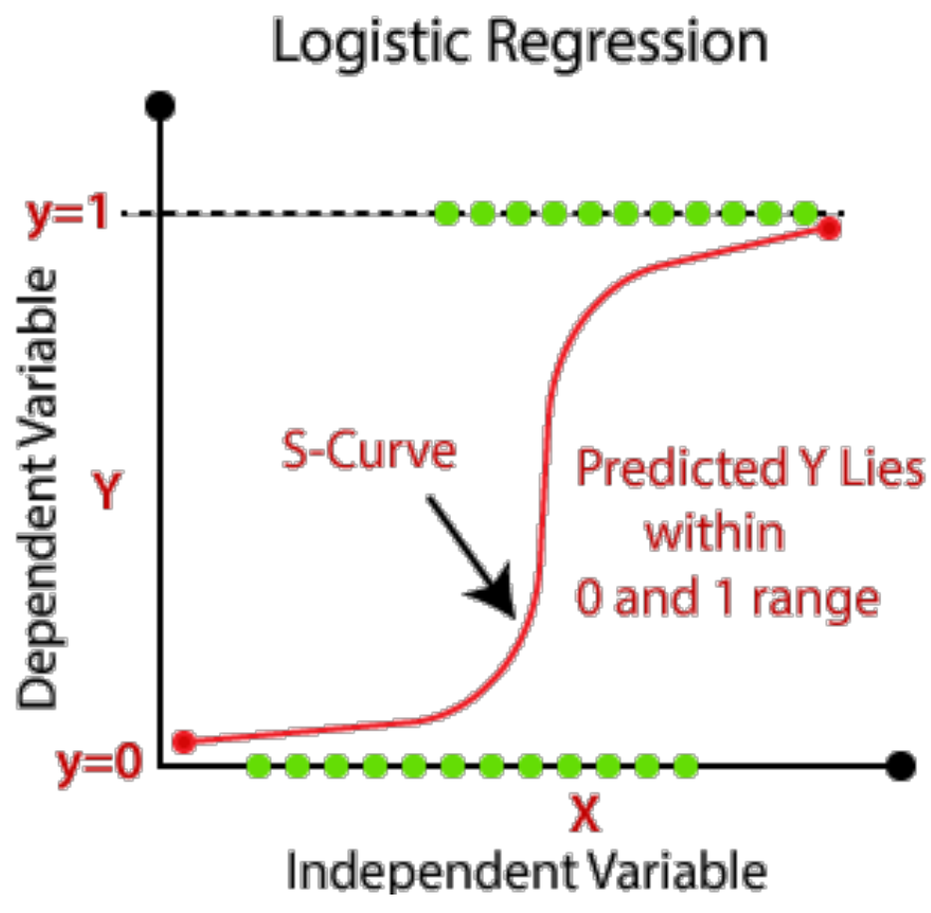




Linear regression to Logistic regression

- Y takes value 0 or 1



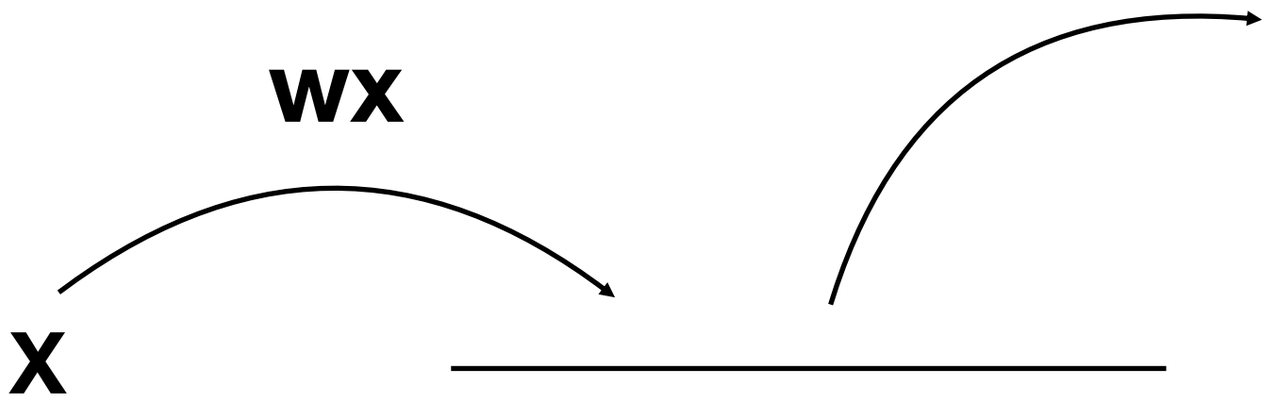


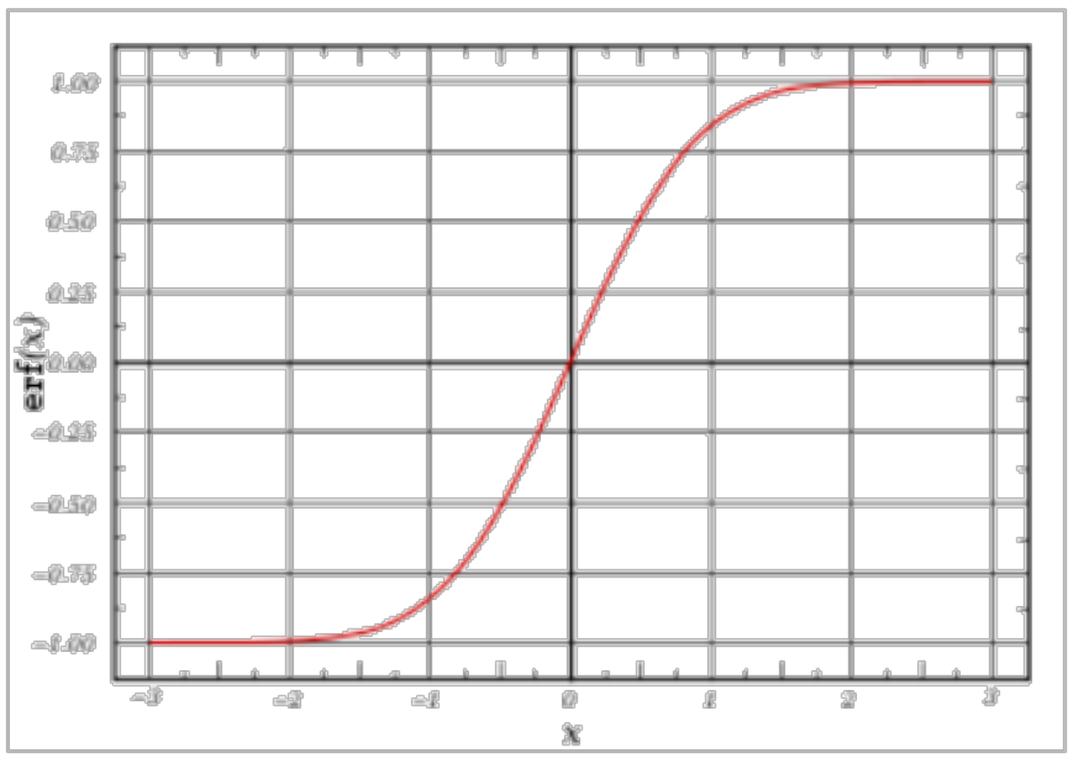
Logistic Regression

- A discriminative approach which directly models p(y|x)
- To predict an outcome variable that is categorical from one or more categorical or continuous predictor variables.
  - Let X be the data instance, and Y be the class label {0,1} :
    Model P(Y|X) directly using a Sigmoid function:

Logistic Sigmoid : $P(Y=1 \mid \mathbf{X}) = \dfrac{1}{1+e^{-\mathbf{wx}}}$

$$\sigma(a) = \frac{1}{1+\exp(-a)}$$





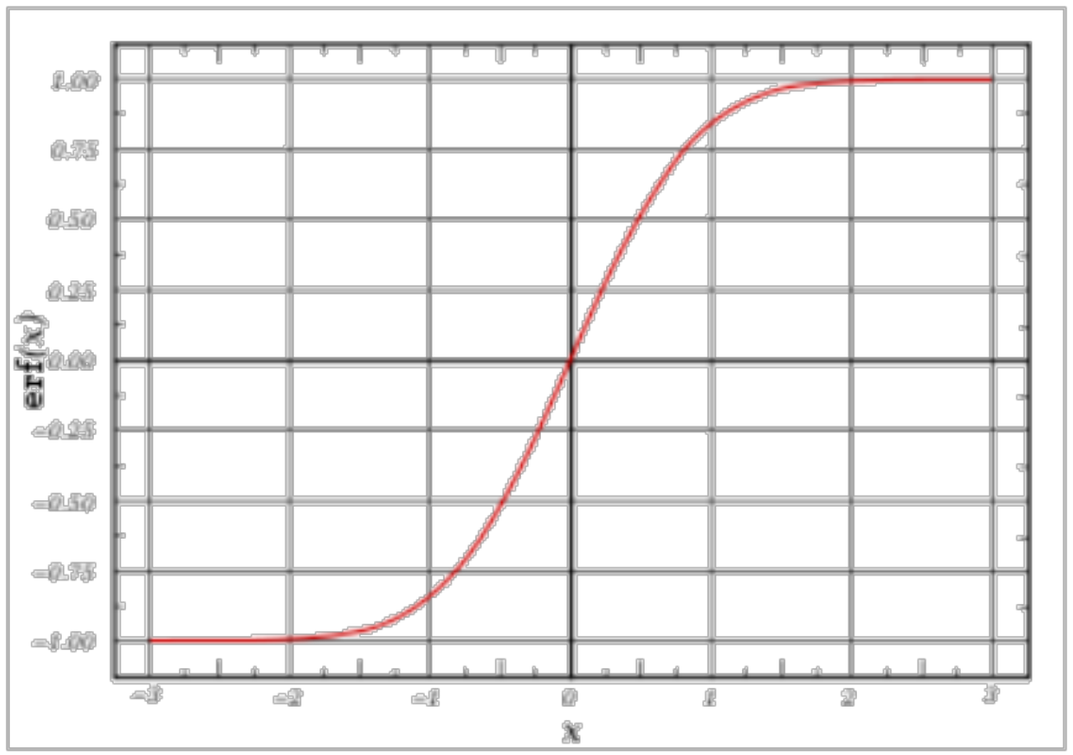
Logistic Regression

- To predict an outcome variable that is categorical from one or more categorical or continuous predictor variables.
  - Let X be the data instance, and Y be the class label:
    Model P(Y|X) directly using a Sigmoid function: Logistic function

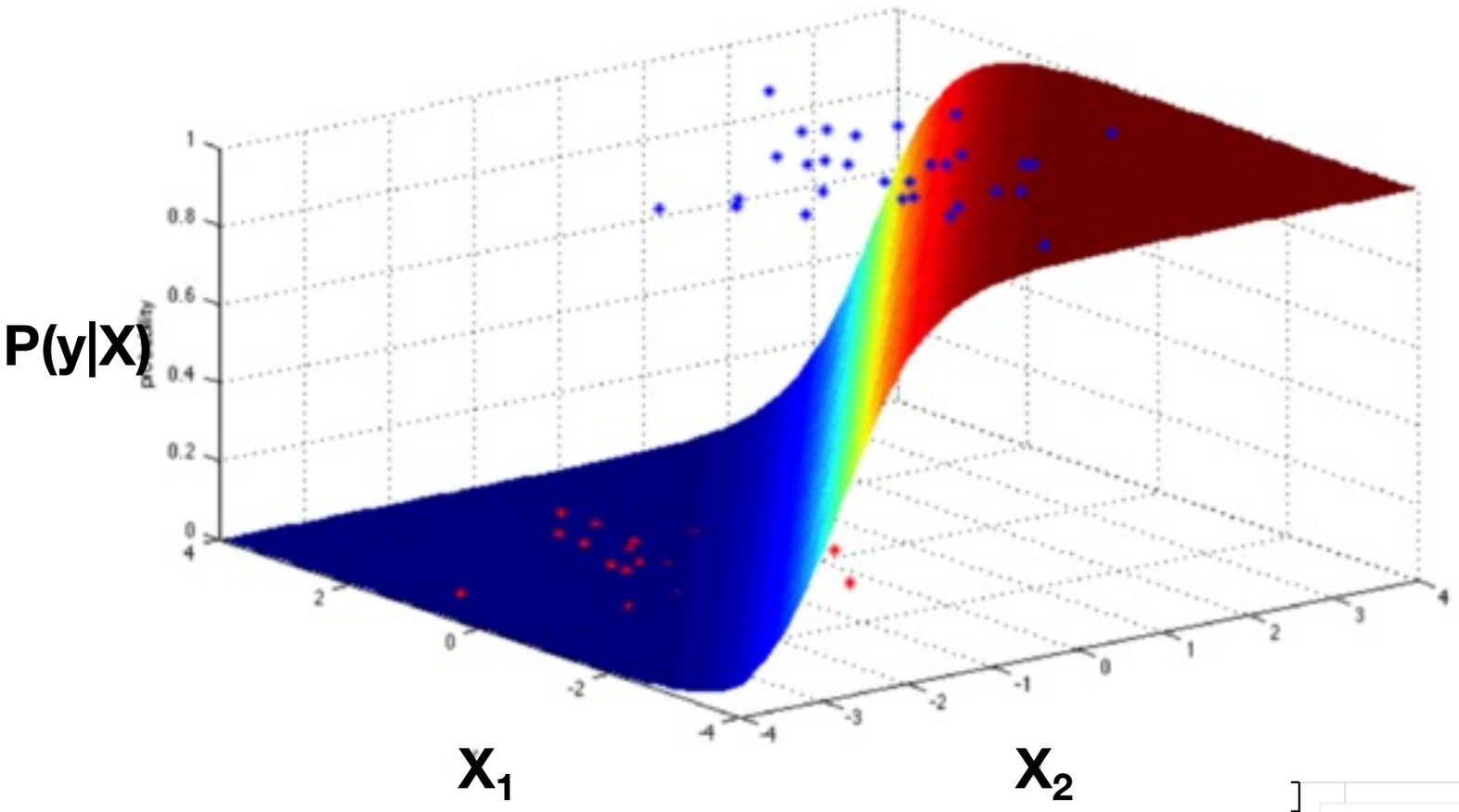
$$P(Y=1|\mathbf{X}) = \frac{1}{1+e^{-\mathbf{wx}}}$$

[HW] Find derivative of s(w) = p(y=1|X)!

$$\Phi(a) = \int_{-\infty}^{a} \mathcal{N}(\theta|0,1)\,\mathrm{d}\theta$$



Logistic Regression

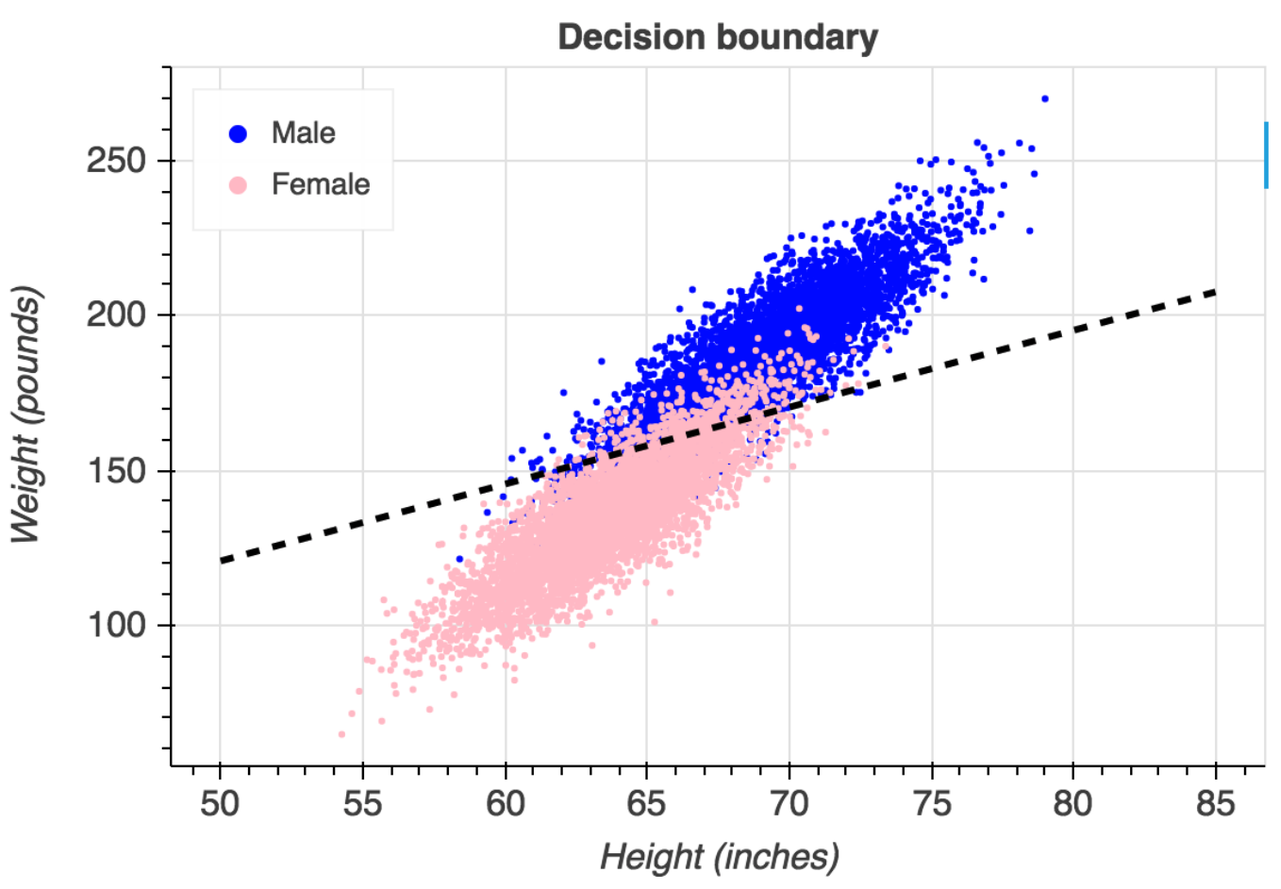


Discriminant Functions

$$P(Y=1 \mid \mathbf{X}) = \frac{1}{1+e^{-\mathbf{wx}}}$$

Decision surfaces are linear functions of x

Decision surfaces correspond to $y(\mathbf{x})$ = constant, so that $\mathbf{w}^T\mathbf{x} + w0 = 0$

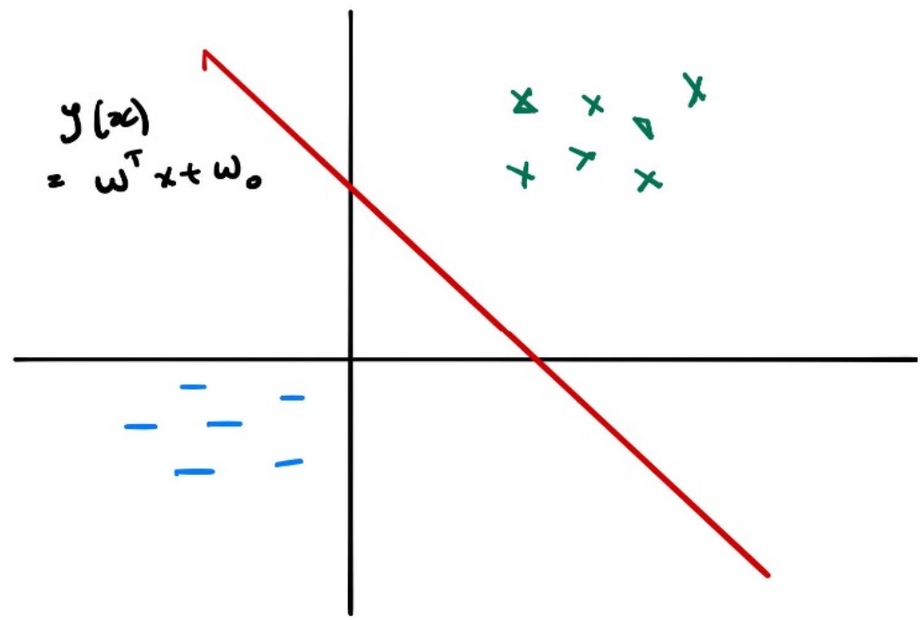


Discriminant function

$$y(\mathbf{x}) = \mathbf{w}^{\mathrm{T}}\mathbf{x} + w_0$$

input vector **x** is assigned to class $C1$ if $y(\mathbf{x}) > 0$ and to class $C2$ otherwise

decision boundary is therefore defined by the relation $y(\mathbf{x}) = 0$



w is orthogonal to every vector lying within the decision surface, and so **w** determines the orientation of the decision surface.

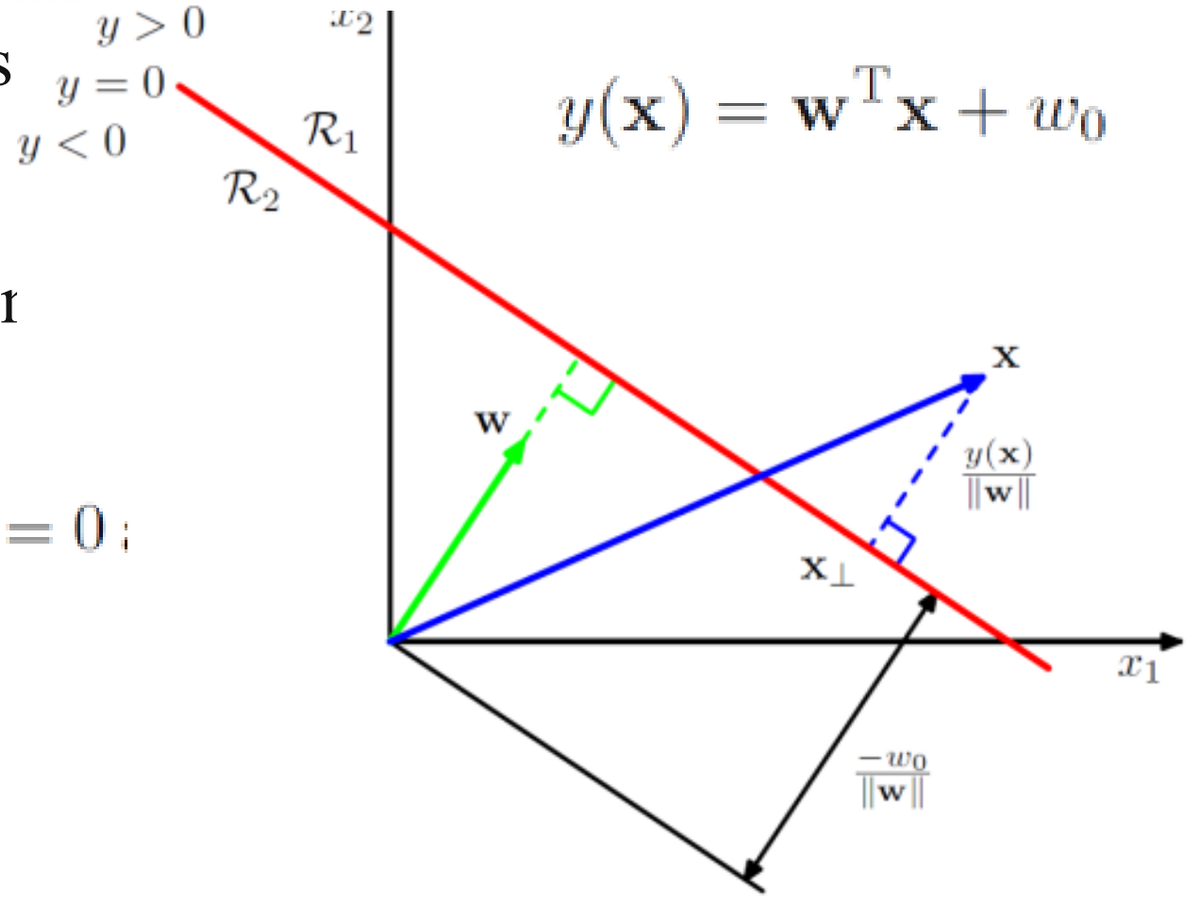
two points **x**A and **x**B both of which lie or decision surface.

$y(\mathbf{x}_{\mathrm{A}}) = y(\mathbf{x}_{\mathrm{B}}) = 0$, we have $\mathbf{w}^{\mathrm{T}}(\mathbf{x}_{\mathrm{A}} - \mathbf{x}_{\mathrm{B}}) = 0$;

$$\mathbf{x} = \mathbf{x}_\perp + r\frac{\mathbf{w}}{\|\mathbf{w}\|}.$$

$$r = \frac{y(\mathbf{x})}{\|\mathbf{w}\|}.$$

$$y(\mathbf{x}_\perp) = \mathbf{w}^{\mathrm{T}}\mathbf{x}_\perp + w_0 = 0,$$



Least squares classification

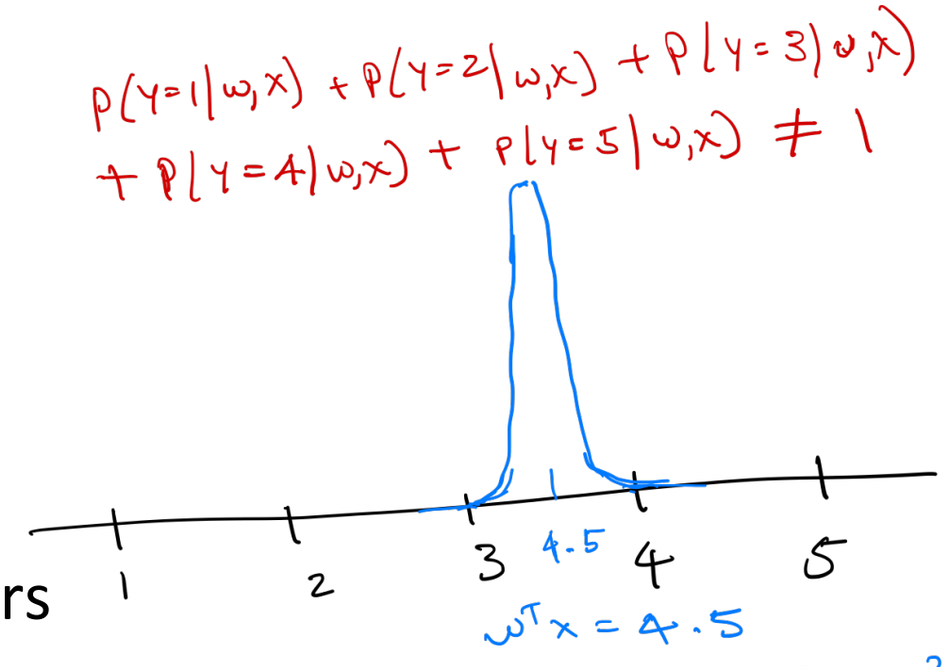
- Loss function

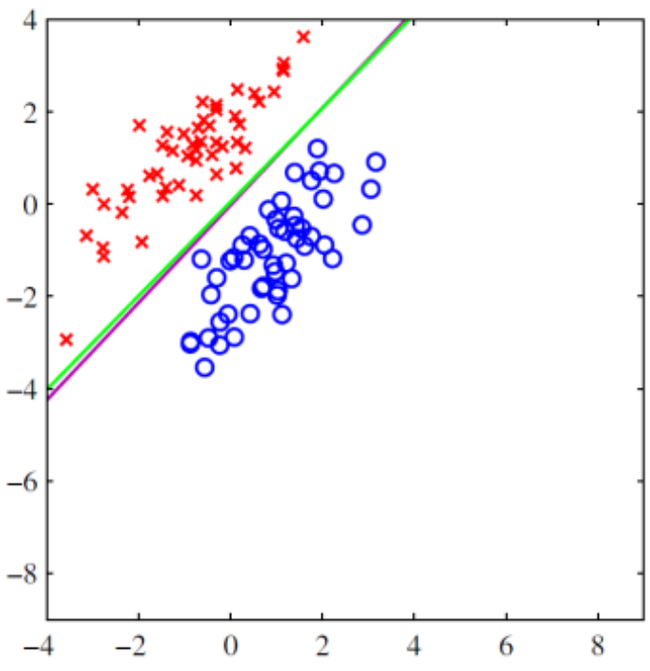
$$E_D(\widetilde{\mathbf{W}}) = \frac{1}{2}\mathrm{Tr}\left\{(\widetilde{\mathbf{X}}\widetilde{\mathbf{W}} - \mathbf{T})^{\mathrm{T}}(\widetilde{\mathbf{X}}\widetilde{\mathbf{W}} - \mathbf{T})\right\}.$$

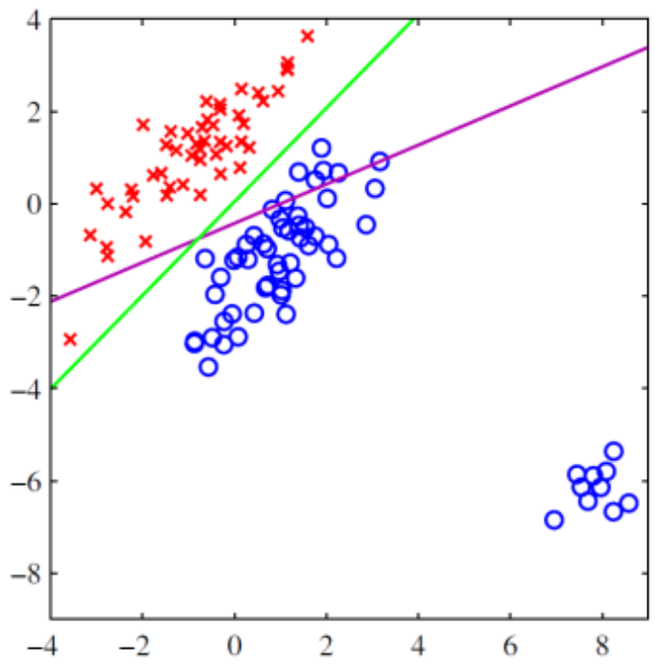
- Solution

$$\widetilde{\mathbf{W}} = (\widetilde{\mathbf{X}}^{\mathrm{T}}\widetilde{\mathbf{X}})^{-1}\widetilde{\mathbf{X}}^{\mathrm{T}}\mathbf{T} = \widetilde{\mathbf{X}}^{\dagger}\mathbf{T}$$

- least-squares solutions lack robustness to outliers







Least squares corresponds to maximum likelihood under the assumption of a **Gaussian conditional** distribution, whereas binary target vectors clearly have a distribution that is far from Gaussian.

Classification : Probabilistic vs Geometric views

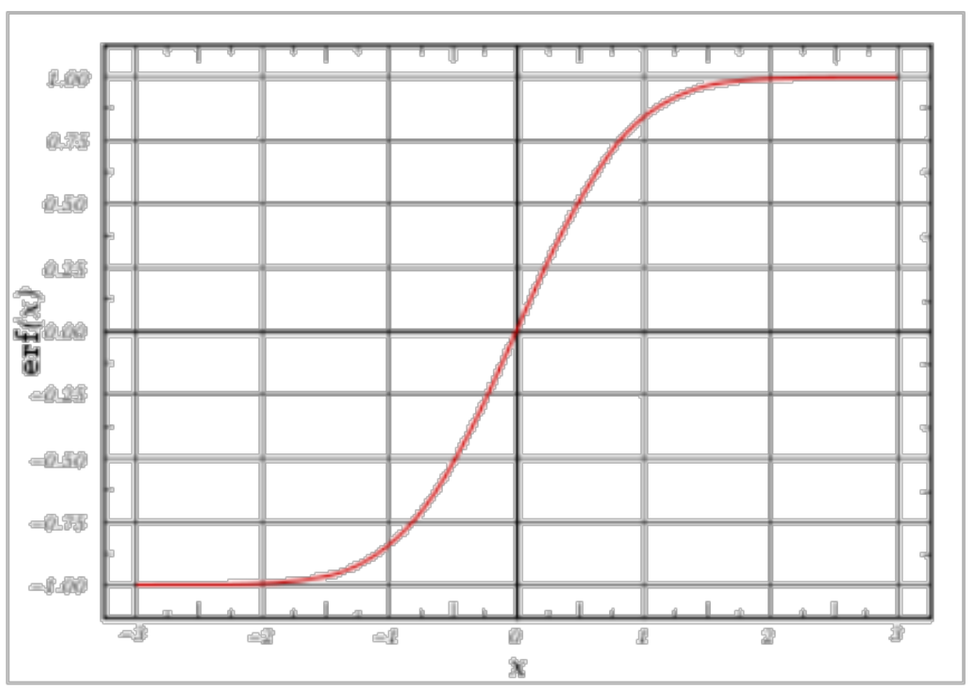
- Logistic Regression
- Model probability predicting y given x and w

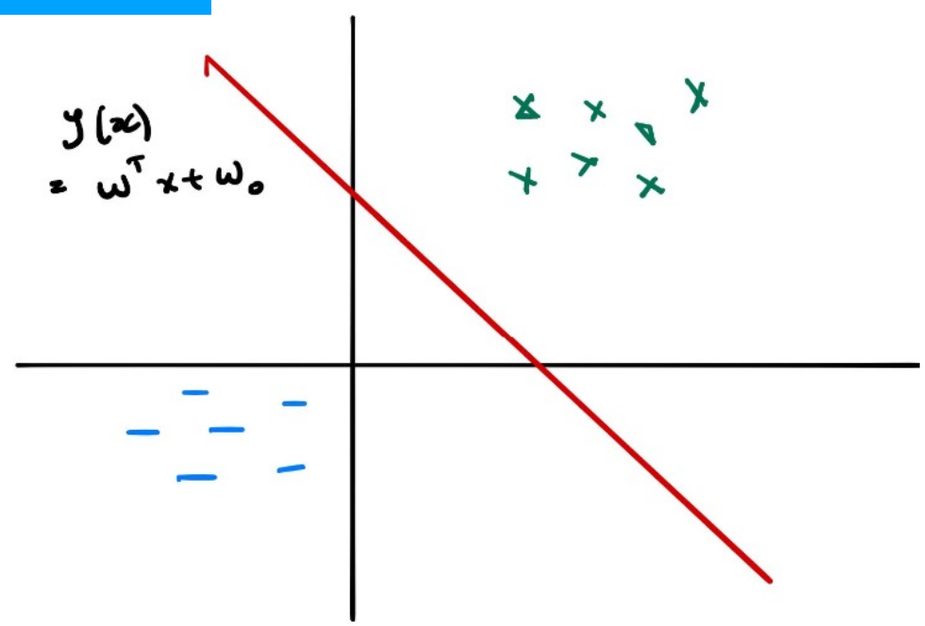
$$P(Y=1|\mathbf{X}) = \frac{1}{1+e^{-\mathbf{wx}}}$$

- Discriminant Analysis
- Models a discriminant function separating classes

$$y(\mathbf{x}) = \mathbf{w}^{\mathrm{T}}\mathbf{x} + w_0$$

How to learn the parameters w ?





Logistic Regression

- In logistic regression, we learn the conditional distribution P(y|x)
- Let $p_y(x;w)$ be our estimate of P(y|x), where w is a vector of adjustable parameters.
- Assume there are two classes, y = 0 and y = 1 and

$$p_1(\mathbf{x};\mathbf{w}) = \frac{1}{1+e^{-\mathbf{wx}}} \qquad p_0(\mathbf{x};\mathbf{w}) = 1 - \frac{1}{1+e^{-\mathbf{wx}}} = \frac{\mathbf{1}}{\mathbf{1+e^{wx}}}$$

- This is equivalent to

$$\log \frac{p_1(\mathbf{x};\mathbf{w})}{p_0(\mathbf{x};\mathbf{w})} = \mathbf{wx}$$

- That is, the log odds of class 1 is a linear function of x
- Q: How to find **W**?

- Alternate representation of p(y|x) : $\mathbf{p_y(x;w) = \frac{1}{1+e^{-ywx}}; y = \{-1,1\}}$

Logistic Regression

- Conditional data likelihood - Probability of observed Y values in the training data, conditioned on corresponding X values.
- We choose parameters w that satisfy

$$\mathbf{w} = \arg\max_{\mathbf{w}} \prod_l P(y^l \mid \mathbf{x}^l, \mathbf{w})$$

- where
  - $\mathbf{w} = \langle w_0, w_1, \ldots, w_n \rangle$ is the vector of parameters to be estimated,
  - y^l denotes the observed value of Y in the *l* th training example, and
  - $\mathbf{x}^l$ denotes the observed value of **X** in the *l* th training example

Logistic Regression

- Equivalently, we can work with log of conditional likelihood:

$$\mathbf{w} = \arg\max_{\mathbf{w}} \sum_l \ln P(y^l \mid \mathbf{x}^l, \mathbf{w})$$

- Conditional data log likelihood, l(W), can be written as

$$l(\mathbf{w}) = \sum_l y^l \ln P(y^l = 1 \mid \mathbf{x}^l, \mathbf{w}) + (1 - y^l) \ln P(y^l = 0 \mid \mathbf{x}^l, \mathbf{w})$$

- Note here that Y can take only values 0 or 1, so only one of the two terms in the expression will be non-zero for any given y^l

Logistic Regression

- We need to estimate:

$$\mathbf{w} = \arg\max_{\mathbf{w}} \sum_l \ln P(y^l \mid \mathbf{x}^l, \mathbf{w})$$

$$l(\mathbf{w}) = \sum_l y^l \ln P(y^l = 1 \mid \mathbf{x}^l, \mathbf{w}) + (1 - y^l) \ln P(y^l = 0 \mid \mathbf{x}^l, \mathbf{w})$$

- Equivalently, we can minimize negative log likelihood using gradient descent technique

- No closed-form solution though. Iterative method required.

- [HW] Find the derivative of l(w) !

Logistic Regression

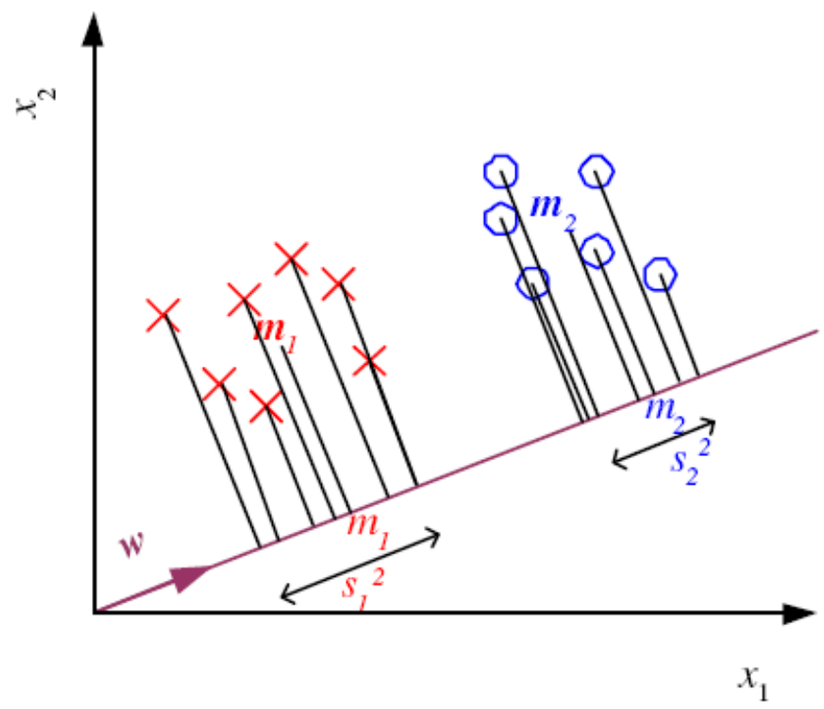
- Overfitting can arise especially when data has very high dimensions and is sparse.
- One approach -> modified "penalized log likelihood function," which penalizes large values of **w**, as before.

$$\mathbf{w} = \arg\max_{\mathbf{w}} \sum_l \ln P(y^l \mid \mathbf{x}^l, \mathbf{w}) - \frac{\lambda}{2} \| \mathbf{w} \|^2$$

- [HW] Find the Derivative !

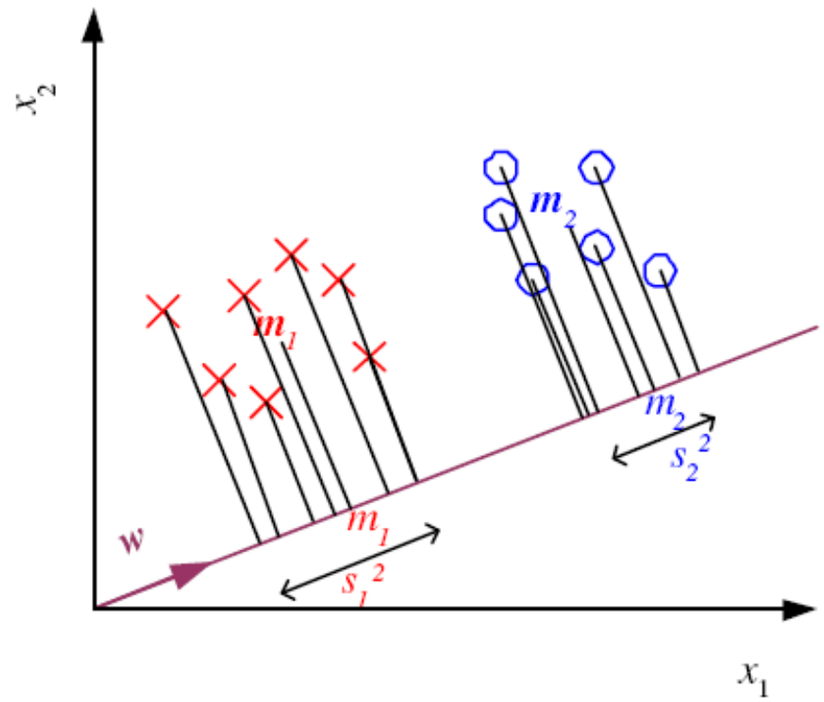
Discriminant Analysis

- Supervised linear discriminant analysis (LDA)
- w as the direction to project x
- Find w such that when ***x*** is projected, classes are well-separated.



Linear Discriminant Analysis

- Supervised linear discriminant analysis (LDA)
- w as the direction to project x
- Find w such that when ***x*** is projected, classes are well-separated.
- Simplest measure of the separation of the classes, when projected onto w, is the separation of the projected class means.



$$\mathbf{m}_1 = \frac{1}{N_1} \sum_{n \in \mathcal{C}_1} \mathbf{x}_n, \qquad \mathbf{m}_2 = \frac{1}{N_2} \sum_{n \in \mathcal{C}_2} \mathbf{x}_n.$$ Maximize $$m_2 - m_1 = \mathbf{w}^{\mathrm{T}}(\mathbf{m}_2 - \mathbf{m}_1)$$

Linear Discriminant Analysis

$$m_2 - m_1 = \mathbf{w}^T(\mathbf{m}_2 - \mathbf{m}_1)$$

Pseudocode

This expression can be made arbitrarily large by increasing the magnitude of $\mathbf{w}$

1. Constrain $\mathbf{w}$ to unit-length, $\sum_i w_i^2 = 1$
2. Use Lagrange multipliers for the constrained maximisation
3. Find the solution, $\mathbf{w} \propto (\mathbf{m}_2 - \mathbf{m}_1)$ $(\star^1)$

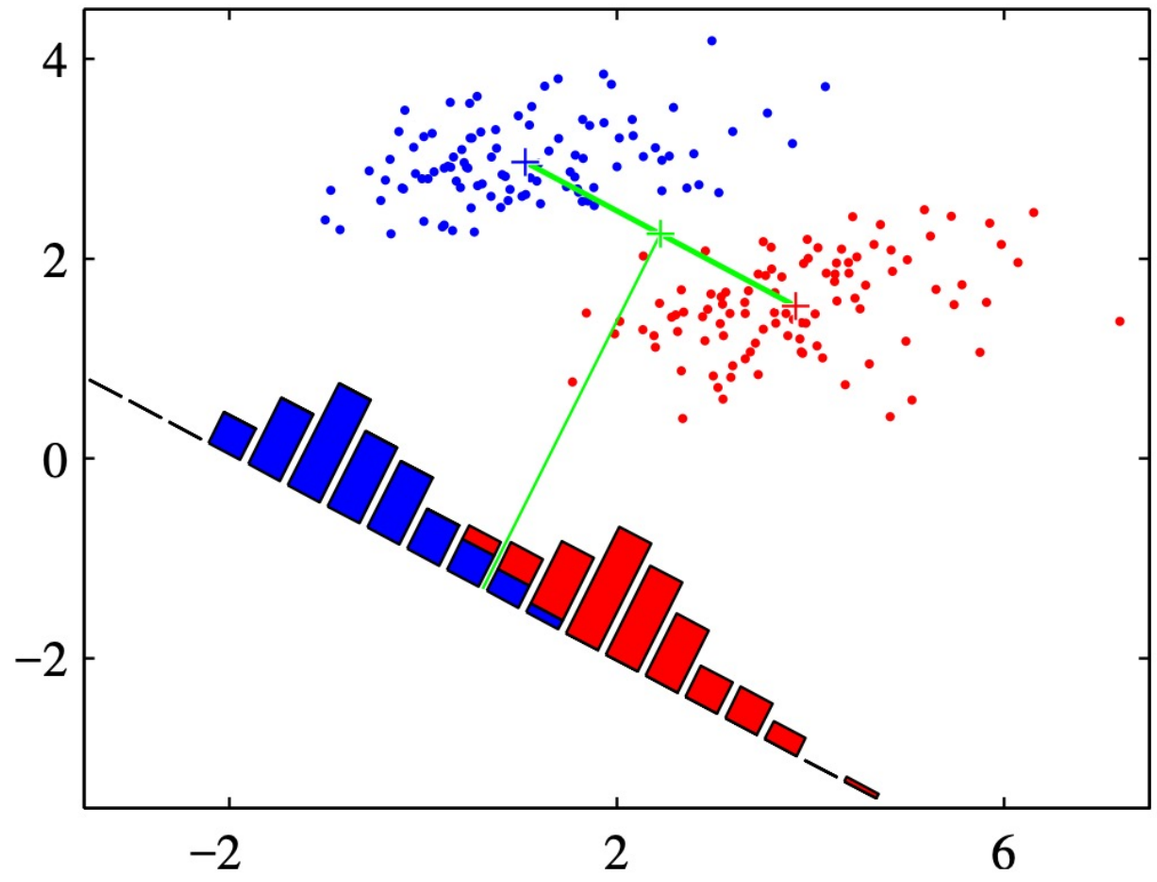
The optimal projection is along the line joining the original class means

$^1 L = \mathbf{w}^T(\mathbf{m}_2 - \mathbf{m}_1) + \lambda(\mathbf{w}^T\mathbf{w} - 1)$, then $\nabla L = \mathbf{m}_2 - \mathbf{m}_1 + 2\lambda\mathbf{w} = 0$ to get $\mathbf{w} = 1/(2\lambda)(\mathbf{m}_2 - \mathbf{m}_1)$

Linear Discriminant Analysis

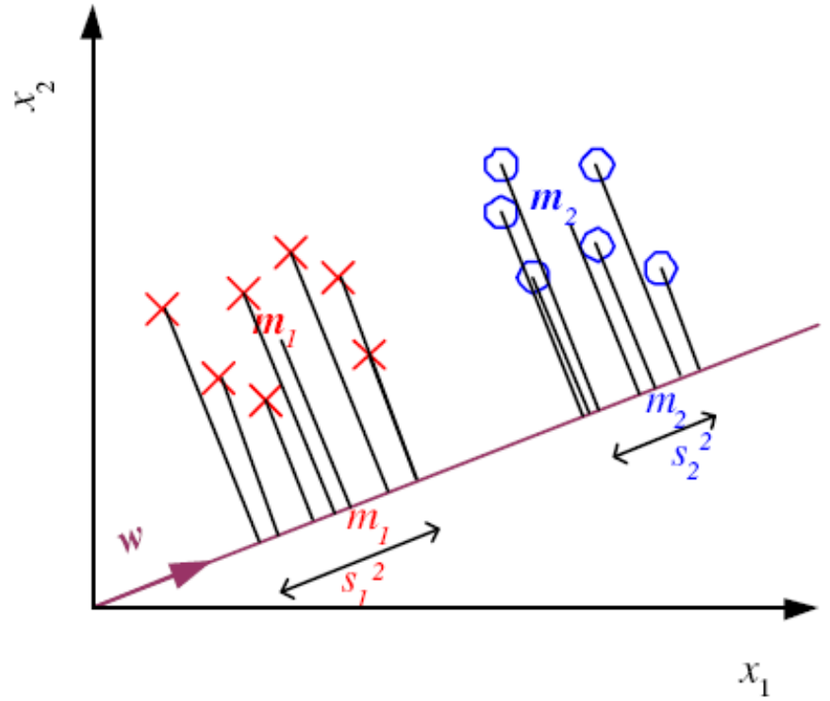
Projection onto the line joining the class means

- Good separation in the original $2D$ space
- Considerable class overlap in the projection $1D$ space



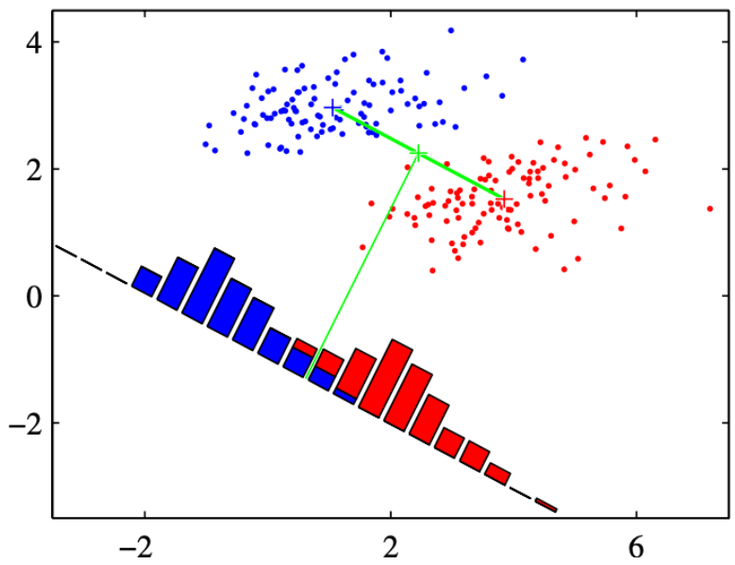
Fishers Linear Discriminant

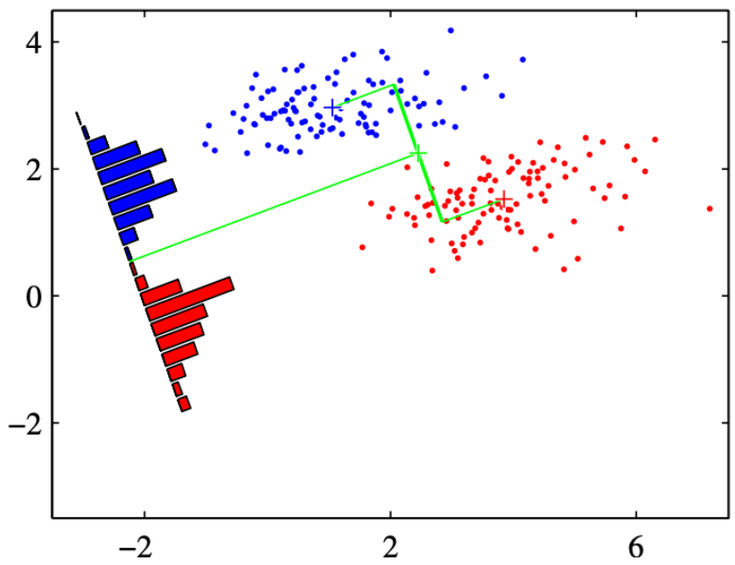
- Idea proposed by Fisher is to maximize a function that will give a large separation between the projected class means while giving a small variance within each class, thereby minimizing the class overlap.
- Find **w** that maximizes



$$J(\mathbf{w}) = \frac{(m_1 - m_2)^2}{s_1^2 + s_2^2}$$

$$m_1 = \frac{\sum_t \mathbf{w}^T \mathbf{x}^t r^t}{\sum_t r^t} \qquad s_1^2 = \sum_t \left(\mathbf{w}^T \mathbf{x}^t - m_1\right)^2 r^t$$





Fishers Linear Discriminant

- Between-class scatter:

$$
\begin{aligned}
(m_1 - m_2)^2 &= \left(\mathbf{w}^T\mathbf{m}_1 - \mathbf{w}^T\mathbf{m}_2\right)^2 \\
&= \mathbf{w}^T(\mathbf{m}_1 - \mathbf{m}_2)(\mathbf{m}_1 - \mathbf{m}_2)^T\mathbf{w} \\
&= \mathbf{w}^T\mathbf{S}_B\mathbf{w} \text{ where } \mathbf{S}_B = (\mathbf{m}_1 - \mathbf{m}_2)(\mathbf{m}_1 - \mathbf{m}_2)^T
\end{aligned}
$$

- Within-class scatter:

$$
\begin{aligned}
s_1^2 &= \sum_t \left(\mathbf{w}^T\mathbf{x}^t - m_1\right)^2 r^t \\
&= \sum_t \mathbf{w}^T\left(\mathbf{x}^t - \mathbf{m}_1\right)\left(\mathbf{x}^t - \mathbf{m}_1\right)^T\mathbf{w}r^t = \mathbf{w}^T\mathbf{S}_1\mathbf{w} \\
\text{where } \mathbf{S}_1 &= \sum_t \left(\mathbf{x}^t - \mathbf{m}_1\right)\left(\mathbf{x}^t - \mathbf{m}_1\right)^T r^t \\
s_1^2 + s_2^2 &= \mathbf{w}^T\mathbf{S}_W\mathbf{w} \text{ where } \mathbf{S}_W = \mathbf{S}_1 + \mathbf{S}_2
\end{aligned}
$$

Fisher's Linear Discriminant

- Find ***w*** that max

$$J(\mathbf{w}) = \frac{\mathbf{w}^T \mathbf{S}_B \mathbf{w}}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}} = \frac{\left|\mathbf{w}^T (\mathbf{m}_1 - \mathbf{m}_2)(\mathbf{m}_1 - \mathbf{m}_2)^T \mathbf{w}\right|}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}}$$

- FLD soln:

$$\mathbf{w} = c \cdot \mathbf{S}_W^{-1}(\mathbf{m}_1 - \mathbf{m}_2)$$

Fisher's Linear Discriminant

- Find ***w*** that max $$J(\mathbf{w}) = \frac{\mathbf{w}^T \mathbf{S}_B \mathbf{w}}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}} = \frac{\left|\mathbf{w}^T (\mathbf{m}_1 - \mathbf{m}_2)(\mathbf{m}_1 - \mathbf{m}_2)^T \mathbf{w}\right|}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}}$$

- FLD soln: $$\mathbf{w} = c \cdot \mathbf{S}_W^{-1}(\mathbf{m}_1 - \mathbf{m}_2)$$

After differentiating with respect to $\mathbf{w}^3$, we get that $J(\mathbf{w})$ is maximised

$$(\mathbf{w}^T \mathbf{S}_B \mathbf{w})\mathbf{S}_W \mathbf{w} = (\mathbf{w}^T \mathbf{S}_W \mathbf{w})\mathbf{S}_B \mathbf{w}$$

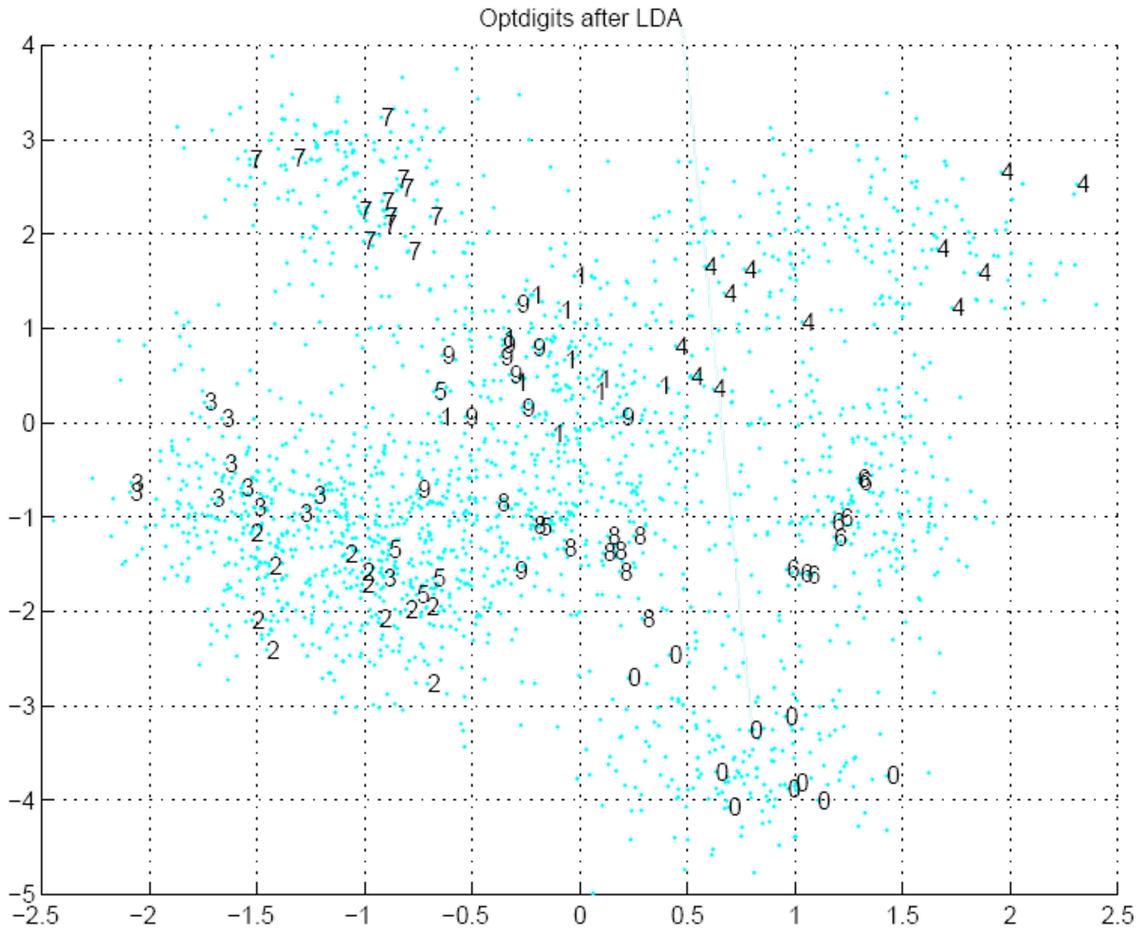
Multiplying both sides of $(\mathbf{w}^T \mathbf{S}_B \mathbf{w})\mathbf{S}_W \mathbf{w} = (\mathbf{w}^T \mathbf{S}_W \mathbf{w})\mathbf{S}_B \mathbf{w}$ by $\mathbf{S}_W^{-1}$

$$\mathbf{w} \propto \mathbf{S}_W^{-1}(\mathbf{m}_2 - \mathbf{m}_1)$$

$$\frac{\partial}{\partial \mathbf{w}}\left(\frac{\mathbf{w}^T \mathbf{S}_B \mathbf{w}}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}}\right) = \frac{2}{(\mathbf{w}^T \mathbf{S}_W \mathbf{w})^2}\left[(\mathbf{w}^T \mathbf{S}_W \mathbf{w})\mathbf{S}_B \mathbf{w} - (\mathbf{w}^T \mathbf{S}_B \mathbf{w})\mathbf{S}_W \mathbf{w}\right]$$

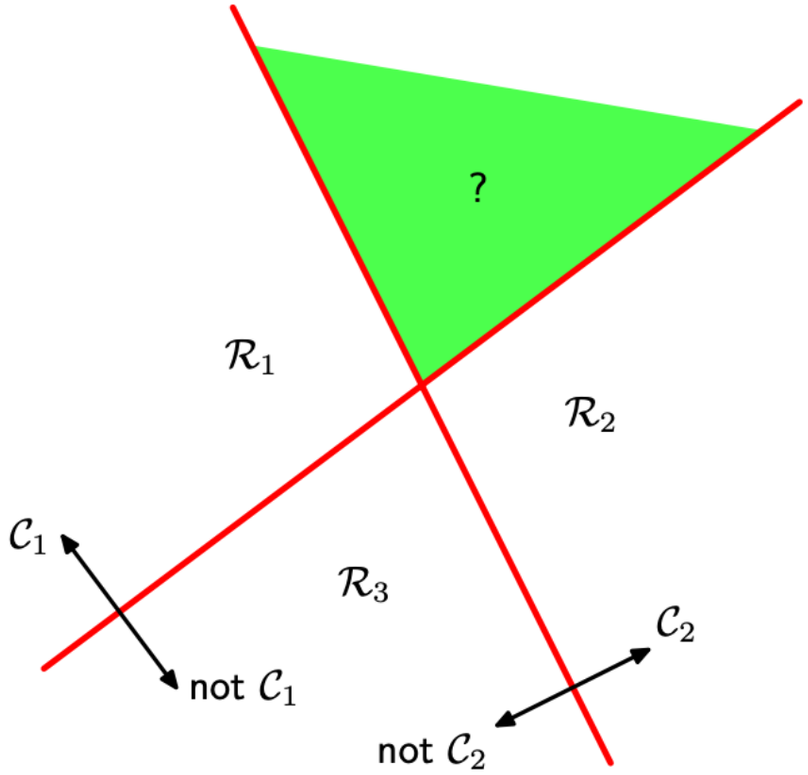
$(\mathbf{m}_1 - \mathbf{m}_2)\mathbf{w}$ is a scalar.

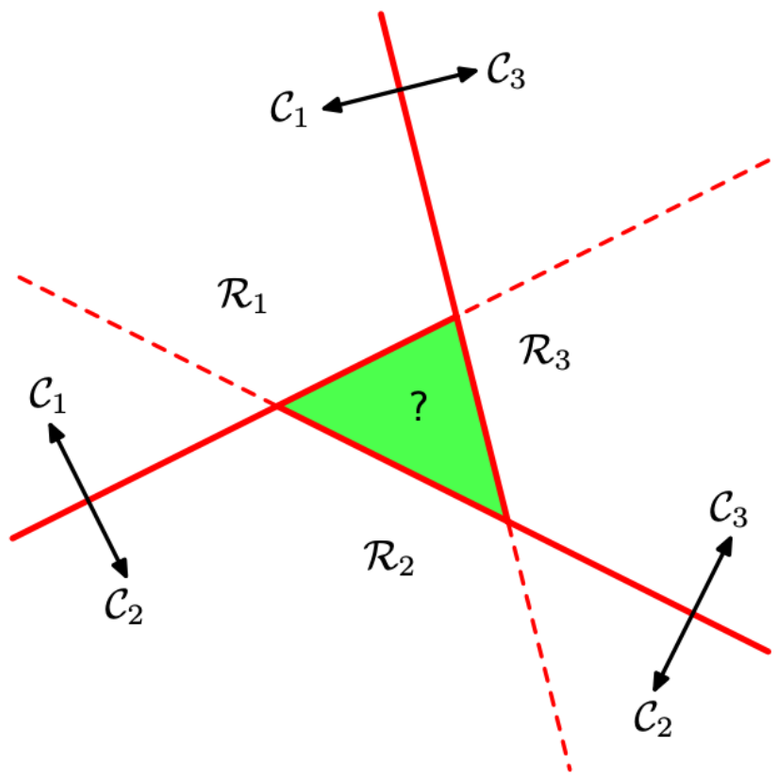
FLD: Illustration



Multi Class Classification

- One vs Rest





- One vs One

- Discriminant function

$$y_k(\mathbf{x}) = \mathbf{w}_k^{\mathrm{T}}\mathbf{x} + w_{k0}$$

$\mathbf{x}$ to class $\mathcal{C}_k$ if $y_k(\mathbf{x}) > y_j(\mathbf{x})$ for all $j \neq k$.

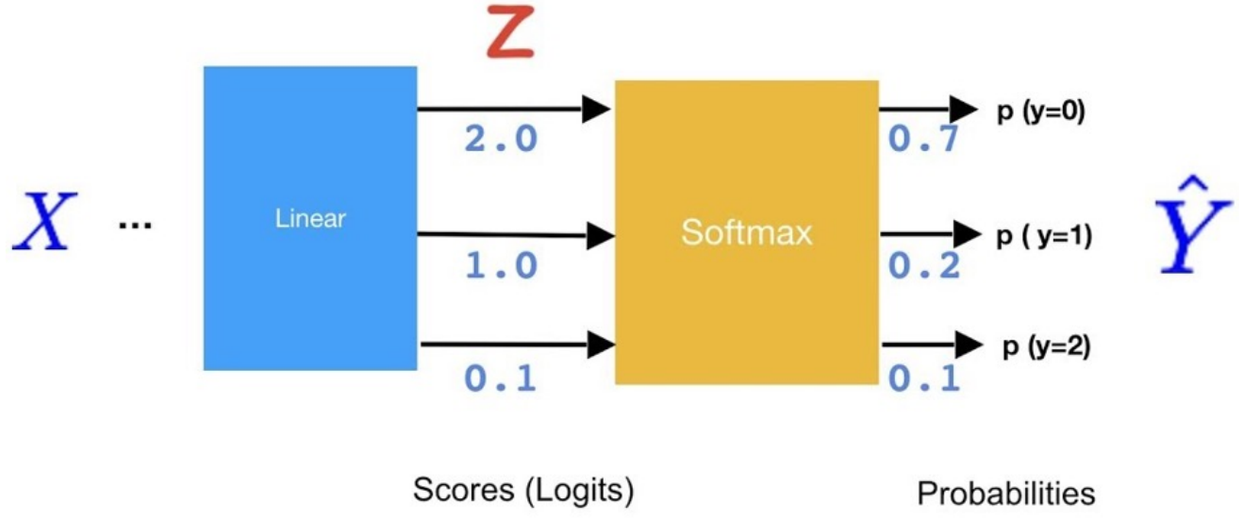
$$(\mathbf{w}_k - \mathbf{w}_j)^{\mathrm{T}}\mathbf{x} + (w_{k0} - w_{j0}) = 0.$$

Multi class classification

- LR: Functional form of P(Y|X), no assumption on P(X|Y)
- LR is a linear classifier
- LR optimized by conditional likelihood
- Extending logistic regression to multiple classes
  - Use softmax for each class k!

$$p(y = k|x) = \frac{\exp(w_k^\top x)}{\sum_{i=1}^{K} \exp(w_i^\top x)}$$

Meet Softmax $\quad \sigma(\mathbf{z})_j = \frac{e^{z_j}}{\sum_{k=1}^{K} e^{z_k}}$ for $j = 1, \ldots, K$.



Thank you !

Reference

[1] Christopher Bishop, Pattern Recognition and Machine Learning
[2] Kevin Murphy, Machine Learning : A Probabilistic Perspective