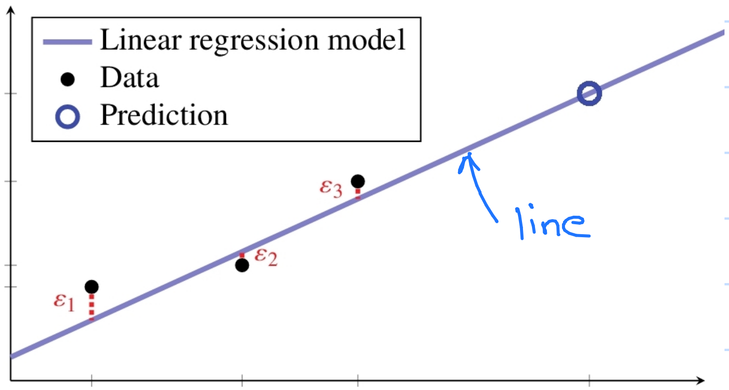
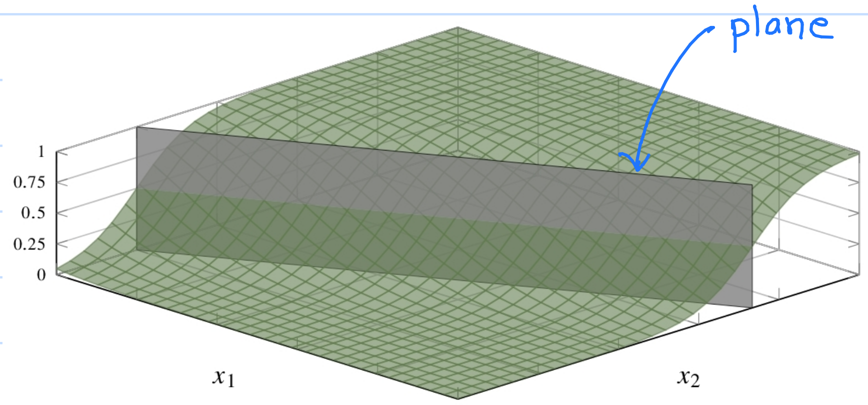
Lecture 7 – Polynomial Regression, Regularization, Generalized linear models

– We looked at two basic parametric models
→ Linear regression
→ Logistic regression (linear regression + logistic function)

– Compared to NON-PARAMETRIC models, linear regression and logistic regression appear to be rigid and not very flexible

- they fit straight lines (or hyperplanes)





– Make linear regression more flexible by increasing the input dimension p

- Question: How to increase input dimension?

- Common Approach: Add non-linear transformation of the input

- A simple nonlinear transformation of one-dimensional input x:

$$\underbrace{y = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \cdots + \theta_p x^p + \epsilon}_{\text{Polynomial regression}}$$

- Recall $y = \underline{x}^T \underline{\theta}$ where $\underline{x} = \begin{bmatrix} 1 \\ x_1 \\ x_2 \\ \vdots \\ x_p \end{bmatrix}$, $\underline{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \vdots \\ \theta_p \end{bmatrix}$

$$\underbrace{y = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \cdots + \theta_p x^p + \epsilon}_{\text{Polynomial regression}}$$

- If $x_1 = x$, $x_2 = x^2$, $x_3 = x^3$, ..., $x_p = x^p$ $\Rightarrow$ $y = \begin{bmatrix} 1 & x & x^2 & x^3 & \cdots & x^p \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \\ \vdots \\ \theta_p \end{bmatrix}$

$$= \underbrace{\underline{x}^T \underline{\theta}}$$

Still a linear model

however "lifted" the input from one-dimension $(p=1)$ to three-dimension $(p=3)$

- The same polynomial expansion can also be applied to logit z in logistic regression

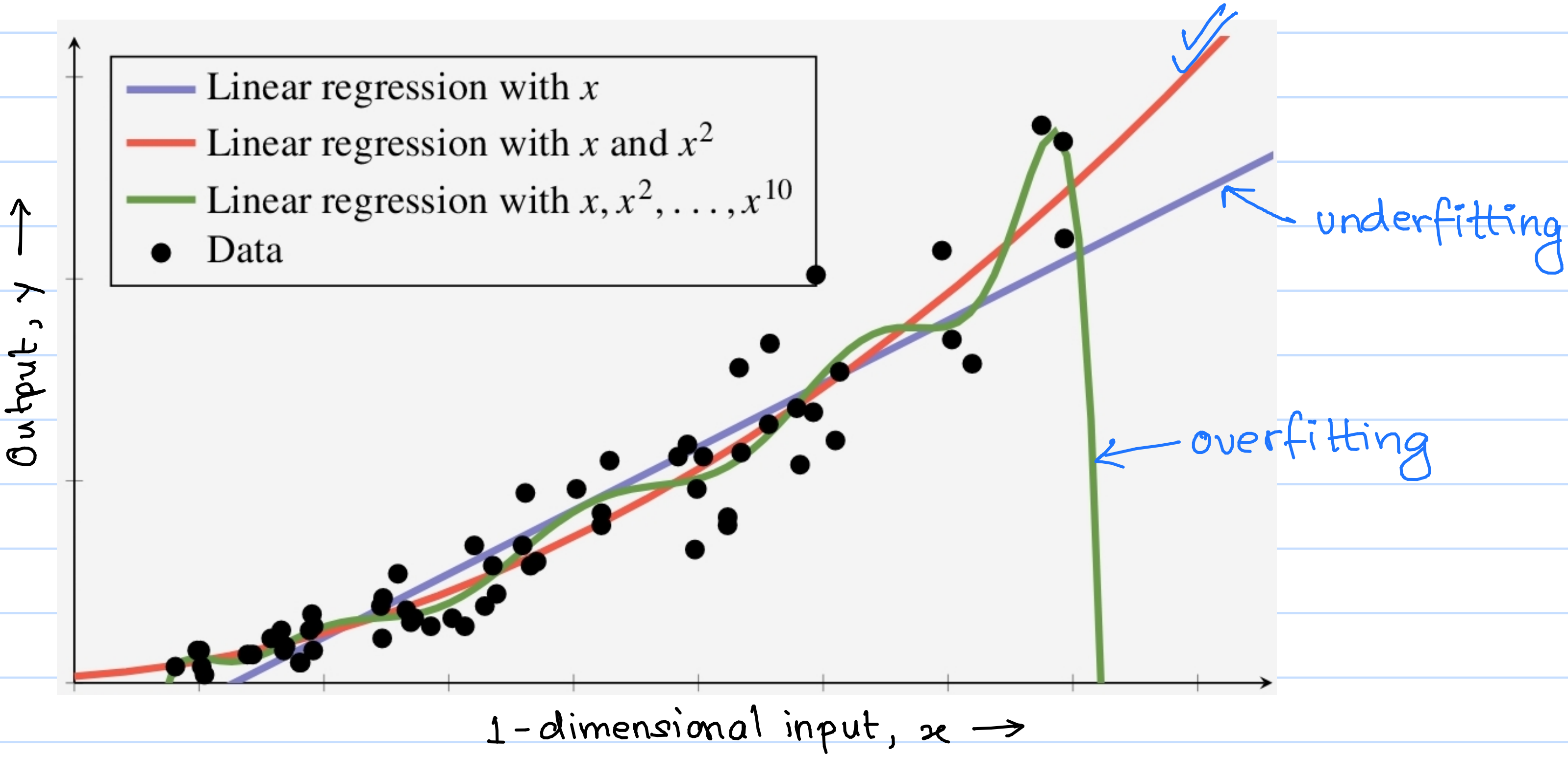
$$z = \begin{bmatrix} 1 & x & x^2 & \cdots & x^p \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \vdots \\ \theta_p \end{bmatrix} = \underline{x}^T \underline{\theta}$$

$y = h(z)$ logistic function

— Using nonlinear transformations are quite useful in practice

- effectively increases input dimension p

— Downside : Can lead to overfitting (the model may fit noise in the training data)



— Ways to avoid overfitting

- Carefully select which input transformations to include → add one inputs at a time; → removing inputs that are redundant
- Use regularization

REGULARIZATION

- Basic idea: Keep the parameters $\hat{\underline{\theta}}$ small unless really required!

- Meaning → if a model with small parameter values $\hat{\underline{\theta}}$ fits the data almost as well as a model with large parameter values, the model with smaller $\hat{\underline{\theta}}$ will be preferred

$$\hat{\underline{\theta}}^{(1)} = \begin{bmatrix} 0.2 \\ 1.5 \\ -0.01 \\ 0.005 \\ 0.01 \end{bmatrix}, \quad \hat{\underline{\theta}}^{(2)} = \begin{bmatrix} 2.3 \\ 10.6 \\ -1.2 \\ 0.1 \\ -1.3 \end{bmatrix}$$

both fit the data well

this set of parameters is more preferrable!

- Several ways to implement the idea of "small parameter values"
  - L_0 - regularization
  - L_1 - regularization

  maybe covered later
  - L_2 - regularization (will look into this here)

L_2 - REGULARIZATION

- Purpose is to prevent overfitting

- To keep $\hat{\underline{\theta}}$ small, an extra penalty term $\lambda \|\hat{\underline{\theta}}\|_2^2$ is added to the cost function

  regularization parameter
  (which is a hyper-parameter)
  chosen by user

- Regularization parameter, $\lambda \geq 0$, controls the strength of regularization effect
  - Larger the λ value, smaller will be the values of $\hat{\underline{\theta}}$
  - $\lambda = 0$ has no effect of regularization
  - $\lambda \to \infty$ will force all parameters $\hat{\underline{\theta}}$ to 0
  - Use cross-validation to select λ or use L-curve method

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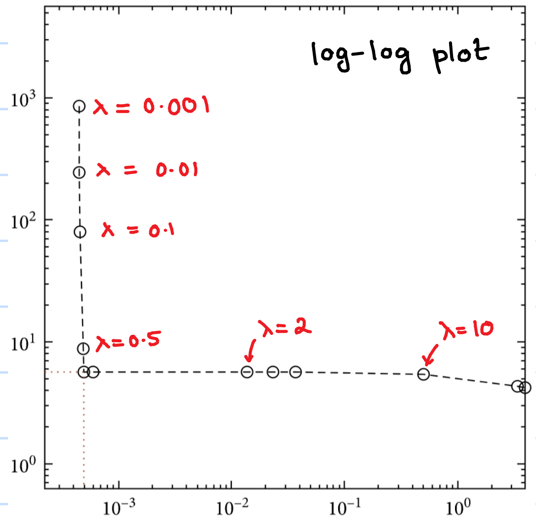
Cross-validation

$\boxed{\text{Training w/ } \lambda = 0.01} \rightarrow$ err = 5 ✗

$\boxed{\text{Training w/ } \lambda = 1} \rightarrow$ err = 1.3 ✓ $\rightarrow$ test err = 1.4

$\boxed{\text{Training w/ } \lambda = 3} \rightarrow$ err = 7 ✗

L-curve method



$\|\hat{\underline{\theta}}_\lambda\|_2$

$\|\underline{y} - \underline{\underline{X}}\,\hat{\underline{\theta}}_\lambda\|_2$

— Previously studied loss function for (non-regularized) linear regression:

$$\underline{\hat{\Theta}} = \underset{\underline{\Theta}}{\operatorname{argmin}} \frac{1}{N} \underbrace{\| \underline{y} - \underline{\underline{X}}\, \underline{\Theta} \|_2^2}_{\text{squared loss}} \longrightarrow (\underline{\underline{X}}^T \underline{\underline{X}})\, \underline{\hat{\Theta}} = \underline{\underline{X}}^T \underline{y}$$

— With L_2-regularization, add a penalty over $\underline{\Theta}$ to the loss

$$\underline{\hat{\Theta}} = \underset{\underline{\Theta}}{\operatorname{argmin}} \left(\underbrace{\frac{1}{N} \| \underline{y} - \underline{\underline{X}}\, \underline{\Theta} \|_2^2}_{\text{tries to fit the data}} + \underbrace{\lambda \| \underline{\Theta} \|_2^2}_{\text{tries to keep parameters small}} \right)$$

* Usually, the intercept parameter Θ_0 is kept out of regularization

— Just like the non-regularized linear regression, the regularized problem also has a closed-form solution

$$(\underline{\underline{X}}^T \underline{\underline{X}} + N \lambda \underline{\underline{I}})\, \underline{\hat{\Theta}} = \underline{\underline{X}}^T \underline{y}$$

$\underline{\underline{I}} \leftarrow$ identity matrix

— This particular application of L_2-regularization is called RIDGE REGRESSION

- L_2-regularization is not just restricted to linear regression
  - The $\|\hat{\underline{\theta}}\|_2^2$ penalty can be applied to any method that involves optimization

Example: Un-regularized logistic regression

$$\hat{\boldsymbol{\theta}} = \underset{\boldsymbol{\theta}}{\operatorname{argmin}}\, J(\boldsymbol{\theta}) = \underset{\boldsymbol{\theta}}{\operatorname{argmin}} \frac{1}{N}\sum_{i=1}^{N} \underbrace{\ln\left(1 + e^{-y^{(i)}(\mathbf{x}^{(i)})^T\boldsymbol{\theta}}\right)}_{\text{logistic loss}}$$

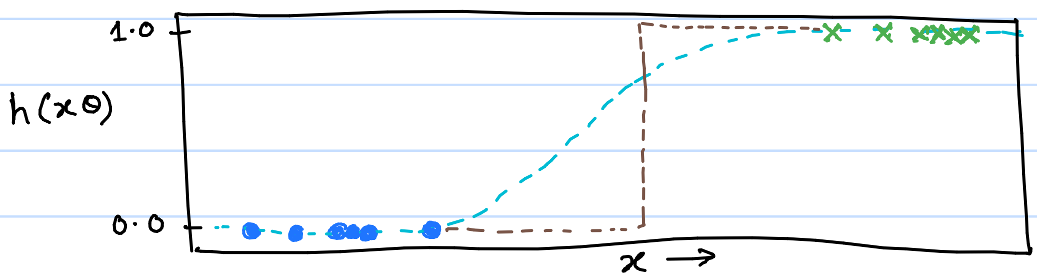
Logistic regression with L_2-regularization (very commonly used)

$$\hat{\underline{\theta}} = \underset{\underline{\theta}}{\operatorname{argmin}} \frac{1}{N}\sum_{i=1}^{N} \ln\left(1 + \exp\left(-y^{(i)}\, \underline{x}^{(i)T}\, \underline{\theta}\right)\right) + \lambda \|\underline{\theta}\|_2^2$$

- Reasons to use L_2-regularization in logistic regression

(a) to prevent overfitting

(b) to prevent unstable (or infinite) values of $\hat{\underline{\theta}}$



Linearly separable data causes a Heaviside step function

Generalized Linear Models

- We saw two basic parametric models:
  - linear regression (used for regression)
  - logistic regression (used for classification)

- In logistic regression, we adapted linear regression by passing the output through a nonlinear (in this case, a logistic) function
  - the output of the nonlinear logistic function was interpreted as class probability

- The same principle can be generalized to adapt linear regression model to different other properties of output as well. Such models are called Generalized linear models

- Different properties of output y
  - Output y corresponds to count of some quantity
    ex. number of cars crossing a bridge, number of earthquakes in a region
  - In such cases, y is a natural number taking values $0, 1, 2, \ldots$
  - Such count data, despite being numerical variables, cannot be well described by linear regression
    Reason: output from linear regression are not restricted to discrete or non-negative values

- To address this issue, we need to change the conditional probability model $p(y \mid \underline{x}; \underline{\theta})$

- First step: Choose a suitable form of $p(y \mid \underline{x}; \underline{\theta})$
  - This step is guided by properties of output data (such as natural numbers only)
  - Compute $z = \underline{x}^T \underline{\theta}$
  - Then let $p(y \mid \underline{x}; \underline{\theta})$ depend upon z in an appropriate way

    logistic function (in logistic regression)

Example: Poisson Regression

The Poisson distribution models natural numbers (including 0)

$$\text{Pois}(y; \mu) = \frac{\lambda e^{-\mu}}{y!} \qquad y = 0, 1, 2, \ldots$$

$\mu \leftarrow$ rate-parameter, $\mu \geq 0$

$\mu = \mathbb{E}[y]$

To use this Poisson distribution for generalized linear models:

- we can let $\mu = \exp(\underline{x}^T \underline{\theta})$ to ensure $\mu \geq 0$
- $p(y \mid \underline{x}; \underline{\theta}) = \text{Pois}\left(y; \exp(\underline{x}^T \underline{\theta})\right)$

- Poisson regression model
  - y has a conditional Poisson distribution $p(y|\underline{x};\underline{\theta})$
  - We can calculate the conditional mean, variance, etc.
    - Conditional mean of output y

$$\mu = \mathbb{E}[y|\underline{x};\underline{\theta}] = \phi^{-1}(z), \quad z = \underline{x}^T\underline{\theta}$$

$$\phi(\mu) \triangleq \log(\mu)$$

- An explicit link between the linear regression term $z = \underline{x}^T\underline{\theta}$ and the conditional mean of the output y in this way is the backbone of generalized linear models

- Generalized linear models consist of:

(a) A choice of output conditional distribution $p(y|\underline{x};\underline{\theta})$

[commonly from exponential family of distributions]

(b) A linear regression term $z = \underline{x}^T\underline{\theta}$

(c) A strictly increasing link function ϕ, s.t. $\mathbb{E}[y|\underline{x};\underline{\theta}] = \phi^{-1}(z)$

(If μ denotes the mean of $p(y|\underline{x};\underline{\theta})$, we can express $\phi(\mu) = \underline{x}^T\underline{\theta}$)