Linear Models: Regression

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$h_\theta = X\theta$

θ ① Normal Eqn

$\rightarrow Nu = k \cdot Pr^{\bar{a}} Re^{\bar{b}}$

$\theta_0 \quad \theta_1$

$\ln Nu = \ln k + a \ln Pr + b \ln Re$

θ_2

Feature x_1 x_2 y

x_1	x_2	y			
Pr	Re	Nu	$\ln Pr$	$\ln Re$	$\ln Nu$

$$Nu = e^{\theta_0} \cdot Pr^{\theta_1} \cdot Re^{\theta_2}$$

Feature Engineering

- The same ideas that we have discussed so far can be used even when the input-output relationship is nonlinear
- The key property of our Linear Model so far is that the loss function that is minimized (the obj. function) is linear in the parameter θ (the decision variable)
- So we can use a model such as

$$h(\boldsymbol{x};\theta) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1 x_2 + \theta_4 x_1^2 + \theta_5 x_2^2$$

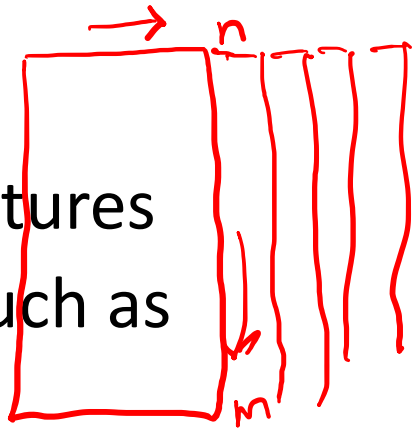
- Here the new polynomial features added are part of our feature engineering process
- It can be anything, really!

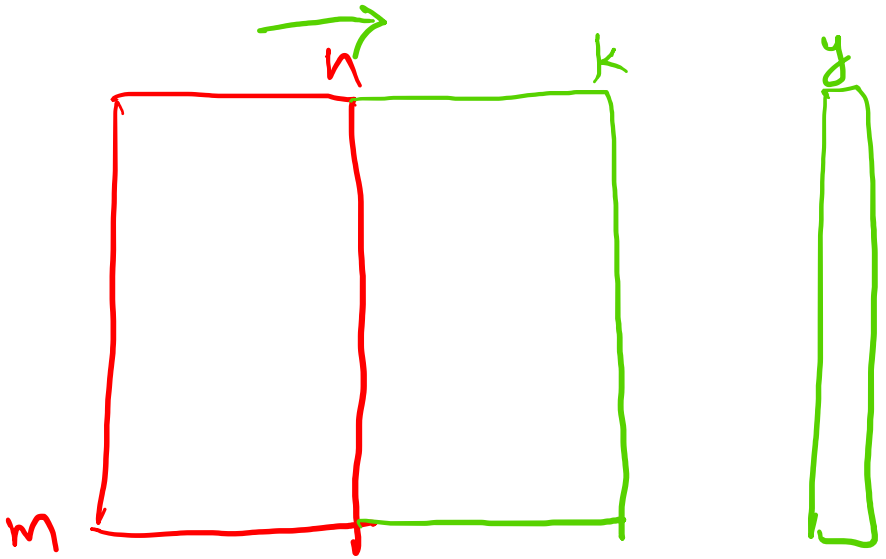
$$h(\boldsymbol{x};\theta) = \theta_0 + \theta_1 \frac{x_1}{x_2} + \theta_2 \frac{x_2 x_3}{x_1^2} + \theta_3 x_1 x_2$$

Polynomial Regression - sklearn

```
from sklearn.preprocessing import PolynomialFeatures
poly_features = PolynomialFeatures(degree=2, include_bias=False)
X_poly = poly_features.fit_transform(X)
```

- X_poly now contains the original features, its square and all pair-wise products as well.
  - Beware of the combinatorial explosion of features!
- Now we can do LinearRegression() with the engineered features
- You can transform data to any other engineered features such as trigonometry, logarithm, etc





$$\theta^* = (X^T X)^{-1} X^T y$$

$k = m$

$X_{m \times m}$

$$\theta^* = \underbrace{(X^T X)^{-1} X^T}_{\downarrow} y$$

$$\theta^* = X^{-1} y$$

$$(X^T X)^{-1} = X^{-1} \underbrace{(X^T)^{-1} X^T}_{} y$$

$$= X^{-1} y$$

$$\hat{y} = X\theta^*$$

$$= X X^{-1} y$$

$$= y$$

Training error = 0

[Complex Model
Large no: of parameters]

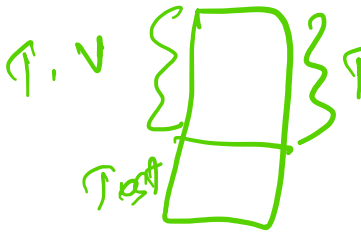
Goodness of Fit

- How do we know that the model that we have is good?
- For Linear Regression problems, traditionally a figure called "Coefficient of Determination" or R^2 is used.
- A linear model explains one variable (the output) in terms of other variables (features/regressors)
- R^2 measures how much explanatory power the linear model has compared to just the natural variability in the data
- $R^2 = 1 - \frac{\sum_j (y_j - \widehat{y_j})^2}{\sum_j (y_j - \bar{y})^2} = 1 - \frac{sum\ of\ squared\ error}{sum\ of\ squared\ deviations\ from\ mean}$
- When error=0, $R^2 = 1$, and when predictions are just the mean, $R^2 = 0$

Problems with R^2

- Can be used only with OLS regression
- High R^2 doesn't necessarily mean a good predictive model and low doesn't mean a bad predictive model
- Just increasing the regressors will increase R^2
- Heavy duty feature engineering, especially using high dimensional polynomials will lead to overfitting the training data and high R^2
- We must have better ways to estimate goodness when other loss functions are used and have a scheme of determining the performance of the data-driven model

Overfit or Underfit?

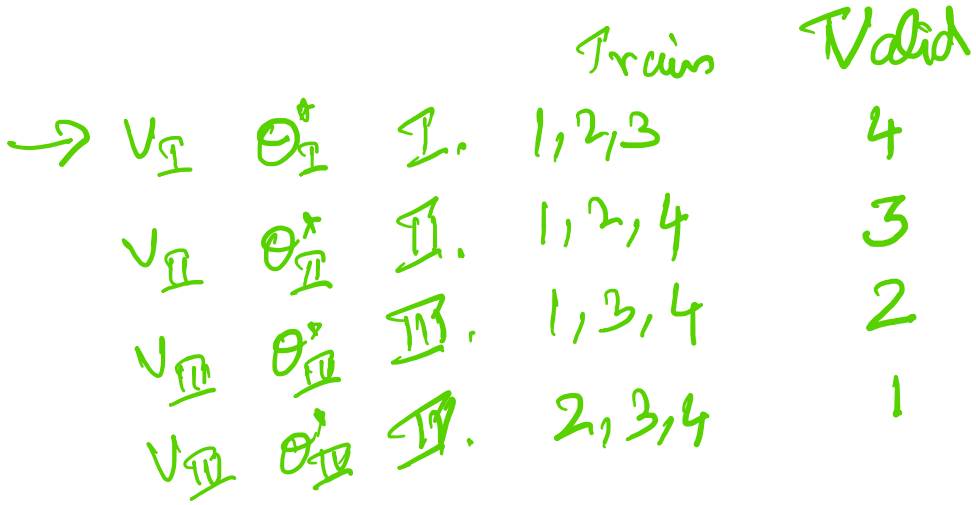


- Question: How to know if you are overfitting or underfitting?
- Answer 1: Cross-Validation
  - If a model performs well on the training data but generalizes poorly according to the cross-validation metrics, then your model is overfitting.
  - If it performs poorly on both, then it is underfitting.
- Answer 2: Learning Curves
  - Plots of the model's performance on the training set and the validation set as a function of the training set size (or the training iteration)
  - Train the model several times on different sized subsets of the training set

Cross-Validation

- Cross-Validation involves using the train set to construct multiple train-validate splits and perform the model building/training activity
- Test set should not be used for model building purpose

- K Fold Cross Validation
  - from sklearn.model_selection import cross_val_score
  - scores = cross_val_score(tree_reg, housing_prepared, housing_labels, scoring="neg_mean_squared_error", cv=10)
  - tree_rmse_scores = np.sqrt(-scores)



- GridSearchCV for Hyper Parameter Tuning

Bias/Variance Trade-off

- A model's generalization error can be expressed as the sum of three very different errors:
  - *Bias:* due to wrong assumptions, such as assuming that the data is linear when it is quadratic.
    - A high-bias model likely underfits the training data.
    - Note: This bias is not the bias-term/intercept.
  - *Variance*: excessive sensitivity to small variations in the training data.
    - A model with many degrees of freedom (such as a high-degree polynomial model) is likely to have high variance and thus overfit the training data.
  - *Irreducible Error*: Due to inherent noise in the data
- Bias-Variance tradeoff
  - Increasing a model's complexity will increase its variance and reduce its bias.
  - Reducing a model's complexity will reduce its variance and increase its bias

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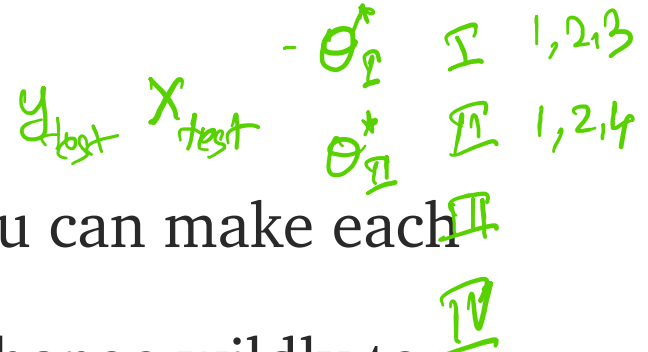
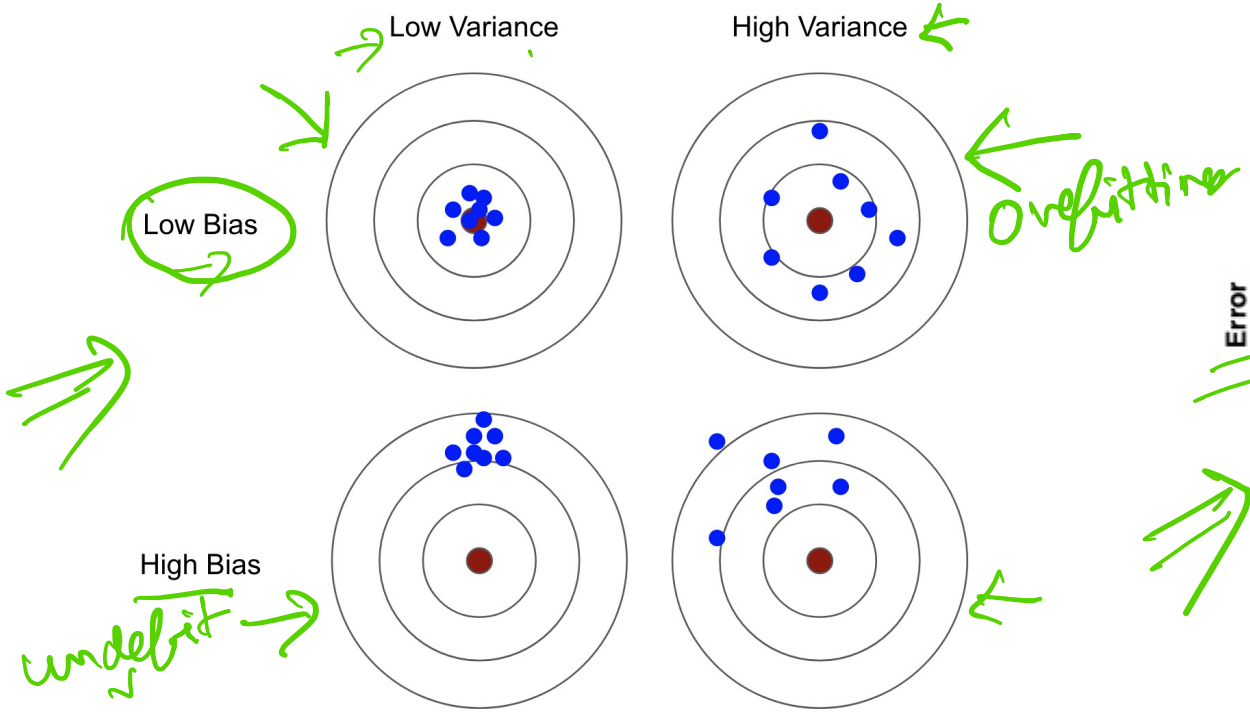
Bias-Variance: Revisit

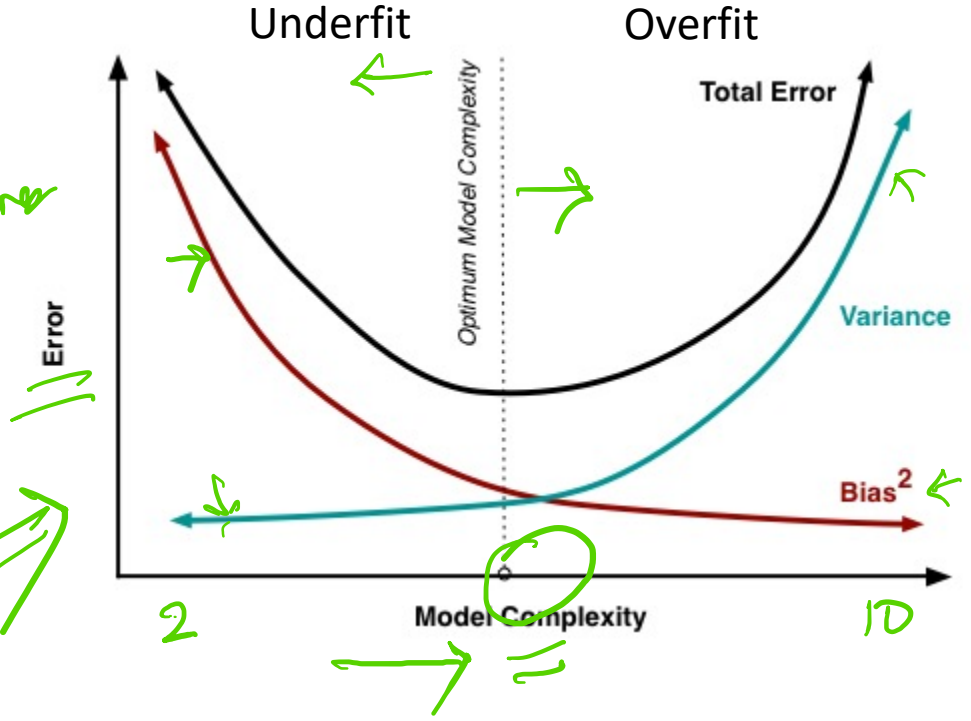
- Bias: Error from erroneous assumptions in the model
  - High bias -> underfitting
  - Model has limited flexibility to learn
  - Analogy: Overly simplistic assumptions about people make you a biased person
- Variance: Error from sensitivity of model to small perturbations in training data
  - High variance -> overfitting
  - Model has too much flexibility to learn
  - If you have a lot of data and over complex model, you can make each parameter of the model "by-heart" one data point
  - When a new data point comes, then the model will change wildly to accommodate the new point



Bias/Variance Equation

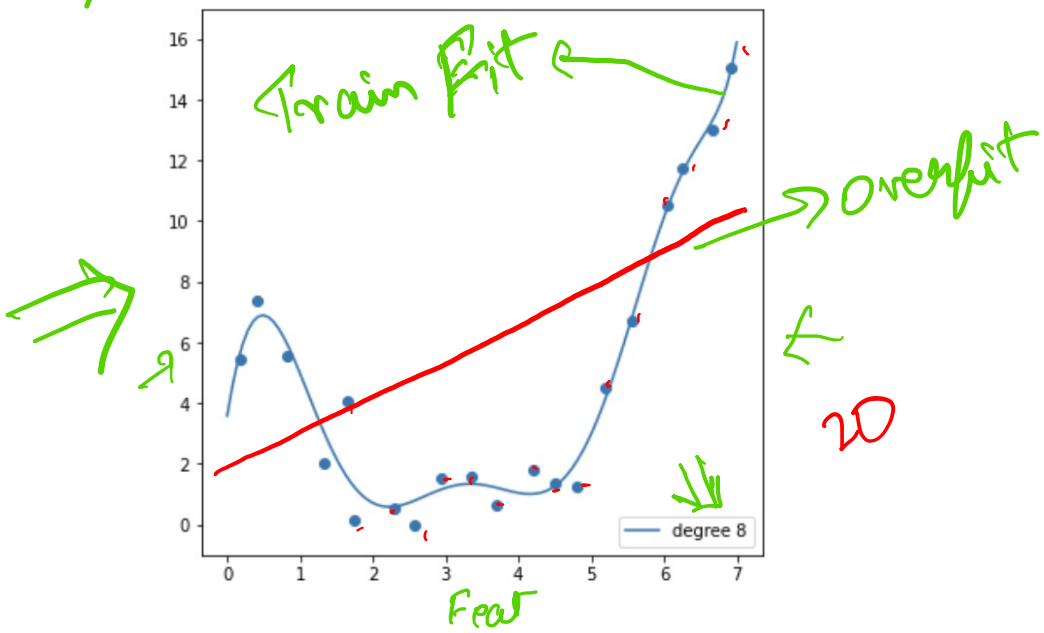
- $Error = E[(y - \hat{y})^2]$ –> RMSE
- $Error = (E[\hat{y}] - y)^2 + E[(\hat{y} - E[\hat{y}])^2] + \sigma_e^2$
- Error = Bias^2 + Variance + Irreducible Error

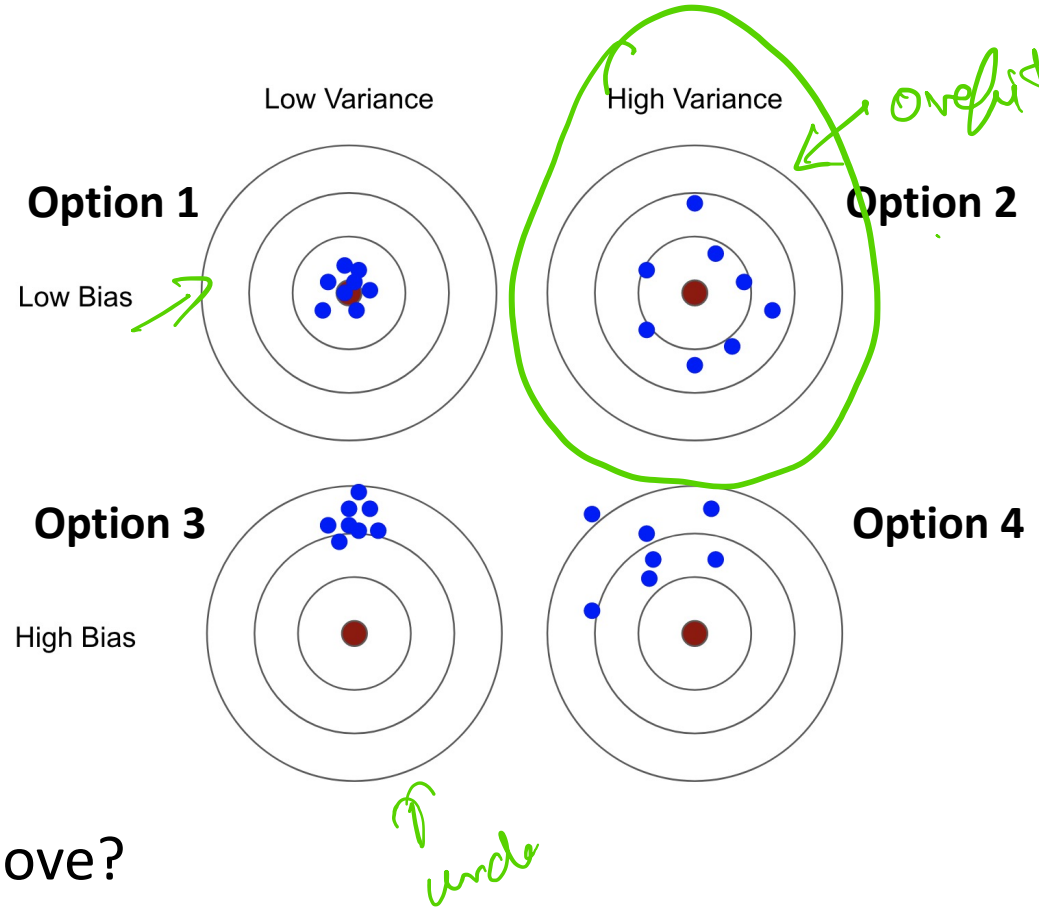




Audience Poll

Question 1: What condition is this fit?





Question 2: What type of fit is the above?

1. Overfit; 2. Underfit; 3. Optimal Fit; 4. None of the above

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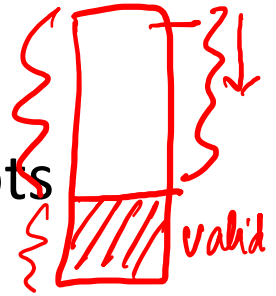
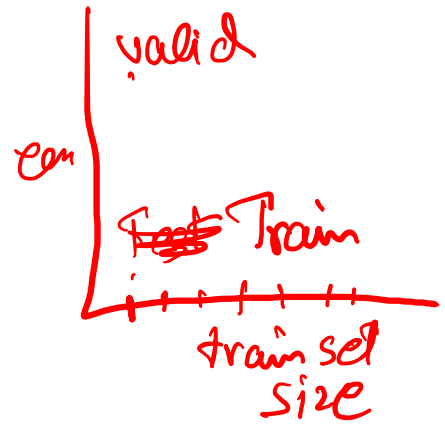
Learning Curves

- To generate learning curves, train the model several times on different sized subsets of the training set.
- The following code defines a function that, given some training data, plots the learning curves of a model
  - **from sklearn.metrics import** mean_squared_error
  - **from sklearn.model_selection import** train_test_split
  - **def** plot_learning_curves(model, X, y):
    - X_train, X_val, y_train, y_val = train_test_split(X, y, test_size=0.2)
    - train_errors, val_errors = [], []
    - **for** m **in** range(1, len(X_train)):
      - model.fit(X_train[:m], y_train[:m])
      - y_train_predict = model.predict(X_train[:m])
      - y_val_predict = model.predict(X_val)
      - train_errors.append(mean_squared_error(y_train[:m], y_train_predict))
      - val_errors.append(mean_squared_error(y_val, y_val_predict))
    - plt.plot(np.sqrt(train_errors), "r-+", linewidth=2, label="train")
    - plt.plot(np.sqrt(val_errors), "b-", linewidth=3, label="val")



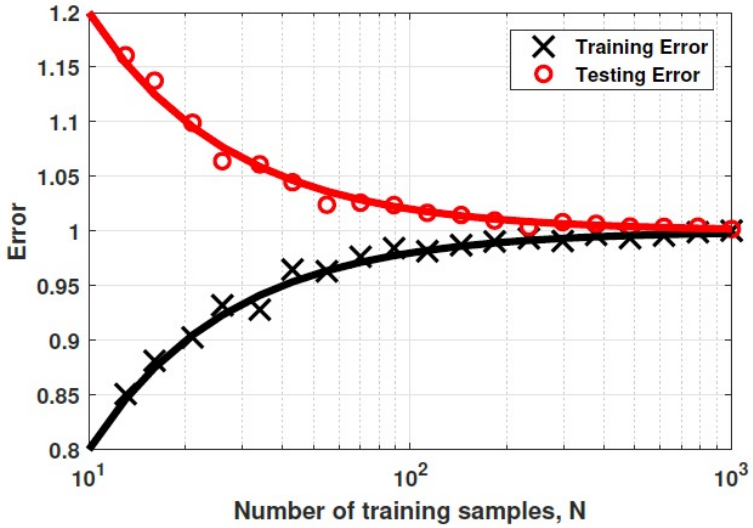


Formula for Linear Regression Errors

- For $m + t$ data points and a linear model with n features
- We fit a linear model $h_\theta(X; \theta)$ from the train set with m data points
  - Consider them first m points
- t data points are used for testing
- Let us analyze the result for train error and test error
- $\epsilon_{train} = MSE(\hat{y}_{1:m}, y_{1:m})$
- $\epsilon_{test} = MSE(\hat{y}_{m+1:m+t}, y_{m+1:m+t})$
- If σ is the variance of y, then we can derive that
  - $\epsilon_{train} = \sigma^2\left(1 - \frac{n}{m}\right)$
  - $\epsilon_{test} = \sigma^2\left(1 + \frac{n}{m}\right)$

Train and Test Errors

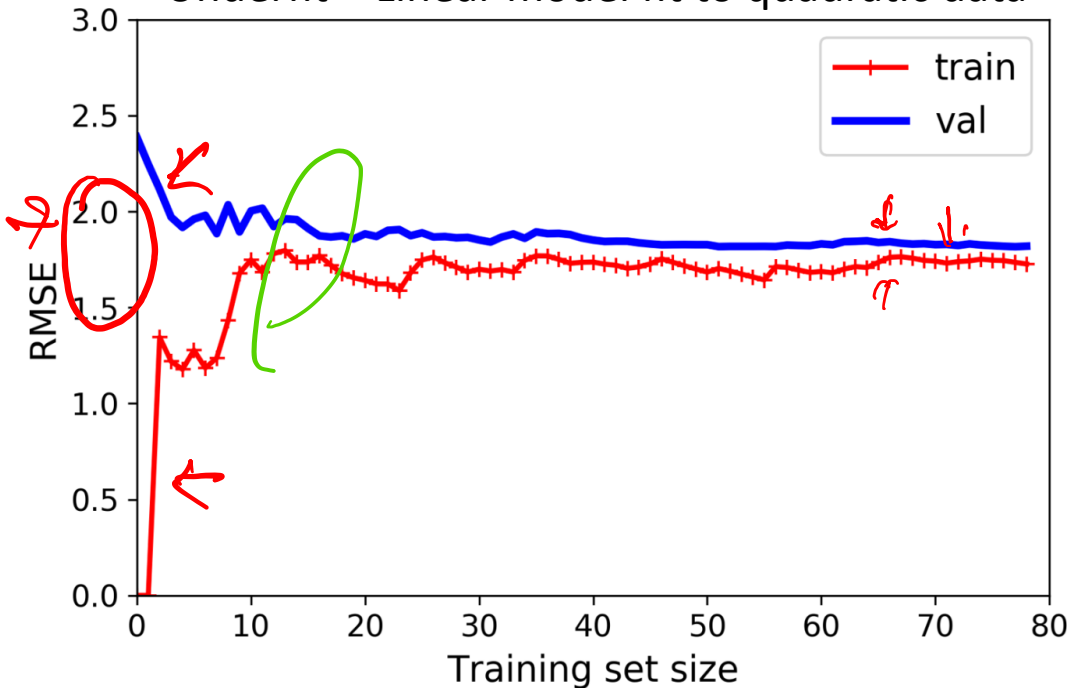
- $\epsilon_{train} = \sigma^2\left(1 - \frac{n}{m}\right)$; $\epsilon_{test} = \sigma^2\left(1 + \frac{n}{m}\right)$
- Usually $n \ll m$ – We want smaller number of parameters than model
  - Else it is over-determined system – infinitely many solution
  - We can always get train error to zero is $n > m$
- Learning curves are formed by increasing m and seeing how $\epsilon_{train}, \epsilon_{test}$ change
- How do train and test error change w.r.t. m?
  - $\epsilon_{train} \uparrow$ as $m \uparrow$. Thus more training samples make fitting harder.
  - $\epsilon_{test} \downarrow$ as $m \uparrow$. Thus more training samples improve generalization.
- How do train and test error change w.r.t. d?
  - $\epsilon_{train} \downarrow$ as $d \uparrow$. Thus a more complex model makes fitting easier.
  - $\epsilon_{test} \uparrow$ as $m \uparrow$. Thus a more complex mode makes generalization harder.



Theoretical learning curve for a perfect linear model with Gaussian noise

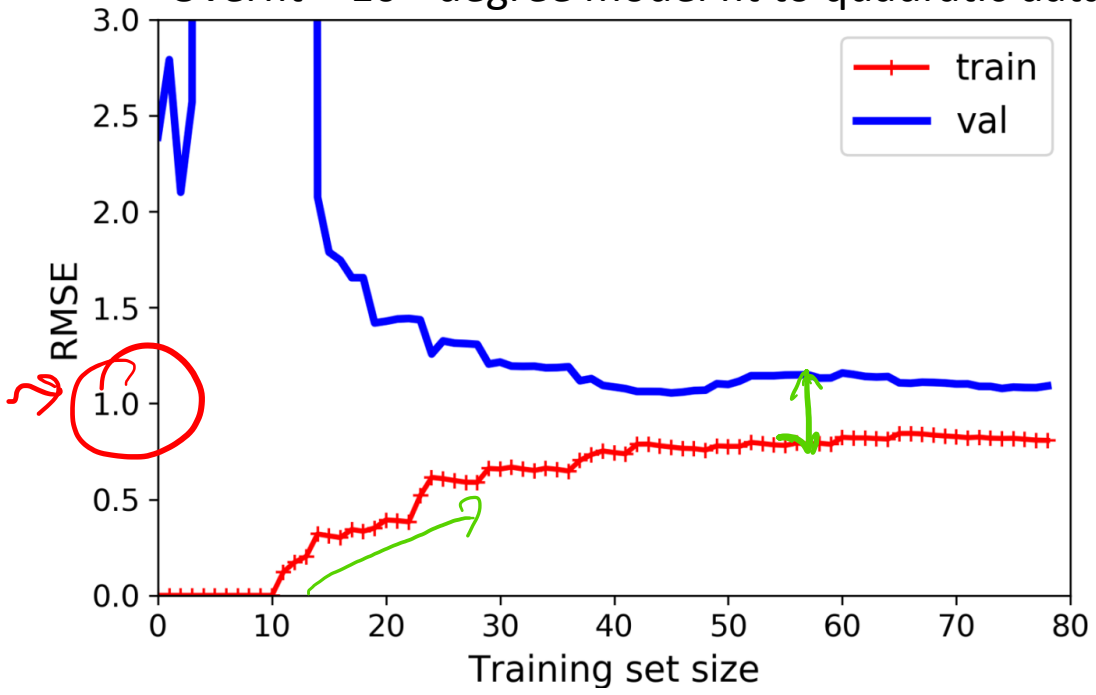
Example of Underfit and Overfit

Underfit – Linear model fit to quadratic data



- With one instance, fit is perfect
- Thereafter training error increases
- Plateaus fairly quickly
- RMSE is high. Magnitude of training is around 2
- RMSE on validation and training are very close

Overfit – 10th degree model fit to quadratic data



- With 10 instances, fit is perfect
- Validation error very high until order of fit
- Difference between training and validation is high
- RMSE of training is lower than underfit

[Figures from Geron]

Regularization

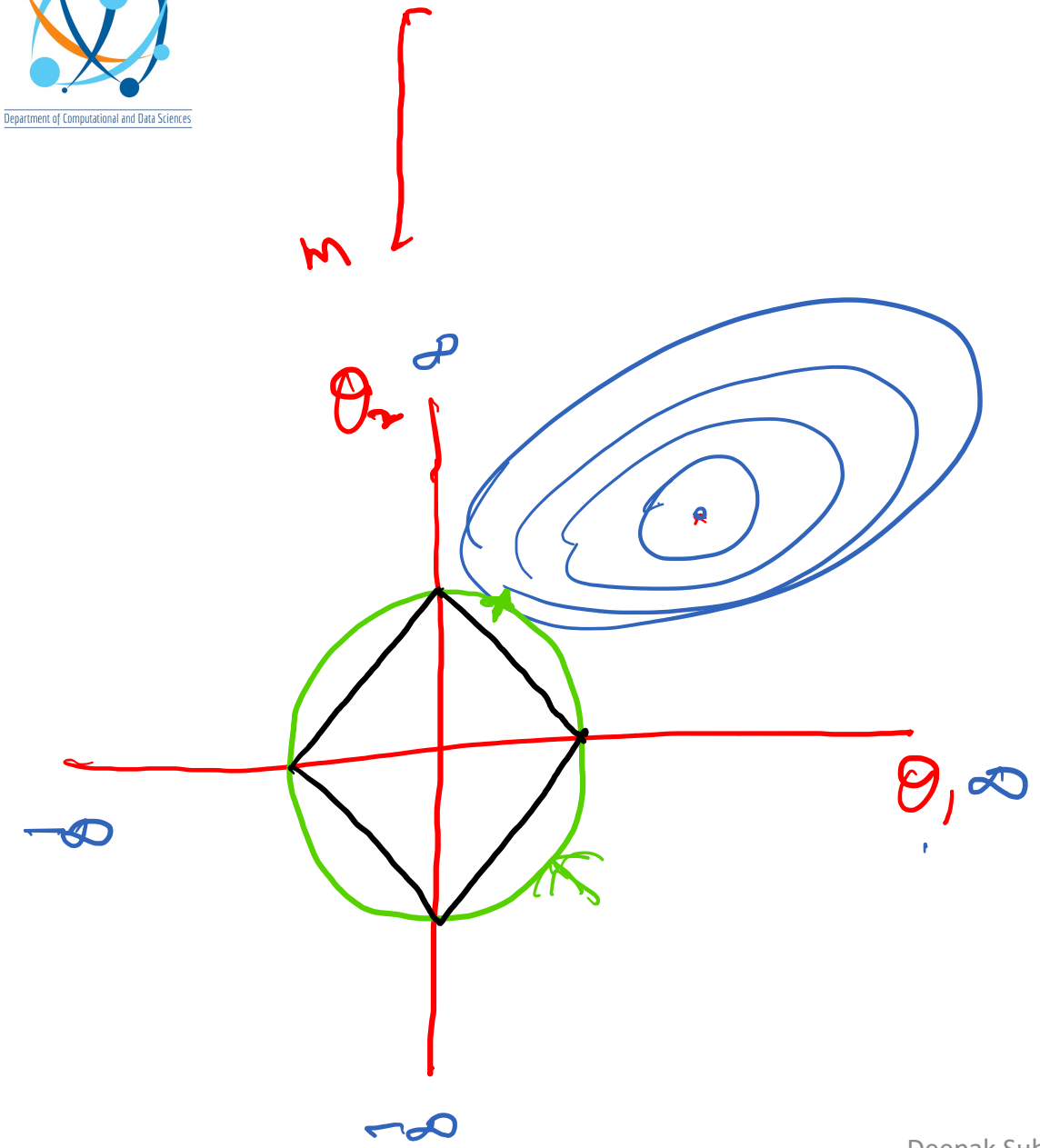
- The fewer degrees of freedom a model has, the harder it will be for overfit
- If we put constraints on θ, it will reduce overfitting and ensure models generalize well beyond training data
- We will study three different ways to constrain the weights
  - Ridge Regression – L2 Regularization, Tikhonov Regularization
  - Lasso Regression – L1 Regularization
  - Elastic Net – L1+L2 Regularization

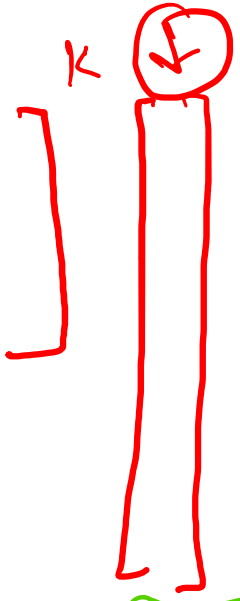
L1, L2 norm vectors

$$L_p = \left[\theta_1^p + \theta_2^2 + \dots + \theta_n^p\right]^{1/p}$$

$$L2 = \sqrt{\theta_1^2 + \theta_2^2 + \dots + \theta_n^2}$$

$$L1 = |\theta_1| + |\theta_2| + |\theta_3| + \dots |\theta_n|$$





Inverse
Prior
constraint

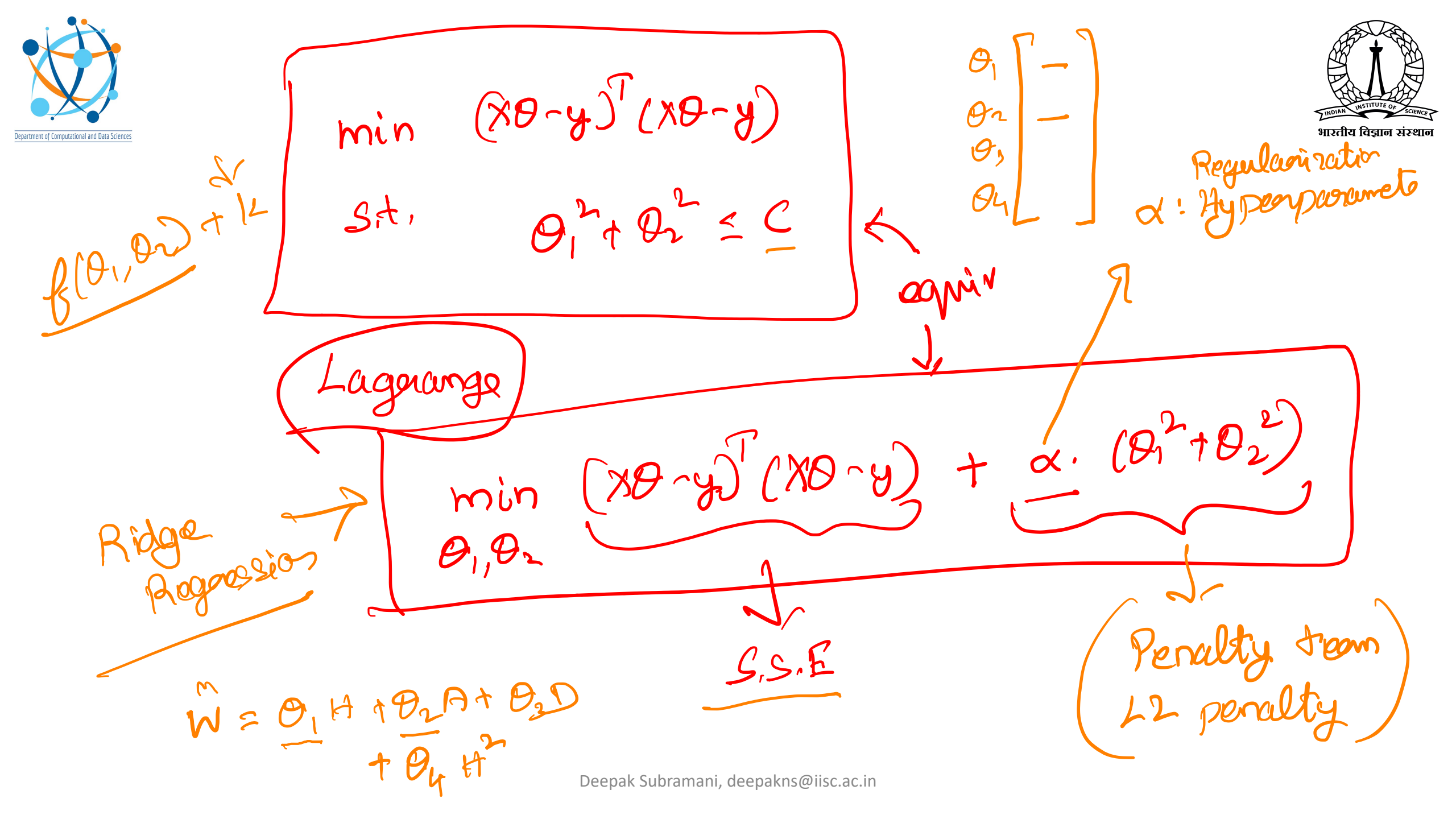
$$\hat{w} = \theta_1 A + \theta_2 A$$

$$\min_{\theta_1,\theta_2} (X\theta - y)^T (X\theta - y)$$

$$\theta_1^2 + \theta_2^2 \leq C_1$$

constrained optim..

$$|\theta_1| + |\theta_2| \leq C_2$$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min (Xθ−y)ᵀ(Xθ−y)
s.t. θ₁² + θ₂² ≤ c
f(θ₁, θ₂) + λ
θ₁ θ₂ θ₃ θ₄
Regularization
α : Hyperparameter
equiv
Lagrange
min θ₁, θ₂ (Xθ−y)ᵀ(Xθ−y) + α·(θ₁² + θ₂²)
Ridge Regression
S.S.E
Penalty term
L2 penalty
W = θ₁H + θ₂A + θ₃D + θ₄H²

Ridge Regression

- Add a regularization term $\alpha \sum_{i=1}^{n} \theta_i^2$ to the cost function

$$f(\theta) = \frac{1}{2} r(\theta)^T r(\theta) + \frac{1}{2} \alpha \sum_{i=1}^{n} \theta_i^2$$

- When using regularization, we don't include the bias term θ_0.
- We only use the weights of the features for regularization
- Hyperparameter α controls amount of regularization
  - If α = 0, then Ridge Regression is just Linear Regression.
  - If α is very large, then all weights end up very close to zero and the result is a flat line going through the data's mean.
- It is important to scale the data (e.g., using a StandardScaler) before performing Ridge Regression, as it is sensitive to the scale of the input features.
- Scaling is needed for most regularized models.

Solution to Ridge Regression

- A closed form solution similar to the normal equation can be found for the Ridge Regression problem
- The final solution is $\theta^* = (X^T X + \alpha A)^{-1} X^T y$, where A is an identity matrix with 0 in the (0,0) location corresponding to the bias term
- Using Cholesky Factorization
  - from sklearn.linear_model import Ridge
  - ridge_reg = Ridge(alpha=1, solver="cholesky")
  - ridge_reg.fit(X, y)
- Using SGD
  - sgd_reg = SGDRegressor(penalty="l2")
  - sgd_reg.fit(X, y.ravel())

Different Loss and Evaluation Functions?

- Use regularized cost function only for training, not for testing
- Apart from regularization, another reason they might be different is that a good training cost function should have optimization-friendly derivatives, while the performance measure used for testing should be as close as possible to the final objective.
- For example, classifiers are often trained using a cost function such as the log loss (discussed shortly) but evaluated using precision/recall.

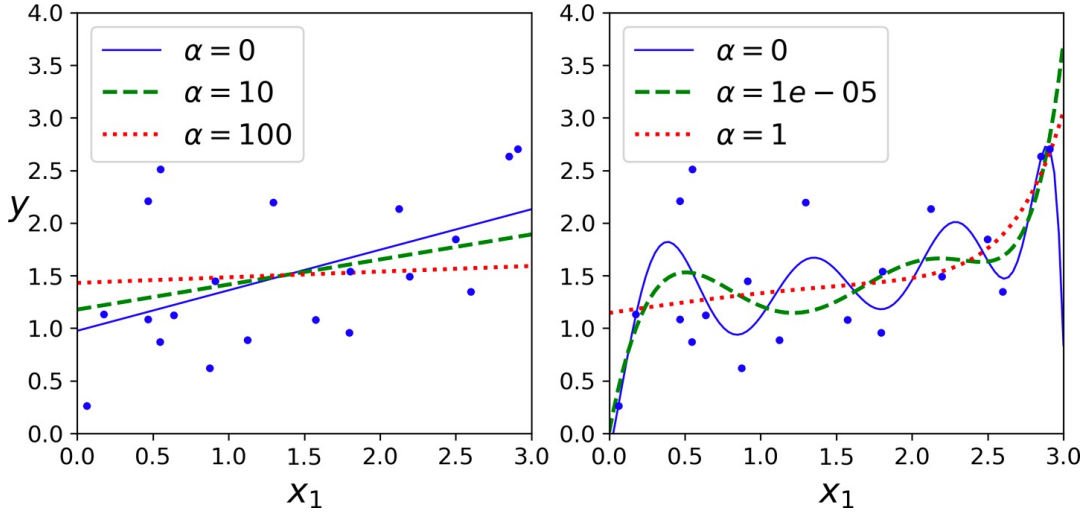
Lasso Regression

- Least Absolute Shrinkage and Selection Operator Regression (usually simply called Lasso Regression) is another regularization technique
- Unlike Ridge Regression, here the ℓ_1 norm is added to the cost function

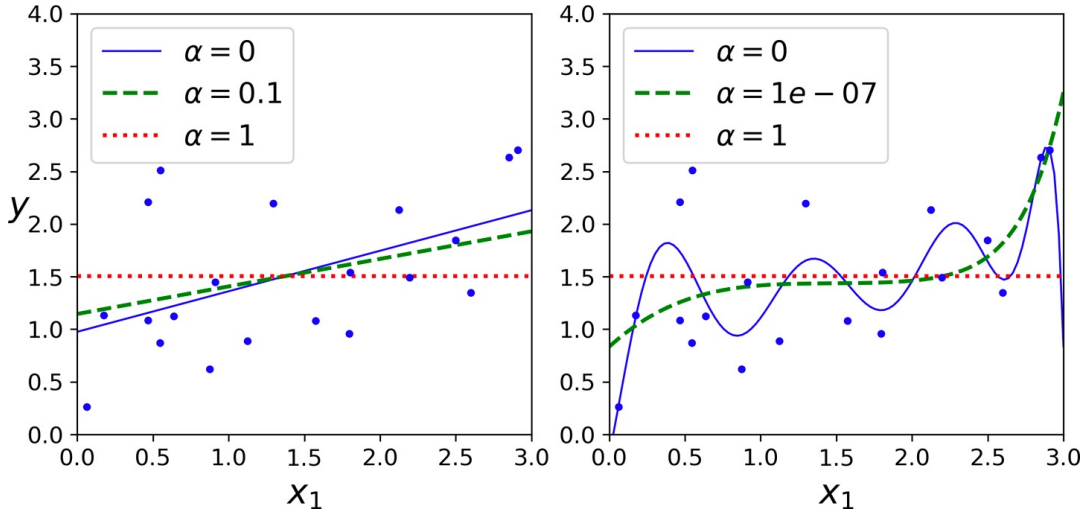
$$f(\theta) = \frac{1}{2} r(\theta)^T r(\theta) + \alpha \sum_{i=1}^{n} |\theta_i|$$

- Like Ridge, here also α is the amount of regularization applied
- LASSO is a sparsity promoting regularizer – it tends to eliminate the weights of the least important features (i.e., set them to zero).
- Notice: There is no ½ in front of the regularization term.

Ridge, Lasso with Different Levels of Regularization



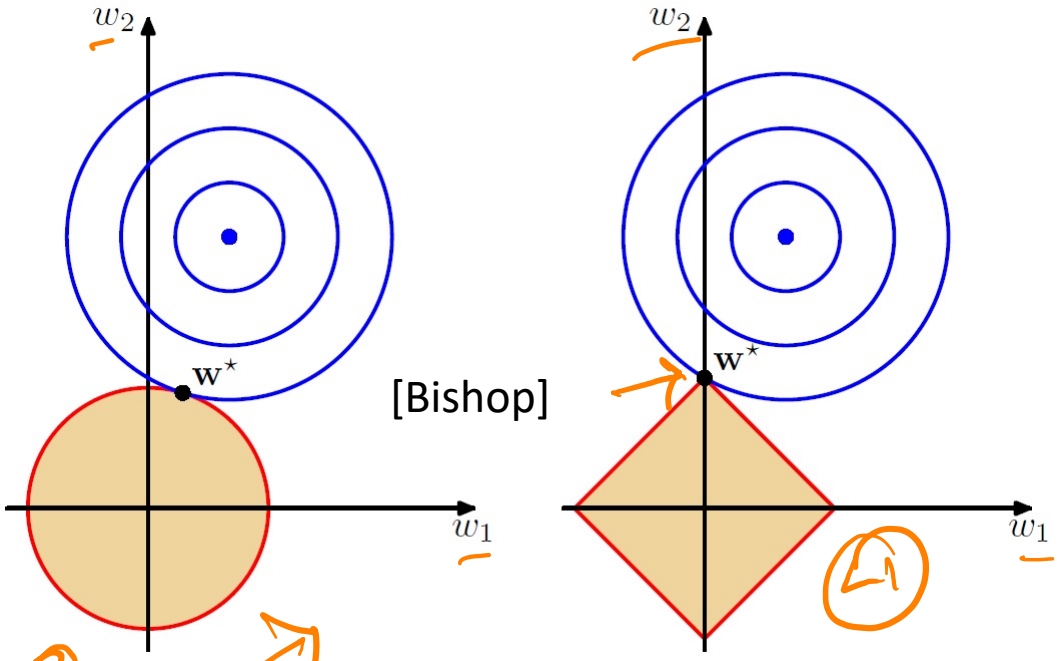
Ridge Regression on Linear Data
Left: Linear Regressors
Right: 10th Degree Polynomial Regressors



LASSO Regression on Linear Data
Left: Linear Regressors
Right: 10th Degree Polynomial Regressors
Lasso promotes sparsity more than Ridge

[Figures from Geron]

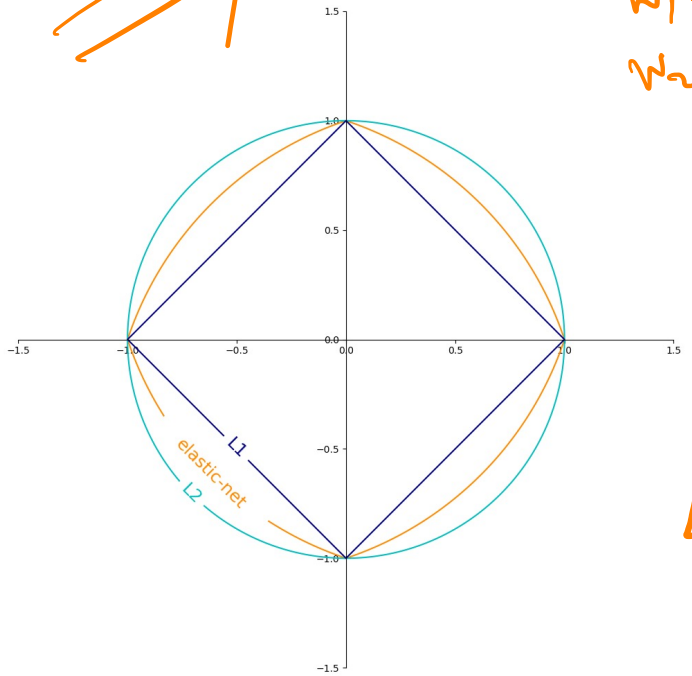
Ridge, Lasso Solutions



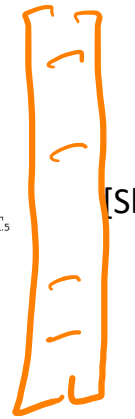
[Bishop]

$w_1 = 0$

$w_2 \neq 0$



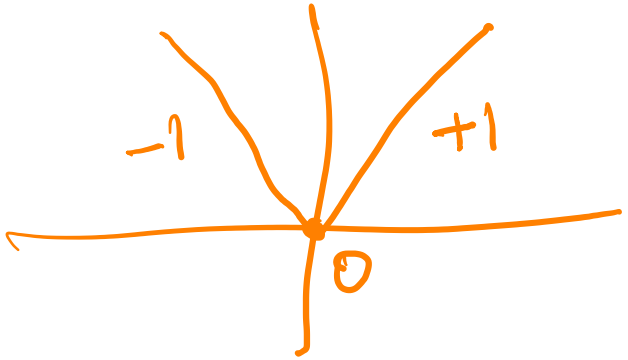
[Sklearn Website]



- A 2-d example
- The minima of the penalty terms is at (0,0)
- Lasso objective function is not differentiable – Needs Sub-Gradients
- Ridge objective function is differentiable
- For large α the optimal point goes close to 0, but never exactly zero
- In Ridge, the gradients reduce magnitude as the iteration gets closer to the true optimal
- In Lasso the iterates oscillate around due to the sub-gradient use

Subgradients for LASSO

- The ℓ_1 cost function is not differentiable at $\theta_i = 0$
- GD still works if a subgradient is used
- $g(\theta) = X^T r(\theta) + \alpha \begin{bmatrix} sign(\theta_1) \\ sign(\theta_2) \\ \cdot \\ sign(\theta_n) \end{bmatrix}$ where $sign(\theta_i) = \begin{cases} -1 \; if \; \theta_j < 0 \\ 0 \; if \; \theta_j = 0 \\ +1 \; if \; \theta_j > 0 \end{cases}$



Elastic Net

- Elastic net uses a combination of l1 and l2 regularization
- The regularization term is $\alpha \left[r \sum_{i=1}^{n} |\theta_i| + (1 - r) \frac{1}{2} \sum_{i=1}^{n} \theta_i^2 \right]$
- r is the mixing ratio –
  - r = 0 -> Elastic Net = Ridge Regression,
  - r = 1 -> Elastic Net = Lasso Regression

Guidelines

- When to use Plain, Ridge, Lasso, Elastic net?
  - Generally avoid plain Linear Regression - almost always preferable to have some regularization
  - Ridge is a good default, but if we believe that only a few features are useful (from domain expertise), then prefer Lasso or Elastic
  - Between lasso and elastic, prefer elastic as lasso may behave irratically when $n > m$

Scikit Learn

- Ridge
  - from sklearn.linear_model import Ridge
  - ridge_reg = Ridge(alpha=0.1)
  - ridge_reg.fit(X, y)
  - SGD - SGDRegressor(penalty="l2", alpha=0.1).
- Lasso
  - from sklearn.linear_model import Lasso
  - lasso_reg = Lasso(alpha=0.1)
  - lasso_reg.fit(X, y)
  - SGD - SGDRegressor(penalty="l1", alpha=0.1).
- Elastic Net
  - from sklearn.linear_model import ElasticNet
  - elastic_reg = ElasticNet(alpha=0.1, l1_ratio=0.5)
  - elastic_reg.fit(X, y)
  - SGD - SGDRegressor(penalty="elasticnet",alpha=0.1,l1_ratio=0.5).
- Ridge Implementation: 'svd', 'cholesky', 'lsqr', 'sparse_cg', 'sag', 'saga'
- Lasso and ElasticNet Implementation: coordinate descent

Audience Poll

1. L1 regularizer is differentiable
   - True, False
2. L2 Regularization with linear regression has an exact closed form solution
   - True, False

$(X^TX + \alpha I)\theta = X^Ty$

3. Elastic Net promotes Sparsity
   - True, False
4. Ridge Regression is L1 regularization
   - True, False

Summary

- Sklearn.linear_model.LinearRegression solves the normal equation
- SGDRegressor solves the regression problem with SGD
  - Different types of loss are possible
- Cross Validation and Learning Curves are used to figure out if a model is overfitting or underfitting
- Regularization helps to build accurate compact models that avoid overfitting
  - Ridge, Lasso, Elastic Net
  - Remember the rules of thumb for choosing regularization

Linear Models: Classification

DA-224-O JAN2022

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The Story So Far

- Sklearn.linear_model.LinearRegression solves the normal equation $h_\theta = X\theta$
- SGDRegressor solves the regression problem with SGD
  - Different types of loss are possible
- Underfit vs Overfit
- Regularization helps to build accurate compact models that avoid overfitting
  - Ridge, Lasso, Elastic Net
  - Remember the rules of thumb for choosing regularization

1) Loss Fn
2) Optimization

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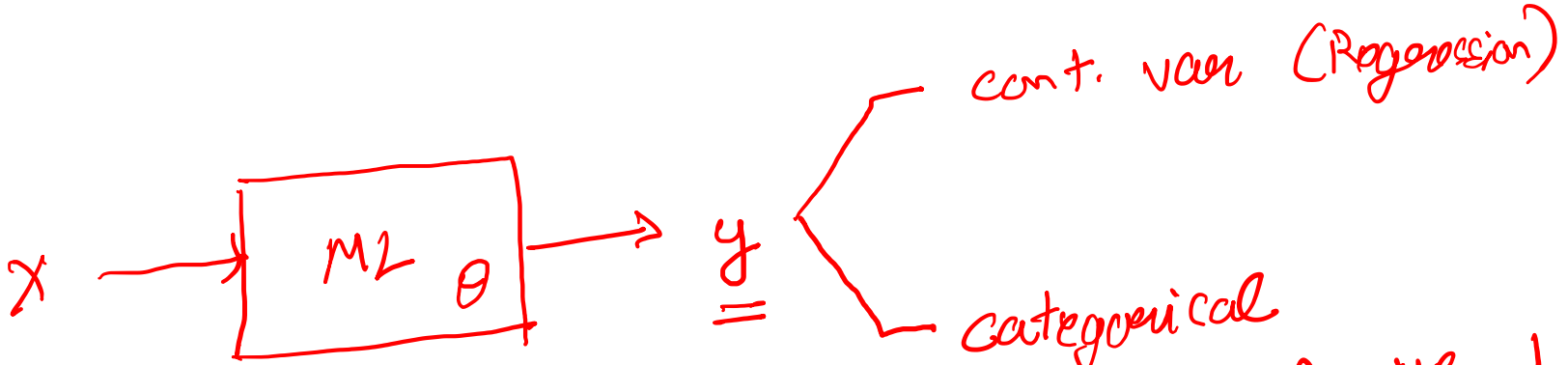
Classification



$\Rightarrow \hat{y} = h_\theta(x; \theta)$

$\min_\theta g(\hat{y} - y)$

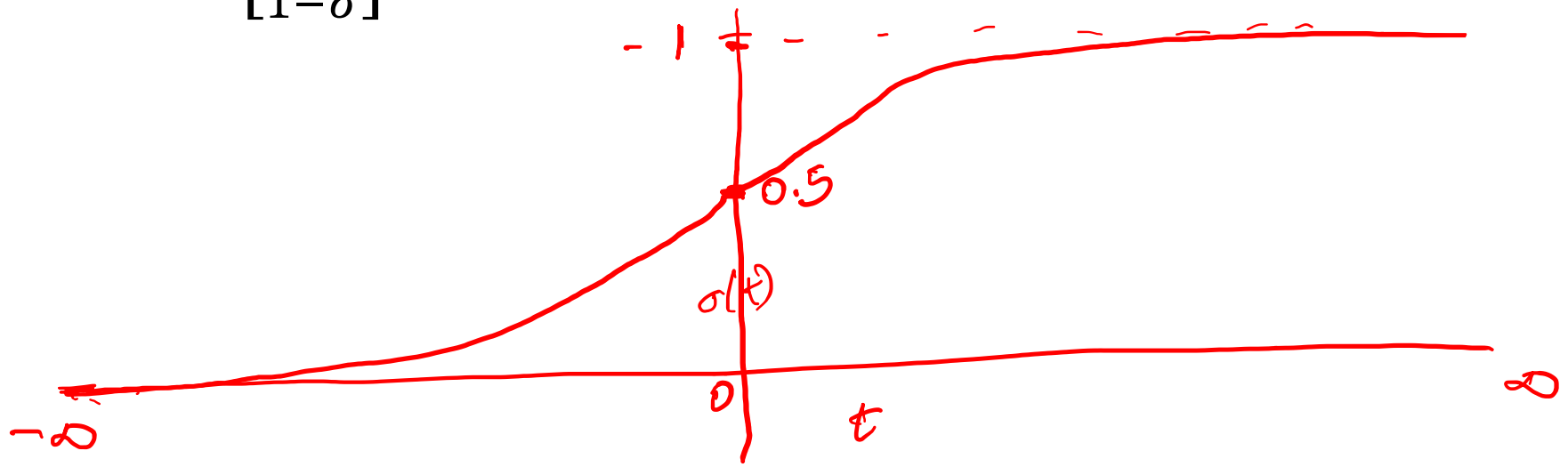
$\underline{x}$ = image
- cat
- dog
- elephant

Logistic Regression

- When the task is binary classification, we can set the target to the probability that a particular label is obtained
- To make regression a binary classification task:
  - Predict a probability
  - If the estimated probability > 50%, predict that the instance is in the positive class, labeled “1”, and
  - otherwise predict that it belongs to the negative class, labeled “0”.
- How to predict the probability?
  - Use a sigmoid function

Logistic or Sigmoid Function

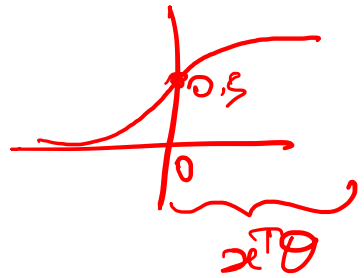
- $\sigma(t) = \frac{1}{1+\exp(-t)}$
- Takes an input in $(-\infty, \infty)$ and returns a value between 0 and 1
- $logit(t) = log\left[\frac{\sigma}{1-\sigma}\right]$



Logistic Regression Model

- Estimate the probability of class using $h(\theta)$
- $\hat{p} = h_\theta(\boldsymbol{x}; \boldsymbol{\theta}) = \sigma(\boldsymbol{x}^T \theta)$ – per instance
- Compare Regular Regression where the output itself is predicted with no modification by the sigmoid function
- After estimating probability, class is predicted as

$$\hat{y} = \begin{cases} 1 \; if \; \hat{p} \geq 0.5 \\ 0 \; otherwise \end{cases}$$

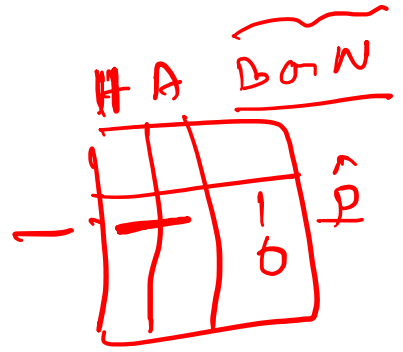


- The sigmoid function is such that $\sigma(t) \geq 0.5$ when t is positive
- When $x^T\theta \geq 0$, the class label is 1, else 0

Audience Poll - 1

- Logistic and Sigmoid Function are the same
  - True, False
- Sigmoid takes any real number as input and outputs a number between 0 and 1
  - True, False
- In Logistic Regression, the output itself is predicted
  - True, False

What and How to Train?



- Loss function for a single training instance
- $c(\theta) = \begin{cases} -\log(\hat{p}) & if\ y = 1 \\ -\log(1-\hat{p}) & if\ y = 0 \end{cases}$
- -log(t) becomes very large when t approaches zero
- When $y = 1$, we want $\hat{p} = 1$, and vice versa.
- The cost function over full training set is

$$f(\theta) = -\frac{1}{m}\sum_{j=1}^{m}\left[y_j \log(\hat{p}_j) + (1-y_j)\log(1-\hat{p}_j)\right]$$

- This is called the ***log loss*** cost function
- No closed form expression to minimize it (no Normal Equation)
- Fortunately, function is convex and gradient descent will find global optima

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Gradients

- Partial derivatives of the cost function are as follows

$$\nabla_i f(\theta) = \frac{1}{m}\sum_{j=1}^{m}\left(\sigma(\boldsymbol{x}_j^T\boldsymbol{\theta}) - \boldsymbol{y}_j\right)x_{j,i}$$

- Use these gradients to perform optimization via
  - 1st order: Batch GD, SGD or Mini-Batch GD,
  - 2nd order: L-BFGS → Quasi Newton
- That is all to train a Logistic Regression model for classification

Gradients

- Implementation in sklearn
  - from sklearn.linear_model import LogisticRegression
  - log_reg = LogisticRegression(penalty='l2',solver='lbfgs')
  - log_reg.fit(X, y)
- This class implements regularized logistic regression using the 'liblinear' library, 'newton-cg', 'sag', 'saga' and 'lbfgs' solvers.
- **Regularization is applied by default**
  - The 'newton-cg', 'sag', and 'lbfgs' solvers support only L2 regularization with primal formulation, or no regularization.
  - The Elastic-Net regularization is only supported by the 'saga' solver.

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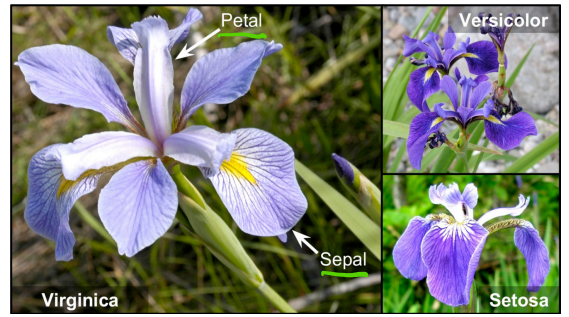
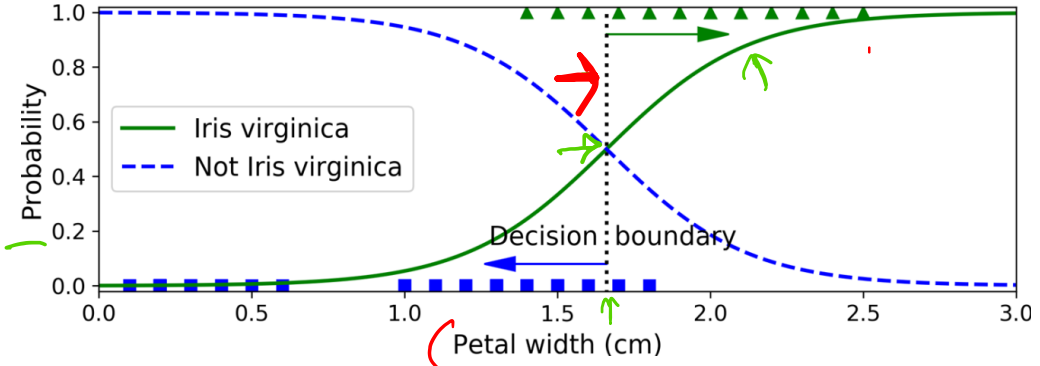
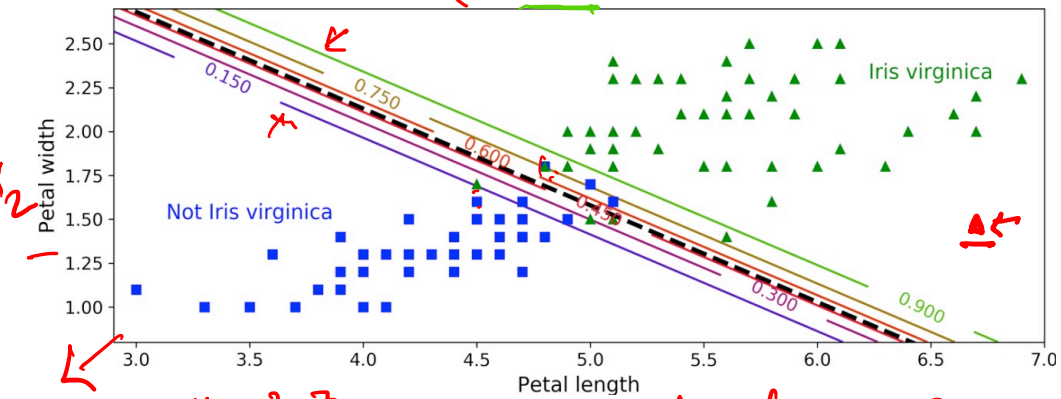
Decision Boundaries: Logistic Regression in Action



- Iris Dataset: 3 species (Iris setosa, Iris versicolor and Iris virginica)
- 150 samples with sepal and petal length and width
- **Binary classifier for Iris virginca or not**
  - **from sklearn import** datasets
  - iris = datasets.load_iris()
  - list(iris.keys())
    - ['data', 'target', 'target_names', 'DESCR', 'feature_names', 'filename']
  - X = iris["data"][:, 3:] *# petal width*
  - y = (iris["target"] == 2).astype(np.int) *# 1 if Iris virginica, else 0*
  - **from sklearn.linear_model import** LogisticRegression
  - log_reg = LogisticRegression()
  - log_reg.fit(X, y)
- Right Middle: 1d decision boundary
- Right Bottom: 2d decision boundary





[Figures from Geron]

```
def predict_can_crash(X):
    return False
```

accuracy 99%

Unbalanced Datasets

- Weighted Logistic Regression
- Consider a data set with 99% of Class 0 and 1% of Class 1
  - 0: Majority Class; 1: Minority Class
- Penalize Label 1's error more than Label 0's error
- Weighted Log-Loss Function

$$f(\theta) = -\frac{1}{m}\sum_{j=1}^{m}\left[w_1 y_j \log(\widehat{p_j}) + w_0\left(1-y_j\right)\log(1-\widehat{p_j})\right]$$

- Sklearn
  - `w = {0:1, 1:99} #define class weights`
  - `lg = LogisticRegression(random_state=42, class_weight=w) # define model`
  - `lg.fit(X_train,y_train) # fit it`

Audience Poll - 2

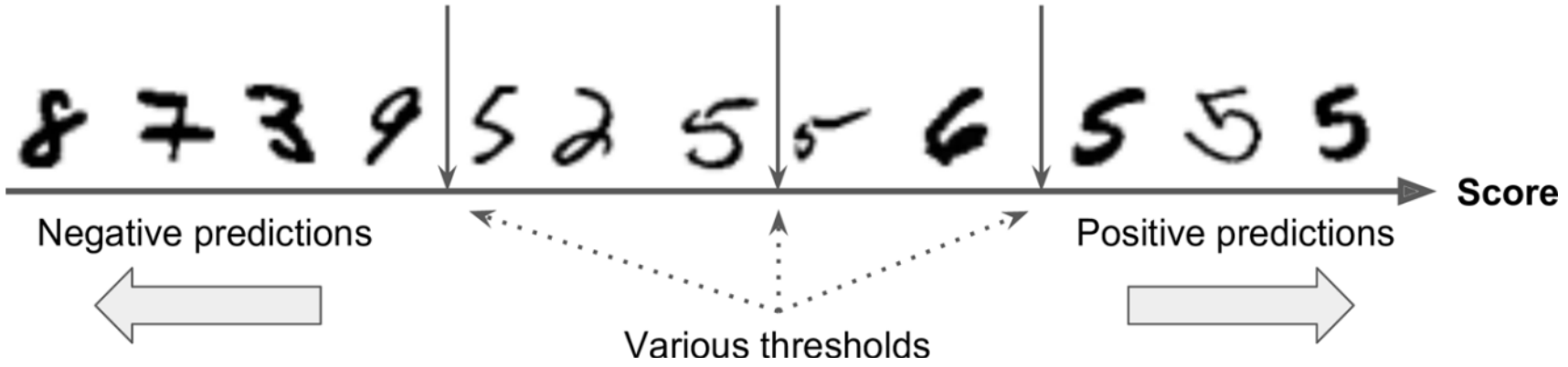
- Logistic Regression returns probability of belonging to a class
  - True, False
- In Classification, we often train with a different loss function than the evaluation metric
  - True, False
- Usual Logistic Regression can be used for imbalanced datasets
  - True, False

Confusion Matrix: Revisit

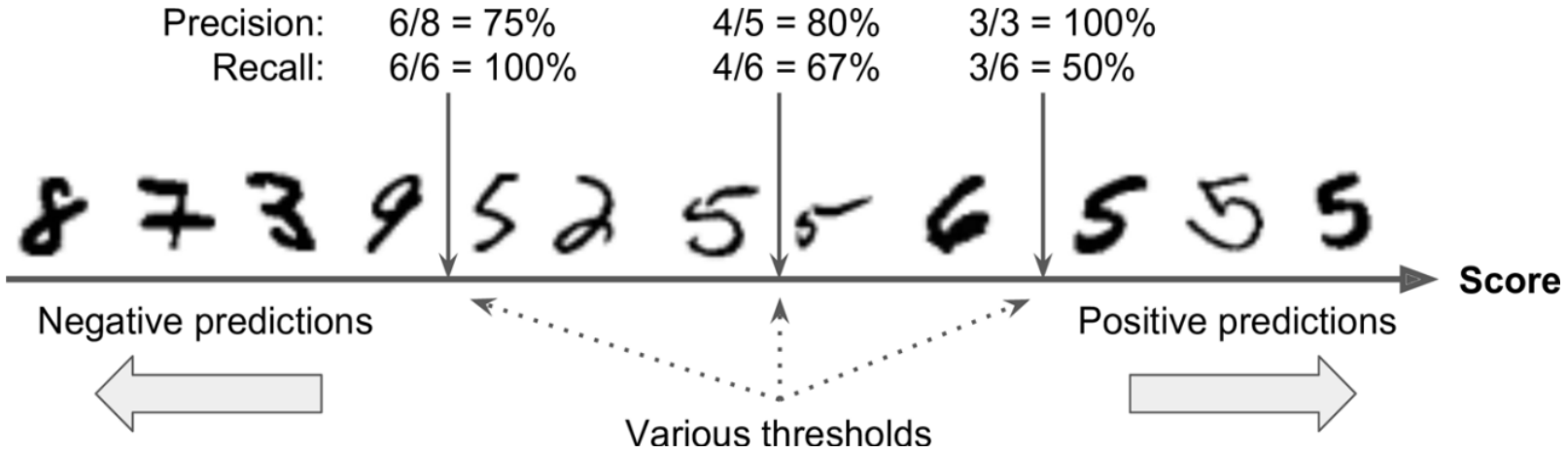
	True Label A	True Label ~A
Pred. Label A	True Positive	False Positive
Pred. Label ~A	False Negative	True Negative

- Precision = $\frac{TP}{TP+FP}$;
  - Among all prediction of Label A, how many are actually Label A
  - Trivial 100% Precision – Make only one Prediction of Label A, and ensure that it is correct. Then TP=1, FP=0, and Precision=1
- Recall = $\frac{TP}{TP+FN}$;
  - Of all true Label A, how many does our classifier predict as Label A
  - Combined with Precision, we now have a good sense of the goodness of our classifier
- Typically, we want high precision and high recall
- F1 Score = $\frac{2}{\frac{1}{precision}+\frac{1}{recall}} = \frac{TP}{TP+\frac{FN+FP}{2}}$
- F1 Score is the harmonic mean of precision and recall. Hence F1 will be high only if precision and recall are high

Precision Recall Tradeoff



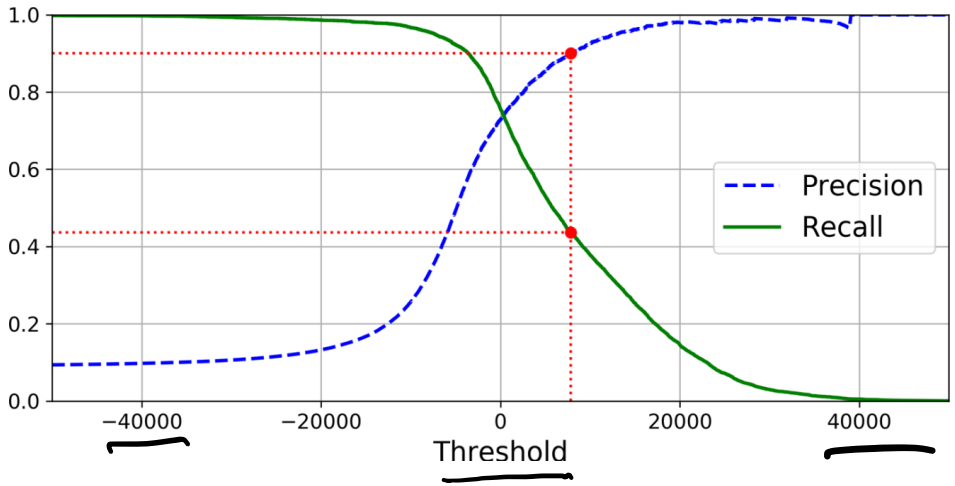
Precision-Recall Tradeoff



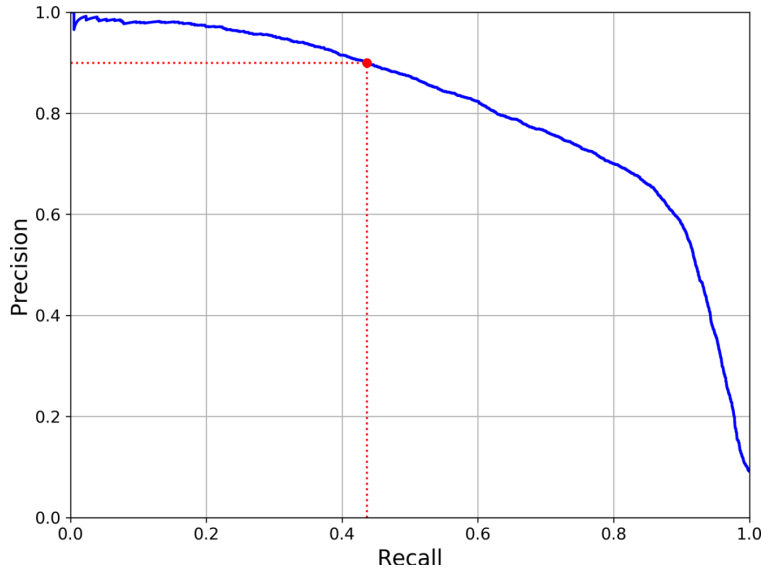
- Classification is based on a score calculation and a threshold set
- Based on where the threshold is placed, precision increases at the expense of recall, and vice versa
- While F1 Score is good, in some applications, we prefer high recall even at the expense of low precision
  - For example, fraud detection. We want to catch all the fraud cases, even if some non fraud cases are also flagged.

Precision-Recall Tradeoff

	True Label A	True Label ~A
Pred. Label A	True Positive	False Positive
Pred. Label ~A	False Negative	True Negative



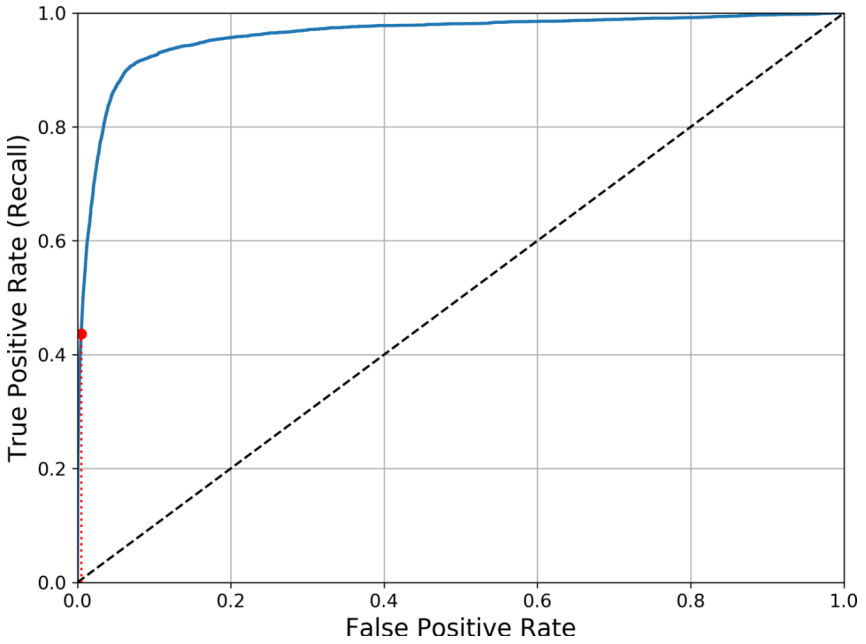
- For different thresholds, we usually plot both precision and recall vs threshold.
- We can also plot Precision vs Recall
- Choose the right threshold from the above curve and settle for a Precision-Recall tradeoff



Plots from Geron Chapter 3

Receiver Operating Characteristic (ROC) Curve

- True Positive Rate (TPR) – Recall or Sensitivity
- True Negative Rate (TNR) – Specificity – Ratio of negative instances correctly classified as negative
- False Positive Rate = 1 – True Negative Rate
- ROC plot is sensitivity vs 1-specificity, i.e., TPR vs FPR
- Compute TPR and FPR for different thresholds and plot it
- The ROC must be as much away from the 45-degree line as possible
- Calculate the Area Under the Curve (AUC) for quantifying goodness of the classifier
- AUC=1 is a perfect classifier, and AUC=0.5 for a random classifier



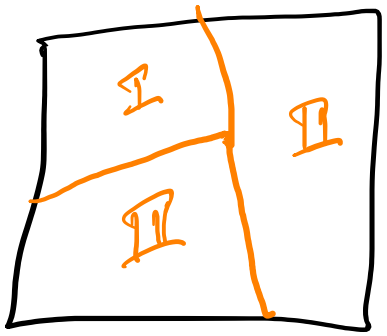
Binary ~~to~~ for Multiclass Approach

- What if we have multiple classes, say K classes?

cat
dog
not

I cat vs oth
II dog vs oth
III not vs oth

- One-vs-Rest (OvR) Strategy
  - Consider a problem of predicting one of 10 lables
  - Convert to Class 0 or Not, Class 1 or Not, etc



- One-vs-Others (OvO) Strategy
  - Convert to Class 0 vs Class 1, Class 0 vs Class 2, etc.
  - There are C(K,2) such classifiers

$^{K}C_{2}$

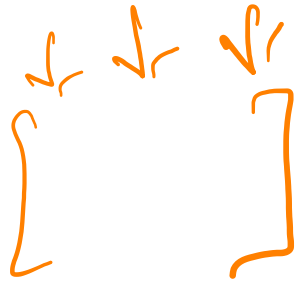
- Use scores (or probabilities) from all classifiers and choose the highest and assign the final class label

Multinomial Logistic Regrssion: Softmax

- Idea
  - Compute a score for each class $s_k(\boldsymbol{x})$
  - Estimate probability of each class by applying the softmax function (a.k.a normalized exponential)
- Softmax score for each input instance $\boldsymbol{x}$ is written as a linear regression model

$$s_k(\boldsymbol{x}) = \boldsymbol{x}^T \theta^{(k)}$$

  - Each class has its own parameter set $\theta^{(k)}$



Multinomial Logistic Regrssion: Softmax

- Probability estimated from softmax score by applying the softmax function

$$\hat{p}_k = \frac{\exp(s_k(\boldsymbol{x}))}{\sum_{k=1}^{K} \exp(s_k(\boldsymbol{x}))}$$

- Final prediction is the class with the highest probability
- $\hat{y} = \underset{k}{\operatorname{argmax}}\, \hat{p}_k = \underset{k}{\operatorname{argmax}}\, s_k(\boldsymbol{x}) = \underset{k}{\operatorname{argmax}}\, \boldsymbol{x}^{\boldsymbol{T}} \theta^{(k)}$
- The above is true for every data instance.
- Question: How to train? How to find the optimal $\boldsymbol{\theta}$

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Training Softmax Regression

- Objective: Model must predict high probabilities for the target class
- What is the objective function or cost function?

$$f(\Theta) = -\frac{1}{m}\sum_{j=1}^{m}\sum_{k=1}^{K} y_{k,j}\log\left(\hat{p}_{k,j}\right)$$

→ cross entropy

$y_{k,j}$ → [0, 1, 2]

- Target $y_{k,j}$ is a one-hot vector
  - 1 for the true class; 0 everywhere else
- If the predicted probability is 1 for the target class, then error = 0.
- The term in the second summation (over K class labels) is called the cross entropy between $\boldsymbol{y}$ and $\hat{\boldsymbol{p}}$
  - K=2 -> Simple Logistic Regression

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Gradient of Softmax Cost Function

- Partial derivatives of the cost function are as follows

$$\nabla_{\theta(k)} f(\boldsymbol{\theta}) = \frac{1}{m} \sum_{j=1}^{m} \left(\hat{p}_{k,j} - y_{k,j} \right) \boldsymbol{x}_j$$

- Gradient vector per class is computed and an optimization method is performed to compute the optimal $\boldsymbol{\theta}$
- Implementation in sklearn
  - from sklearn.linear_model import LogisticRegression
  - Softmax_reg = LogisticRegression(multi_class="multinomial",solver="lbfgs", C=10)
  - This applies a l2 regularization by default controlled using C
    - C is the inverse of alpha that we used in LinearRegression

Audience Poll - 3

- Which of the following is a multiclass classification algorithm
  - OvO
  - Linear Regression
  - Logistic Regression
  - OvB
- If the softmax score of 3 classes A,B,C are log(10), log(20) and log(30). What is the probability of class B
  - 1/3
  - 1/6
  - 1/2
  - 2/3

$$\frac{20}{10+20+30} = \frac{20}{60} = \frac{1}{3}$$

- There are three classes A,B and C. What is the one-hot vector for a data point of Class C?
  - [0,0,1]
  - [0,1,0]
  - [1,0,0]
  - [1,1,0]

What is in a name?

- Log-Linear Models – direct name!
- (Multinomial) Logistic Regression – in traditional stats/data analytics
- Softmax Regression – in Machine Learning
- Generalized Linear Models – by theoretical CS/AI/Math/Stats folks
  - With a Binomial Distribution MaxEnt
- Very Shallow (Sigmoidal) Neural Networks – to sound cool today!

Summary of Logistic Regression

- sklearn.linear_model.LogisticRegression solves a classification problem
- SGDClassifier solves the classification problem with SGD
- Softmax Regression can be used for multiclass classification
- Log Loss in SGD solves the logistic regression problem

Comparison of algorithms for Linear Regression

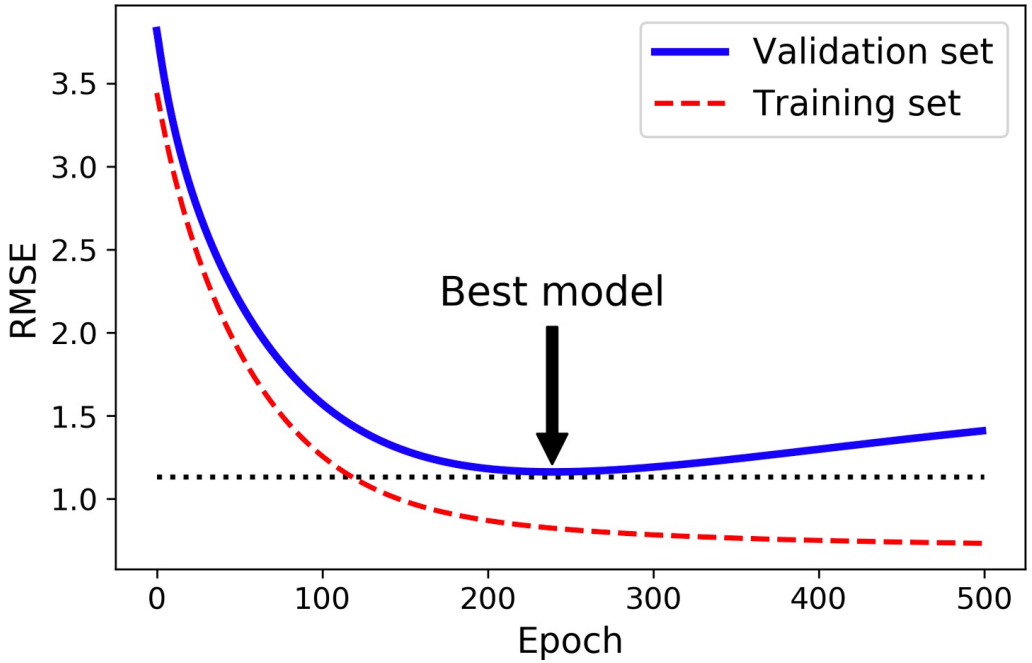
Algorithm	Large *m*	Out-of-core support	Large *n*	Hyperparams	Scaling required	Scikit-Learn
Normal Equation	Fast	No	Slow	0	No	N/A
SVD	Fast	No	Slow	0	No	`LinearRegression`
Batch GD	Slow	No	Fast	2	Yes	`SGDRegressor`
Stochastic GD	Fast	Yes	Fast	≥2	Yes	`SGDRegressor`
Mini-batch GD	Fast	Yes	Fast	≥2	Yes	`SGDRegressor`

Geron Chapter 4, Page 128, Table 4-1

Out of core algorithms are those that can process data that are too large to fit into a computer's main memory at once.

Early Stopping as a Regularizer

- The Free Regularizer – Just stop the training (i.e., optimization of parameters) as soon as the validation error takes a U-turn
- Calculate and plot the RMSE on the training set and test set with epochs
- As soon as the validation error reaches a minimum and starts increasing stop
- This U-turn indicates that the model has started overfitting the train data
- With SGD and MiniBatch, the curves won't be smooth. So what to do?
  - Stop only when validation error has been above the last known minimum for some time
  - Then roll back to the minimum



[Figures from Geron]