Lecture 2
Machine Learning Review
CMSC 35246: Deep Learning

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  - Formal Setup for Supervised Learning

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  - Formal Setup for Supervised Learning
  - Empirical Risk, Risk, Generalization
  - Define and derive a linear model for Regression
  - Revise Regularization
  - Define and derive a linear model for Classification
  - (Time permitting) Start with Feedforward Networks

Note: Most slides in this presentation are adapted from, or taken (with permission) from slides by Professor Gregory Shakhnarovich for his TTIC 31020 course

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- Gregory Shakhnarovich: Make predictions and pay the price if the predictions are incorrect. Goal of learning is to reduce the price.
- How can you specify T, P and E?

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- Finite $\mathcal{Y} \implies$ Classification
- Continuous $\mathcal{Y} \implies$ Regression

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- Does it make sense to use learning here?

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- Let us begin with considering one of the simpled model classes: linear functions

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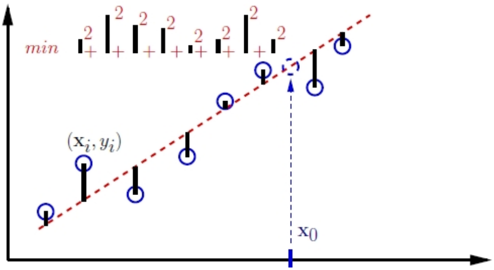

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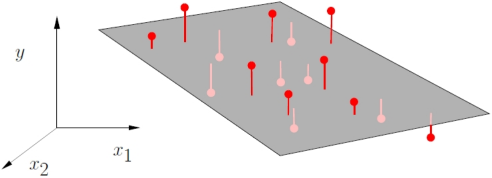
- *Hyperplane* in general d-D case



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- Standard choice for regression: $L(\hat{y}, y) = (\hat{y} - y)^2$

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- When does empirical loss minimization help us in doing that?

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- The **goal** is to minimize the *expected loss*, also known as **risk**:

$$R(\theta) = \mathbb{E}_{(\mathbf{x}_0, y_0) \sim p(\mathbf{x}, y)} [L(f(\mathbf{x}_0; \theta), y_0)]$$

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- In essence: Estimate $p(\mathbf{x}, y)$ by the *empirical distribution* of the data

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- How do we find $\theta^* = [\theta_0, \theta_1, \ldots, \theta_d]$?

Least Squares: Estimation

- Necessary condition to minimize L:
  $\frac{\partial L(\theta)}{\partial \theta_0}, \frac{\partial L(\theta)}{\partial \theta_1}, \ldots, \frac{\partial L(\theta)}{\partial \theta_d}$

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- Let us switch to vector notation for convenience

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- What next? Take derivative of $L(\theta)$ and set it to zero

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$$\frac{\partial L(\theta)}{\partial \theta} = \frac{1}{N}\frac{\partial}{\partial \theta}[\mathbf{y}^T\mathbf{y} - \theta^T X^T \mathbf{y} - \mathbf{y}^T X\theta + \theta^T X^T X\theta]$$

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&= \frac{1}{N}[0 - X^T\mathbf{y} - (\mathbf{y}^T X)^T + 2X^T X\theta] \\
&= -\frac{2}{N}(X^T\mathbf{y} - X^T X\theta)
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- Prediction: $\hat{y} = {\theta^*}^T \begin{bmatrix} 1 \\ \mathbf{x}_0 \end{bmatrix} = \mathbf{y}^T {X^\dagger}^T \begin{bmatrix} 1 \\ \mathbf{x}_0 \end{bmatrix}$

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- Back to familiar linear regression!

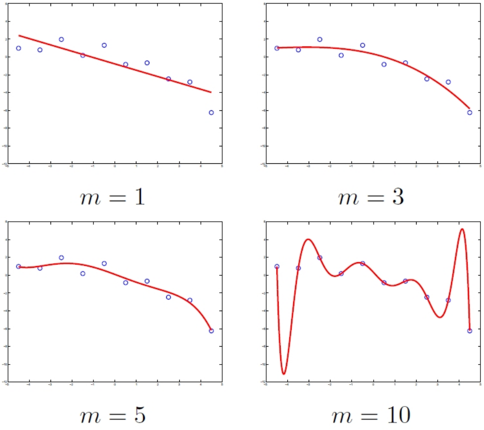
Polynomial Regression

- Transform $\mathbf{x} \to \phi(\mathbf{x})$
- For example consider 1D for simplicity:
- $f(x;\theta) = \theta_0 + \theta_1 x + \theta_2 x^2 + \cdots + \theta_m x^m$
- Above $\phi(\mathbf{x}) = [1, x, x^2, \ldots, x^m]$
- No longer linear in x, but still linear in θ!
- Back to familiar linear regression!
- Generalized Linear models:
  $f(\mathbf{x};\theta) = \theta_0 + \theta_1 \phi_1(\mathbf{x}) + \theta_2 \phi_2(\mathbf{x}) + \cdots + \theta_m \phi_m(\mathbf{x})$

A Short Primer on Regularization

Model Complexity and Overfitting

Consider data drawn from a 3rd order model:



Avoiding Overfitting: Cross Validation

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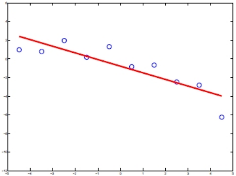
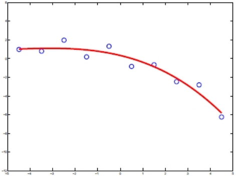
- k-fold cross validation. Extreme case: *leave one out* cross validation
- What is the source of overfitting?

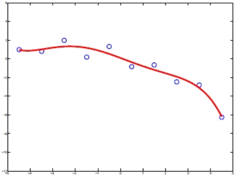
Cross Validation Example



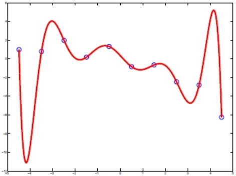
$m = 1 : L = 1.4, \hat{L}_{\text{CV}} = 2.6$



$m = 3 : L = 0.4, \hat{L}_{\text{CV}} = 1.3$



$m = 5 : L = 0.3, \hat{L}_{\text{CV}} = 2.7$



$m = 10 : L = 0, \hat{L}_{\text{CV}} = 4 \times 10^4$

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- Complex model $\implies$ more sensitive to data $\implies$ more likely to overfit
- Simple model $\implies$ more rigid $\implies$ more likely to underfit
- Find the model with the right "bias-variance" balance

Penalizing Model Complexity

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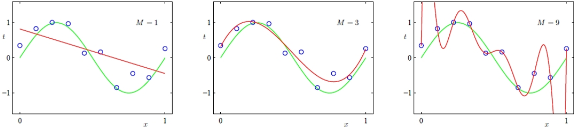
- Since the parameters might not be independent, we would like to penalize the complexity in a more sophisticated way

Problems



	$m = 0$	$m = 1$	$m = 3$	$m = 9$
w_0^*	0.19	0.82	0.31	0.35
w_1^*		-1.27	7.99	232.37
w_2^*			-25.43	-5321.83
w_3^*			17.37	48568.31
w_4^*				-231639.30
w_5^*				640042.26
w_6^*				-1061800.52
w_7^*				1042400.18
w_8^*				-557682.99
w_9^*				125201.43

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- Regularization is basically a way to implement Occam's Razor

Shrinkage Regression

- Shrinkage methods: We penalize the L2 norm

$$\theta^*_{ridge} = \arg\min_{\theta} \sum_{i=1}^{N} L(f(x_i;\theta), y_i) + \lambda \sum_{j=1}^{m} (\theta_j)^2$$

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- This is called Ridge regression: Closed form solution for squared loss $\hat{\theta}_{ridge} = (\lambda I + X^T X)^{-1} X^T \mathbf{y}$!

LASSO Regression

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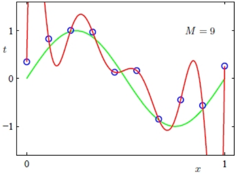
- Still convex, but no longer smooth. Solve using Lagrange multipliers!

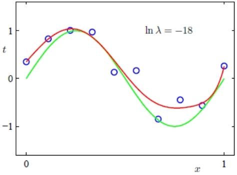
Effect of λ

$\lambda = 0$



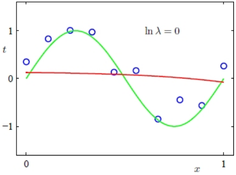
$\|\mathbf{w}^*\|^2 > 10^{12}$

$\lambda = e^{-18}$



$\|\mathbf{w}^*\|^2 \approx 21595$

$\lambda = 1$



$\|\mathbf{w}^*\|^2 \approx 0.027$

The Principle of Maximum Likelihood

- Suppose we have N data points $X = \{x_1, x_2, \ldots, x_N\}$ (or $\{(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)\}$)

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- If $P1$ is very small, it means that such a dataset is very unlikely to occur, thus perhaps θ_1 was not a good guess

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- The procedure:
  - Write the log likelihood function: $\log p(x;\theta)$ (we'll see later why log)
  - Want to maximize - So differentiate $\log p(x;\theta)$ w.r.t θ and set to zero
  - Solve for θ that satisfies the equation. This is θ_{ML}

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  - "Optimal" for large data sizes
- Disadvantages of ML Estimation
  - Not optimal for small sample sizes
  - Can be computationally challenging (numerical methods)

Linear Classifiers

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- We need to find the (direction) θ and (the location) θ_0
- Want to minimize the expected 0/1 loss for classifier $h : \mathcal{X} \to \mathcal{Y}$

$$L(h(\mathbf{x}), y) = \begin{cases} 0, & \text{if } h(\mathbf{x}) = y \\ 1, & \text{if } h(\mathbf{x}) \neq y \end{cases}$$

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$$

- Clearly, it suffices to minimize the conditional risk:

$$
R(h|\mathbf{x}) = \sum_{c=1}^{C} L(h(\mathbf{x}), c) p(y = c|\mathbf{x})
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Conditional Risk of a Classifier

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\end{aligned}$$

- To minimize the conditional risk given $\mathbf{x}$, the classifier must decide

$$h(\mathbf{x}) = \arg\max_{c} p(y = c|\mathbf{x})$$

Log Odds Ratio

- Optimal rule $h(\mathbf{x}) = \arg\max_c p(y = c|\mathbf{x})$ is equivalent to:

$$h(\mathbf{x}) = c^* \quad \Longleftrightarrow \quad \frac{p(y = c^*|\mathbf{x})}{p(y = c|\mathbf{x})} \geq 1 \forall c$$

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$$\iff \log \frac{p(y = c^*|\mathbf{x})}{p(y = c|\mathbf{x})} \geq 0 \forall c$$

- For the binary case:

$$h(\mathbf{x}) = 1 \iff \frac{p(y = 1|\mathbf{x})}{p(y = 0|\mathbf{x})} \geq 0$$

The Logistic Model

- The unknown decision boundary can be modeled directly:

$$\frac{p(y=1|\mathbf{x})}{p(y=0|\mathbf{x})} = \theta_0 + \theta^T \mathbf{x} = 0$$

- Since $p(y=1|\mathbf{x}) = 1 - p(y=0|\mathbf{x})$, exponentiating, we have:

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$$\begin{aligned} \frac{p(y=1|\mathbf{x})}{1-p(y=1|\mathbf{x})} &= \exp(\theta_0 + \theta^T\mathbf{x}) = 1 \\ \implies \frac{1}{p(y=1|\mathbf{x})} &= 1 + \exp(-\theta_0 - \theta^T\mathbf{x}) = 2 \end{aligned}$$

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$$\begin{aligned} \frac{p(y=1|\mathbf{x})}{1-p(y=1|\mathbf{x})} &= \exp(\theta_0 + \theta^T\mathbf{x}) = 1 \\ \implies \frac{1}{p(y=1|\mathbf{x})} &= 1 + \exp(-\theta_0 - \theta^T\mathbf{x}) = 2 \\ \implies p(y=1|\mathbf{x}) &= \frac{1}{1+\exp(-\theta_0 - \theta^T\mathbf{x})} = \frac{1}{2} \end{aligned}$$

The Logistic Function

$$p(y = 1|\mathbf{x}) = \frac{1}{1 + \exp(-\theta_0 - \theta^T \mathbf{x})}$$

- Properties?

The Logistic Function

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- Properties?
- With linear logistic model we get a linear decision boundary

Likelihood under the Logistic Model

$$p(y_i|\mathbf{x};\theta) = \begin{cases} \sigma(\theta_0 + \theta^T \mathbf{x}_i) \text{ if } y_i = 1 \\ 1 - \sigma(\theta_0 + \theta^T \mathbf{x}_i) \text{ if } y_i = 0 \end{cases}$$

- We can rewrite this as:

Likelihood under the Logistic Model

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- The log-likelihood of θ:

$$\log p(Y|X;\theta) = \sum_{i=1}^{N} \log p(y_i|\mathbf{x}_i;\theta)$$

$$= \sum_{i=1}^{N} y_i \log \sigma(\theta_0 + \theta^T \mathbf{x}_i) + (1 - y_i) \log(1 - \sigma(\theta_0 + \theta^T \mathbf{x}_i))$$

The Maximum Likelihood Solution

$$\log p(Y|X;\theta) = \sum_{i=1}^{N} y_i \log \sigma(\theta_0 + \theta^T \mathbf{x}_i) + (1 - y_i) \log(1 - \sigma(\theta_0 + \theta^T \mathbf{x}_i))$$

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- Setting derivatives to zero:

$$\frac{\partial \log p(Y|X;\theta)}{\partial \theta_0} = \sum_{i=1}^{N} (y_i - \sigma(\theta_0 + \theta^T \mathbf{x}_i)) = 0$$

$$\frac{\partial \log p(Y|X;\theta)}{\partial \theta_j} = \sum_{i=1}^{N} (y_i - \sigma(\theta_0 + \theta^T \mathbf{x}_i)) \mathbf{x}_{i,j} = 0$$

The Maximum Likelihood Solution

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$$\frac{\partial \log p(Y|X;\theta)}{\partial \theta_0} = \sum_{i=1}^{N}(y_i - \sigma(\theta_0 + \theta^T \mathbf{x}_i)) = 0$$

$$\frac{\partial \log p(Y|X;\theta)}{\partial \theta_j} = \sum_{i=1}^{N}(y_i - \sigma(\theta_0 + \theta^T \mathbf{x}_i))\mathbf{x}_{i,j} = 0$$

- Can treat $y_i - p(y_i|\mathbf{x}_i) = y_i - \sigma(\theta_0 + \theta^T \mathbf{x}_i)$ as the prediction error

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- But $\log p(Y|X; \mathbf{x})$ is jointly concave in all components of θ
- Or, equivalently, the error is convex
- Gradient Descent/ascent (descent on $-\log p(y|\mathbf{x}; \theta)$, log loss)

Next time

- Feedforward Networks

Next time

- Feedforward Networks
- Backpropagation