Overfitting and Regularization

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Plan

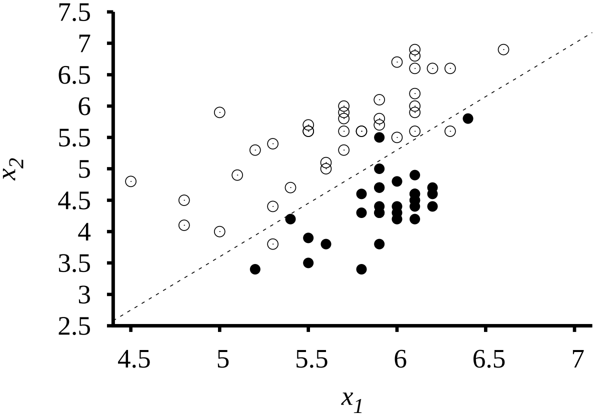
- What is Overfitting?
- How to Diagnose Overfitting
- Regularization

What is Overfitting?

Demo: polynomials

What is Overfitting?

Complex decision boundaries



What is Overfitting?

Overfitting is learning a model that fits the training data very well, but does not generalize well.

(Generalize = predict accurately for new examples.)

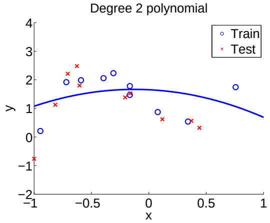
How to Diagnose Overfitting?

Exercise

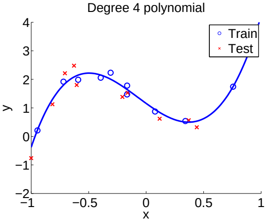
How to Diagnose Overfitting?

Exercise

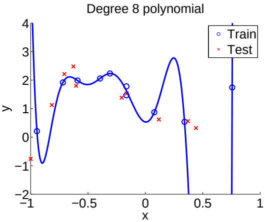
Reserve some data to test whether hypothesis generalizes well



(a) underfitting: average of our estimate differs from the true mean (high bias)



(b) good fit



(c) overfitting: variance of estimate is high

Train Data vs. Test Data: Regression

- Start with m training examples

$$(\mathbf{x}^{(1)}, y^{(1)}), (\mathbf{x}^{(2)}, y^{(2)}), \ldots, (\mathbf{x}^{(m)}, y^{(m)})$$

- Split into *train* and *test* sets (usually random)
- To fit the model, minimize cost on train data only

$$J_{\text{train}}(\boldsymbol{\theta}) = \sum_{i \in \text{train}} \text{cost}(h_{\boldsymbol{\theta}}(x^{(i)}), y^{(i)})$$

- To evaluate the fit, measure cost on test set

$$J_{\text{test}}(\boldsymbol{\theta}) = \sum_{i \in \text{test}} \text{cost}(h_{\boldsymbol{\theta}}(x^{(i)}), y^{(i)})$$

- *regression* $\text{cost}(h_{\boldsymbol{\theta}}(x^{(i)}), y^{(i)}) = (h_{\boldsymbol{\theta}}(x^{(i)}) - y^{(i)})^2$

Train Data vs. Test Data: Classification

- Start with m training examples $(\mathbf{x}^{(1)}, y^{(1)}), (\mathbf{x}^{(2)}, y^{(2)}), \ldots, (\mathbf{x}^{(m)}, y^{(m)})$
- Split into *train* and *test* sets (usually random)
- To fit the model, minimize cost on train data only. Cost depends on classifier
- To evaluate the fit, measure error on test set.

  $$\frac{1}{n_{\text{test}}} \sum_{i \in \text{test}} I(y_{est} \neq y^{(i)})$$

  where y_{est} is the label estimated by the classifier and $I(z)$ is the indicator of event z
- For logistic regression $y_{est} = 1 \quad \text{if} \quad h(x^{(i)}) \geq 1/2 \; y_{est} = 0 \quad \text{if} \quad h(x^{(i)}) < 1/2$

How to Diagnose Overfitting?

Example: cost function vs. degree of polynomial

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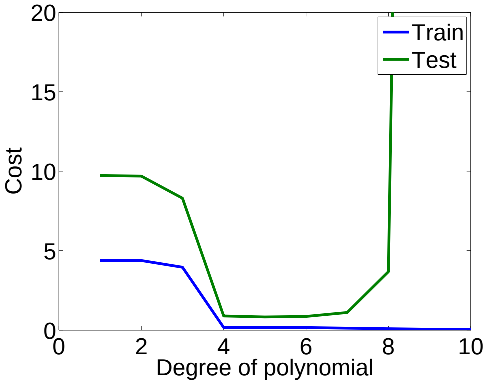


How to Diagnose Overfitting?

Example: feature expansion for book data

Width x_1	Thickness x_2	Height x_3	Weight y
8	1.8	10	4.4
8	0.9	9	2.7
	...		

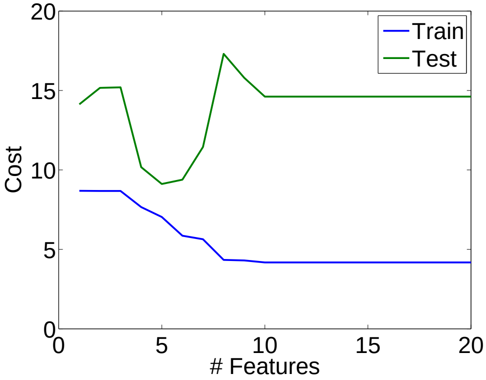
Suppose you add "quadratic" features:

$$(x_1, \ldots, x_n,) \mapsto (\underbrace{x_1, \ldots, x_n}_{\text{original features}}, \underbrace{x_1^2, x_1x_2, x_1x_3, \ldots, x_{n-1}x_n, x_n^2}_{\text{products of two original features}})$$

Do more features help?

How to Diagnose Overfitting?

Example: cost function vs. number of features in book data



Cost vs. Complexity

General phenomenon: training/test cost vs. model "complexity"

What is complexity?

- Deterministic classifiers that can represent more complex decision boundaries are said to have higher capacity than classifiers that can only represent simpler boundaries
- Probabilistic classifiers that can represent more complex sets of conditionals $P(Y|X)$ are said to have higher capacity than probabilistic classifiers that can only represent simpler sets of conditionals.
- the same statements can be formulated for regression: substitute hypothesis (regression function) to boundary

Bias and Variance (classifiers)

- **Bias:** A classifier is said to have low bias if the true decision boundary conditionals $P(Y|X)$ can be approximated closely by the model.
- **Variance:** A classifier is said to have low variance if the decision boundary or conditionals $P(Y|X)$ it constructs are stable with respect to small changes to the training data.
- **Bias-Variance Dilemma:** To achieve low generalization error, we need classifiers that are low-bias and low-variance, but this isn't always possible.
- **Bias-Variance and Capacity:** On complex data, models with low capacity have low variance, but high bias; while models with high capacity have low bias, but high variance.

Hyperparameters

- In order to control the capacity of a classifier or regressor, it needs to have capacity control parameters.
- Because capacity control parameters can not be chosen based on training error, they are often called hyperparameters.
- Question: What are the capacity control parameters for linear regression? Question: What are the capacity control parameters for logistic regression?
- we will cover other classifiers (KNN , neural networks, and trees) with specific hyperparameters.

What Makes a Model Complex?

- Polynomial: higher degree
- Book data: more features
- Linear functions ($h_{\boldsymbol{\theta}}(\mathbf{x}) = \boldsymbol{\theta}^T \mathbf{x}$): large weights (steep hyperplanes), therefore in logistic regression $P_{\boldsymbol{\theta}}(y|\mathbf{x})$ is also sensitive to large weights
- for KNN the complexity is the ratio: (# of neighbors) / (# of training points) $= k/N$

Large Weights

Example

Width x_1	Thickness x_2	Height x_3	Weight y
8	1.8	10	4.4
8	0.9	9	2.7

...

Which is more complex?

$$y = -3.94 + 0.18x_1 + .34x_2 + 0.4x_3$$

vs.

$$y = 2842 - 957x_1 + 300x_2 + 69712x_3$$

Solution to Overfitting: Regularization

Intuition: large weights $\rightarrow$ high complexity

Modify the cost function to penalize large weights = "regularization"

For squared error, we get:

$$J(\boldsymbol{\theta}) = \frac{\lambda}{2} \sum_{j=1}^{n} \theta_j^2 + \frac{1}{2} \sum_{i=1}^{m} (h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) - y^{(i)})^2$$

λ controls trade-off between model complexity and fit

Notes

Penalty / regularization term:

$$\frac{\lambda}{2}\sum_{j=1}^{n}\theta_j^2$$

- Best practice not to regularize θ_0. Why?
- Often written as $\frac{\lambda}{2}\|\boldsymbol{\theta}\|^2$ (Need to be careful to specify whether $\boldsymbol{\theta}$ include θ_0 or not!).

Discussion

Regularization is really important!!!

Why?

Learning with Regularization

Let's see how to solve two learning problems with regularized cost functions:

- Linear regression
- Logistic regression

Linear Regression: Normal Equations with Regularization

Find $\boldsymbol{\theta}$ to minimize regularized $J(\boldsymbol{\theta})$

$$\boldsymbol{\theta} = (X^T X + \lambda \hat{I})^{-1} X^T y$$

Linear Regression: Normal Equations with Regularization

Find $\boldsymbol{\theta}$ to minimize regularized $J(\boldsymbol{\theta})$

$$\boldsymbol{\theta} = (X^T X + \lambda \hat{I})^{-1} X^T y$$

$$\hat{I} = \begin{bmatrix} {\color{red}0} & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 1 \end{bmatrix}$$

(Identity matrix with top left entry replaced by 0)

Normal Equations Derivation: Vectorized Cost Function

$$
\begin{aligned}
J(\boldsymbol{\theta}) &= \frac{1}{2}\sum_{i=1}^{m}(h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) - y^{(i)})^2 + \frac{\lambda}{2}\sum_{j=1}^{n}\theta_j^2 \\
&= \frac{1}{2}(X\boldsymbol{\theta} - \mathbf{y})^T(X\boldsymbol{\theta} - \mathbf{y}) + \frac{\lambda}{2}\hat{\boldsymbol{\theta}}^T\hat{\boldsymbol{\theta}}.
\end{aligned}
$$

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\end{aligned}
$$

$$
\hat{\boldsymbol{\theta}} = \begin{bmatrix} 0 \\ \theta_1 \\ \theta_2 \\ \vdots \\ \theta_n \end{bmatrix} = \hat{I}\boldsymbol{\theta}
$$

Normal Equations Derivation

$$J(\boldsymbol{\theta}) = \frac{1}{2}(X\boldsymbol{\theta} - \mathbf{y})^T(X\boldsymbol{\theta} - \mathbf{y}) + \frac{\lambda}{2}\hat{\boldsymbol{\theta}}^T\hat{\boldsymbol{\theta}}$$

Set derivative to zero and solve (review on your own)

$$\begin{aligned}
0 = \frac{d}{d\boldsymbol{\theta}}J(\boldsymbol{\theta}) &= X^T(X\boldsymbol{\theta} - \mathbf{y}) + \lambda\hat{\boldsymbol{\theta}}^T \\
0 &= X^T(X\boldsymbol{\theta} - \mathbf{y}) + \lambda\hat{I}\boldsymbol{\theta} \\
X^TX\boldsymbol{\theta} + \lambda\hat{I}\boldsymbol{\theta} &= X^T\mathbf{y} \\
(X^TX + \lambda\hat{I})\boldsymbol{\theta} &= X^T\mathbf{y} \\
\boldsymbol{\theta} &= (X^TX + \lambda\hat{I})^{-1}X^T\mathbf{y}
\end{aligned}$$

Linear Regression: Regularized Gradient Descent

$$J(\boldsymbol{\theta}) = \frac{\lambda}{2}\sum_{j=1}^{n}\theta_j^2 + \frac{1}{2}\sum_{i=1}^{m}(h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) - y^{(i)})^2$$

Repeat until convergence

Linear Regression: Regularized Gradient Descent

$$J(\boldsymbol{\theta}) = \frac{\lambda}{2}\sum_{j=1}^{n}\theta_j^2 + \frac{1}{2}\sum_{i=1}^{m}(h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) - y^{(i)})^2$$

Repeat until convergence

$$\theta_0 \leftarrow \theta_0 - \alpha\sum_{i=1}^{m}(h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) - y^{(i)})$$

$$\theta_j \leftarrow \theta_j - \alpha\left(\lambda\theta_j + \sum_{i=1}^{m}(h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) - y^{(i)})x_j^{(i)}\right), \quad j = 1, \ldots, n$$

Linear Regression: Regularized Gradient Descent

Update rule for θ_j after simplification:

$$\theta_j \leftarrow \underbrace{\theta_j(1-\alpha\lambda)}_{\text{shrink}} - \underbrace{\alpha\sum_{i=1}^{m}(h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) - y^{(i)})x_j^{(i)}}_{\text{old gradient}}, \quad j = 1, \ldots, n$$

Interpretation: first "shrink" weights, then take gradient step for *unregularized* cost function

Logistic Regression: Regularized Gradient Descent

$$J(\boldsymbol{\theta}) = \frac{\lambda}{2}\sum_{j=1}^{n}\theta_j^2+\sum_{i=1}^{m}\left(-y^{(i)}\log h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)})-(1-y^{(i)})\log\left(1-h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)})\right)\right)$$

Algorithm:

Repeat until convergence

$$\theta_0 \leftarrow \theta_0 - \alpha\sum_{i=1}^{m}(h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) - y^{(i)})$$

$$\theta_j \leftarrow \theta_j(1-\alpha\lambda) - \alpha\sum_{i=1}^{m}(h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) - y^{(i)})x_j^{(i)}, \quad j = 1,\ldots,n$$

(Again: same as linear regression, but different $h_{\boldsymbol{\theta}}(\mathbf{x})$)

What You Need To Know

- Concept of overfitting
- Diagnosis: train/test sets
- Regularized cost function (penalize weights)
- Regularized gradient descent ("weight shrinking")
- See it work: polynomial regularization demo