Day 3: Generalization Error

Summer STEM: Machine Learning

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Outline

1. Lab: Simple Linear Regression
2. Review of Day 2
3. Lab: Robot Arm Calibration
4. Polynomial Regression
5. Train and Test Error, Overfitting
6. Regularization
7. Non-Linear Optimization

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Lab: Find/Build and fit your own data

1. Find your a data set
   - Google: "[subject you're interested in] dataset"
   - `https://archive.ics.uci.edu/ml/datasets.php`
   - `https://toolbox.google.com/datasetsearch`

– or –

2. Build your own data set
   - Only need 10+ samples

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- Find parameters that minimize the error function
  - Select b, w to minimize the error function

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Extending the Model to Multi-variable Data

- Model: $\hat{y} = w_0 \times 1 + w_1 x_1 + w_2 x_2 + \ldots + w_D x_D$
- Design Matrix: Let, $X = \begin{bmatrix} 1 & x_{1_1} & \cdots & x_{1_D} \\ 1 & x_{2_1} & \cdots & x_{2_D} \\ \vdots & & \ddots & \\ 1 & x_{N_1} & \cdots & x_{N_D} \end{bmatrix}$
- We say $\mathrm{w}^\star$ solves $\mathrm{y} = X\mathrm{w}$ in the least squares sense, where

$$\mathrm{w}^\star = X^\dagger \mathrm{y}$$

- This $\mathrm{w}^\star$ is the unique set of parameters that minimize the squared error

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Robot Arm Calibration

- Let's train a model based on the given data.
- In this lab we're going to:
  - Predict the *current* drawn
  - Predictors, X: Robot arm's joint angles, velocity, acceleration, strain gauge readings (load measurement).

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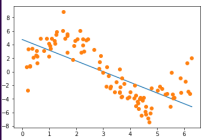
Polynomial Fitting

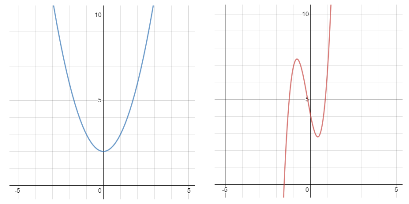
- We have been using linear model to fit our data. But it doesn't work well every time
- Some data have more complex relation that cannot be fitted well using a straight line
  - Ex: Projectile motion, Coulomb's law, Exponential growth/decay, ...



- Linear model does not look like a good fit for this data
- Can we use some other model to fit this data?

Polynomial Fitting

- Can we use a polynomial to fit our data?
- Polynomial: A sum of different powers of a variable
  - Examples: $y = x^2 + 2$, $y = 5x^3 - 3x^2 + 4$



- Polynomial Model: $y = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + \ldots$

Polynomial Fitting

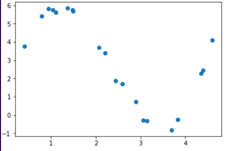
- Polynomial Model: $y = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + \ldots$
- The process of fitting a polynomial is similar to linearly fitting multivariate data
- Recall the linear model for multivariable
- $y = w_0 + w_1 x_1 + w_2 x_2 + w_3 x_3 + \ldots$
  - Where x_1, x_2, x_3... are different features
- If we treat x^2 as our second feature, x^3 as our third feature, x^4 as our fourth feature.... We can use the same procedure in multivariate regression for linear fit!

Polynomial Fitting

- Design Matrix for Linear: $A = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_N \end{bmatrix}$
- Design Matrix for Polynomial: $X = \begin{bmatrix} 1 & x_1 & x_2^2 & \cdots & x_1^D \\ 1 & x_2 & x_2^2 & \cdots & x_2^D \\ \vdots & & \ddots & & \vdots \\ 1 & x_N & x_N^2 & \cdots & x_N^D \end{bmatrix}$
- For the polynomial fitting, we just added columns of features that are powers of the original feature

Lab: Fit a polynomial

- You are given the data set below with x and y values



- Try to fit the data using a polynomial with a certain degree
- Calculate mean square error between the sample y and your predicted y
- Try different polynomial degree and see if you can improve the mse
- Plot your polynomial over the data points

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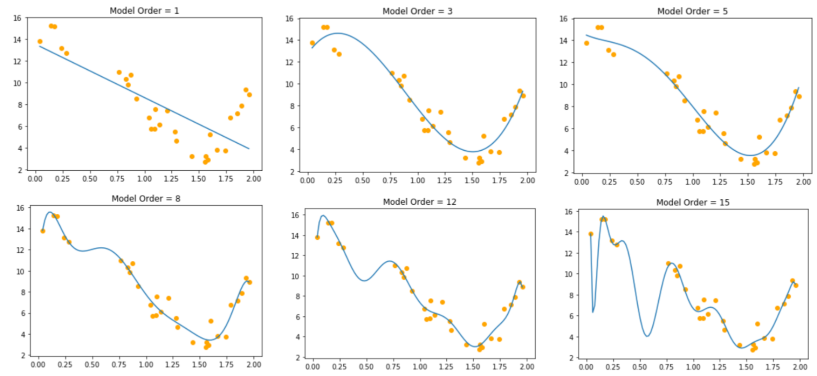
Overfitting

- We learned how to fit our data using polynomials of different order
- With a higher model order, we can fit the data with increasing accuracy
- As you increase the model order, at certain point it is possible find a model that fits your data perfectly (ie. zero error)
- What could be the problem?

Overfitting



- Which of these model do you think is the best? Why?

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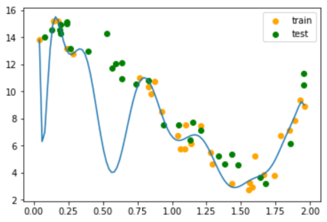
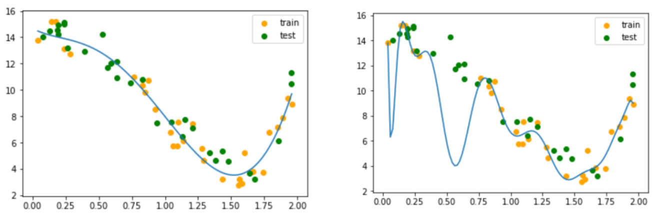
Overfitting

- The problem is that we are only fitting our model using data that is given
- Data usually contains noise
- When a model becomes too complex, it will start to fit the noise in the data
- What happens if we apply our model to predict some data that the model has never seen before? It will not work well.
- This is called over-fitting



Overfitting

- Split the data set into a train set and a test set
- Train set will be used to train the model
- The test set will not be seen by the model during the training process
- Use test set to evaluate the model when a model is trained



- With the training and test sets shown, which one do you think is the better model now?

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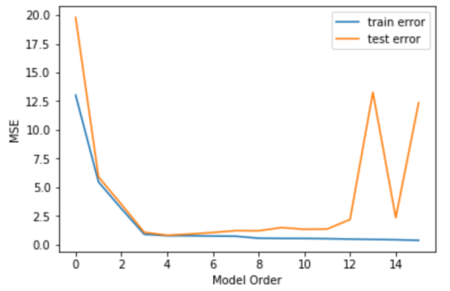
Train and Test Error

- Plot of train error and test error for different model order
- Initially both train and test error go down as model order increase
- But at a certain point, test error start to increase because of overfitting



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How can we prevent overfitting without knowing the model order before-hand?

- **Regularization**: methods to prevent overfitting
  - We just covered regularization by model order selection
- Running K-folds for cross-validation is intensive
- Is there another way?
  - Solution: We can change our cost function.

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Weight Based Regularization

- Looking back at the polynomial overfitting
- Notice that weight-size increases with overfitting

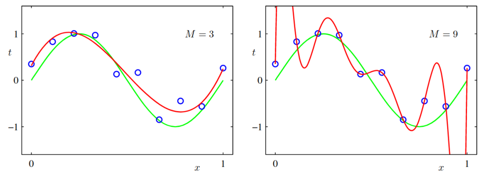

Table 1.1 Table of the coefficients $\mathbf{w}^\star$ for polynomials of various order. Observe how the typical magnitude of the coefficients increases dramatically as the order of the polynomial increases.

	$M = 0$	$M = 1$	$M = 6$	$M = 9$
$w_0^\star$	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

New Cost Function

$$J = \sum_{i=1}^{N} (y_i - y_{i\,pred})^2 + \lambda \sum_{j=1}^{D} (w_j)^2$$

- Penalize complexity by simultaneously minimizing weight values.
- We call λ a **hyperparameter**
  - λ determines relative importance

Table 1.2 Table of the coefficients $\mathbf{w}^\star$ for $M = 9$ polynomials with various values for the regularization parameter λ. Note that $\ln \lambda = -\infty$ corresponds to a model with no regularization, i.e., to the graph at the bottom right in Figure 1.4. We see that, as the value of λ increases, the typical magnitude of the coefficients gets smaller.

	$\ln \lambda = -\infty$	$\ln \lambda = -18$	$\ln \lambda = 0$
$w_0^\star$	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

Cross-Validation

- Motivation: never determine a hyper-parameter based on training data
- **Hyper-Parameter**: a parameter of the algorithm that is not a model-parameter solved for in optimization.
  - Ex: λ weight regularization value vs. model weights (w)
- Solution: split dataset into three
  - **Training set**: to compute the model-parameters (w)
  - **Validation set**: to tune hyper-parameters (λ)
  - **Test set**: to compute the performance of the algorithm (MSE)

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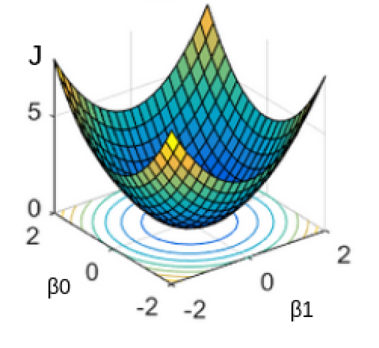
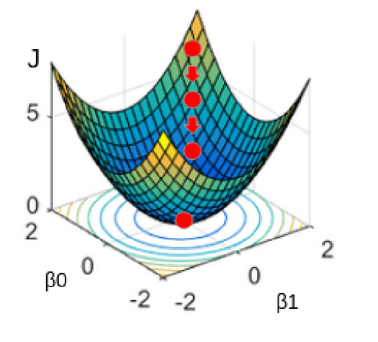
Motivation

- Cannot rely on closed form solutions
  - Computation efficiency: operations like inverting a matrix is not efficient
  - For more complex problems, like neural network, a closed form solution is not always available
- Need an optimization technique to find an optimal solution
  - Machine learning practitioners use gradient based methods

Understanding Optimization

- *Recap* $\hat{y} = w_0 + w_1 x$
- *Loss*, $J = \Sigma_{i=1}^{N}(y_i - \hat{y}_i)^2 \implies J = \Sigma_{i=1}^{N}(y_i - w_0 - w_1 x_i)^2$
- Want to find $w_0 and w_1$ that minimizes J





Gradient Descent Algorithm

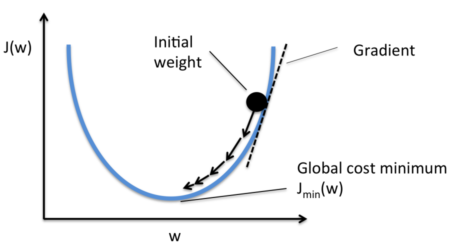
- Update Rule

  $Repeat\{$

  $$w_{new} = w - \alpha \frac{dJ}{dw}$$

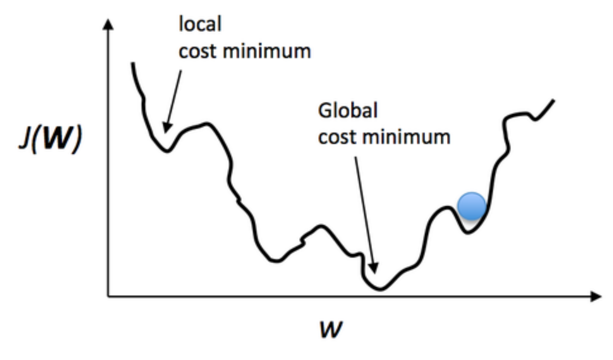
  $\}$

  α is the learning rate

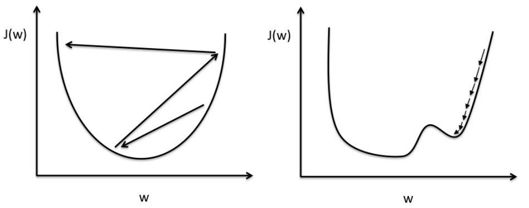


General Loss Function Contours

- Most loss function contours are not perfectly parabolic
- Our goal is to find a solution that is very close to global minimum by the right choice of hyper parameters

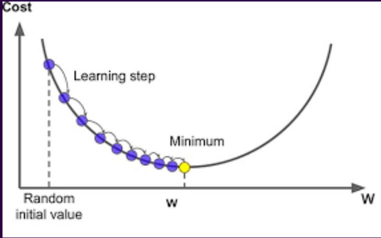


Understanding Learning Rate



Large learning rate: Overshooting.

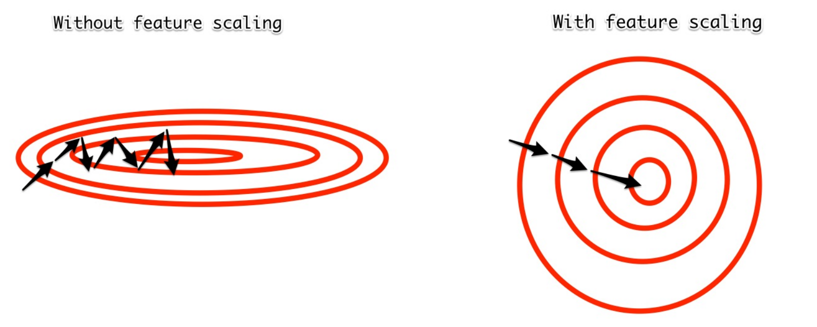
Small learning rate: Many iterations until convergence and trapping in local minima.



Correct learning rate

Importance of Feature Normalization

- Helps improve the performance of gradient based optimization



Some Gradient Based Algorithms

- Gradient descent
  - Stochastic gradient descent
  - Mini-batch gradient descent
- Gradient descent with momentum
- RMSprop
- Adam optimization algorithm

We have many frameworks that help us use these techniques in a single line of code (Eg: TensorFlow, PyTorch, Caffe, etc).

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Thank You!

- Next Class: Linear Classification