Introduction to Machine Learning - CS725
Instructor: Prof. Ganesh Ramakrishnan
Lecture 4 - Linear Regression - Probabilistic
Interpretation and Regularization

Recap: Linear Regression is **not Naively Linear**

- Need to determine **w** for the linear function
  $f(\mathbf{x}, \mathbf{w}) = \sum_{i=1}^{n} w_i \phi_i(\mathbf{x_j}) = \phi \mathbf{w}$ which minimizes our error
  function $E(f(\mathbf{x}, \mathbf{w}), \mathcal{D})$
- Owing to basis function ϕ, "Linear Regression" is *linear* in **w**
  but NOT in **x** (which could be arbitrarily non-linear)!

$$
\phi = \left[\begin{array}{cccc} \phi_1(\mathbf{x_1}) & \phi_2(\mathbf{x_1}) & ...... & \phi_p(\mathbf{x_1}) \\ . & & & \\ . & & & \\ \phi_1(\mathbf{x_m}) & \phi_2(\mathbf{x_m}) & ...... & \phi_n(\mathbf{x_m}) \end{array} \right] \tag{1}
$$

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$$

- Least Squares error and corresponding estimates:

$$
E^* = \min_{\mathbf{w}} E(\mathbf{w}, \mathcal{D}) = \min_{\mathbf{w}} \left(\mathbf{w^T} \phi^\mathbf{T} \phi \mathbf{w} - \mathbf{2y^T} \phi \mathbf{w} + \mathbf{y^T y} \right) \quad (2)
$$

$$
\mathbf{w}^* = \arg\min_{\mathbf{w}} \mathbf{E(\mathbf{w}, \mathcal{D})} = \arg\min_{\mathbf{w}} \left\{ \sum_{j=1}^{m} \left(\sum_{i=1}^{n} \mathbf{w_i} \phi_i(\mathbf{x_j}) - \mathbf{y_j} \right)^2 \right\}
$$

- Let $\mathbf{y}^*$ be a solution in the column space of ϕ
- The least squares solution is such that the distance between $\mathbf{y}^*$ and $\mathbf{y}$ is minimized
- Therefore, the line joining $\mathbf{y}^*$ to $\mathbf{y}$ should be orthogonal to the column space of $\phi \Rightarrow$

$$\mathbf{w} = (\phi^{\mathbf{T}}\phi)^{-\mathbf{1}}\phi\mathbf{y} \qquad (4)$$

- Here $\phi^T\phi$ is invertible only if ϕ has full column rank

1. Is there a probabilistic interpretation?
   - Gaussian Error, Maximum Likelihood Estimate
2. Addressing overfitting
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Probabilistic Modeling of Linear Regression

- Linear Model: Y is a linear function of $\phi(x)$, subject to a random noise variable ε which we believe is 'mostly' bounded by some threshold σ:

$$Y = w^T \phi(x) + \varepsilon$$
$$\varepsilon \sim \mathcal{N}(0, \sigma^2)$$

- Motivation: $\mathcal{N}(\mu, \sigma^2)$, has maximum entropy among all real-valued distributions with a specified variance σ^2
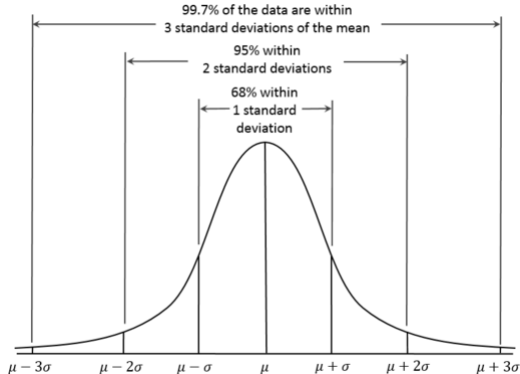
- $3 - \sigma$ rule: About 68% of values drawn from $\mathcal{N}(\mu, \sigma^2)$ are within one standard deviation σ away from the mean μ; about 95% of the values lie within 2σ; and about 99.7% are within 3σ.

Figure 1: $3 - \sigma$ rule: About 68% of values drawn from $\mathcal{N}(\mu, \sigma^2)$ are within one standard deviation σ away from the mean μ; about 95% of the values lie within 2σ; and about 99.7% are within 3σ. Source: https://en.wikipedia.org/wiki/Normal_distribution

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- This allows for the Probabilistic model

$$P(y_j | \mathbf{w}, \mathbf{x}_j, \sigma^2) = \mathcal{N}(\mathbf{w}^T \phi(\mathbf{x}_j), \sigma^2)$$
$$P(y | \mathbf{w}, \mathbf{x}_j, \sigma^2) = \prod_{j=1}^{m} P(y_j | \mathbf{w}, \mathbf{x}_j, \sigma^2)$$

- Another motivation: $E[Y(\mathbf{w}, \mathbf{x}_j)] =$

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- Another motivation: $E[Y(\mathbf{w}, \mathbf{x}_j)] = \mathbf{w}^T \phi(\mathbf{x}_j)$
  $= \mathbf{w}_0^T + \mathbf{w}_1^T \phi_1(\mathbf{x}_j) + ... + \mathbf{w}_n^T \phi_n(\mathbf{x}_j)$

- If $\epsilon \sim \mathcal{N}(0, \sigma^2)$ and $y = \mathbf{w}^\mathsf{T}\phi(\mathbf{x}) + \epsilon$ where $\mathbf{w}, \ \phi(\mathbf{x}) \in \mathbf{R^m}$ then, given dataset $\mathcal{D}$, find the most likely $\hat{\mathbf{w}}_{ML}$

- Recall: $\Pr(y_j|\mathbf{x}_j, \mathbf{w}) = \dfrac{1}{\sqrt{2\pi\sigma^2}} exp\left(\dfrac{(y_j - \mathbf{w}^\mathsf{T}\phi(\mathbf{x}_j))^2}{2\sigma^2}\right)$

- From *Probability of data* to *Likelihood of parameters*:
  $\Pr(\mathcal{D}|\mathbf{w}) = \Pr(\mathbf{y}|\mathbf{x}, \mathbf{w}) =$

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- Maximum Likelihood Estimate
  $\hat{\mathbf{w}}_{ML} = \underset{\mathbf{w}}{\operatorname{argmax}} \Pr(\mathcal{D}|\mathbf{w}) = \Pr(\mathbf{y}|\mathbf{x}, \mathbf{w}) = L(\mathbf{w}|\mathcal{D})$

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  $$-\frac{m}{2}ln(2\pi\sigma^2) - \frac{1}{2\sigma^2}\sum_{j=1}^{m}(\mathbf{w}^{\mathsf{T}}\phi(\mathbf{x_j}) - \mathbf{y_j})^2$$
  For a fixed σ^2
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  $\hat{\mathbf{w}_{ML}} = \text{argmax } LL(y_1...y_m|\mathbf{x}_1 \ldots \mathbf{x}_m, \mathbf{w}, \sigma^2)$

  $\qquad = \text{argmax } \sum_{j=1}^{m}(\mathbf{w}^T\phi(\mathbf{x}_j) - y_j)^2$

- Note that this is same as the Least square solution!!

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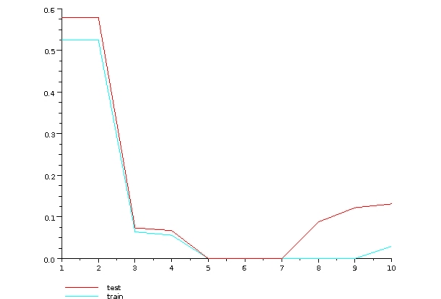
Redundant ϕ and Overfitting

Figure 2: Root Mean Squared (RMS) errors on sample train and test datasets as a function of the degree t of the polynomial being fit

- Too many bends (t=9 onwards) in curve $\equiv$ high values of some $w_i's$. Try plotting values of w_i's using applet at

  http://mste.illinois.edu/users/exner/java.f/leastsquares/#simulation

- Train and test errors differ significantly

- The Bayesian interpretation of probabilistic estimation is a logical extension that enables reasoning with uncertainty **but in the light of some background belief**
- **Bayesian linear regression**: A Bayesian alternative to **Maximum Likelihood** least squares regression
- Continue with Normally distributed errors
- Model the **w** using a prior distribution and use the posterior over **w** as the result
- Intuitive Prior:

Bayesian Linear Regression

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- Model the **w** using a prior distribution and use the posterior over **w** as the result
- Intuitive Prior: Components of **w** should not become too large!
- Next: Illustration of Bayesian Estimation on a simple Coin-tossing example