CS229 Section: Midterm Review

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Content from past CS229 teams and ML Cheatsheets from Shervine & Afshine Amidi

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Outline

Supervised Learning: Recap

- **Given**: a set of data points (or attributes) $\{x^{(1)}, x^{(2)}, ..., x^{(m)}\}$ and their associated labels $\{y^{(1)}, y^{(2)}, ..., y^{(m)}\}$
- **Dimensions**: x usually d-dimensional $\in \mathbb{R}^d$, y typically scalar
- **Goal**: build a model that predicts y from x for unseen x

Supervised Learning: Recap

Types of predictions

- y is continuous, real-valued: Regression
- Example: Linear regression
- y is discrete classes: Classification
- Example: Logistic regression, SVM, Naive Bayes

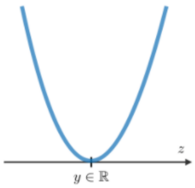
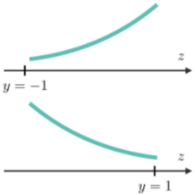
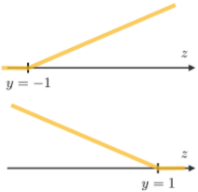
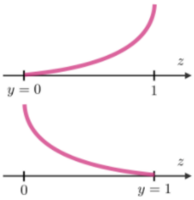
Supervised Learning: Recap

Types of models

- **Discriminative**
- Directly estimate $p(y|x)$ by learning decision boundary
- Example: Logistic regression, SVM
- **Generative**
- Estimate $p(x|y)$ and infer $p(y|x)$ from it
- Can generate new samples
- Example: GDA, Naive Bayes

Notations and Concepts

- **Hypothesis**: Denoted by h_θ. Given an input $x^{(i)}$, predicted output is $h_\theta(x^{(i)})$
- **Loss Function**: Function $L(z, y) : \mathbb{R} \times \mathbb{Y} \mapsto \mathbb{R}$ computes how different the predicted value z and the ground truth label are

Least squared error	Logistic loss	Hinge loss	Cross-entropy
$\frac{1}{2}(y-z)^2$	$\log(1+\exp(-yz))$	$\max(0, 1-yz)$	$-\left[y\log(z)+(1-y)\log(1-z)\right]$
			
Linear regression	Logistic regression	SVM	Neural Network

Notations and Concepts

- **Cost function**: Function J taking model parameters θ as input and giving a score to reflect how badly the model performs. Sum of loss over all predictions

$$J(\theta) = \sum_{i=1}^{m} L(h_\theta(x^{(i)}), y^{(i)})$$

- **Likelihood**: Maximizing likelihood $L(\theta)$ corresponds to finding the "best" distribution of data given a set of parameters. We usually find the log likelihood $\ell(\theta) = \log L(\theta)$ and maximize it.

$$\theta^* = \text{argmax}_\theta \; \ell(\theta)$$

Outline

Optimization: Gradient Descent

- To find the optimal θ that minimizes the cost function $J(\theta)$, we can use gradient descent with a learning rate $\alpha \in \mathbb{R}$

$$\theta^{(t+1)} = \theta^{(t)} - \alpha \nabla_\theta J(\theta^{(t)})$$

Stochastic Gradient Descent

- In Stochastic gradient descent (SGD), we update the parameter based on **each** training example, whereas in batch gradient descent we update based on a batch of training examples.

Optimization: Newton's method

- Numerical method to estimate θ such that $J'(\theta)$ is 0
- We update θ as follows:

$$\theta^{(t+1)} = \theta^{(t)} - \frac{J'(\theta^{(t)})}{J''(\theta^{(t)})}$$

- For the multi-dimensional case:

$$\theta^{(t+1)} = \theta^{(t)} - \left[\nabla^2_\theta J(\theta^{(t)})\right]^{-1} \nabla_\theta J(\theta^{(t)})$$

Recap: Gradients and Hessians

- Gradient and Hessian (differentiable function $f : \mathbb{R}^d \mapsto \mathbb{R}$)

$$\nabla_x f = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \cdots & \frac{\partial f}{\partial x_d} \end{bmatrix}^T \in \mathbb{R}^d$$

$$\nabla_x^2 f = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_d} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_d \partial x_1} & \cdots & \frac{\partial^2 f}{\partial x_d^2} \end{bmatrix} \in \mathbb{R}^{d \times d}$$

Outline

Linear Regression

- Model: $h_\theta(x) = \theta^T x$
- Training data: $\left\{\left(x^{(i)}, y^{(i)}\right)\right\}_{i=1}^{n}$, $x^{(i)} \in \mathbb{R}^d$
- Loss: $J(\theta) = \frac{1}{2}\sum_{i=1}^{n}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2$
- Update rule:

$$\theta^{(t+1)} = \theta^{(t)} - \alpha \sum_{i=1}^{n}\left(h_\theta(x^{(i)}) - y^{(i)}\right) x^{(i)}$$

Stochastic Gradient Descent (SGD)

Pick one data point $x^{(i)}$ and then update:

$$\theta^{(t+1)} = \theta^{(t)} - \alpha\left(h_\theta(x^{(i)}) - y^{(i)}\right) x^{(i)}$$

Solving Least Squares: Closed Form

- Loss in matrix form: $J(\theta) = \frac{1}{2}\|X\theta - y\|_2^2$, where $X \in \mathbb{R}^{n\times d}$, $y \in \mathbb{R}^n$
- Normal Equation (set gradient to 0):

$$X^T(X\theta^\star - y) = 0$$

- Closed form solution:

$$\theta^\star = \left(X^T X\right)^{-1} X^T y$$

Connection to Newton's Method

$$\theta^\star = \left[\nabla_\theta^2 J\right]^{-1} \nabla_\theta J, \quad \text{when the gradient is evaluated at } \theta = 0$$

Newton's method is exact with only one step iteration if we started from $\theta^{(0)} = 0$.

Outline

Logistic Regression

A binary classification model and $y^{(i)} \in \{0, 1\}$

- Assumed model:

$$p(y \mid x; \theta) = \begin{cases} g_\theta(x) & \text{if } y = 1 \\ 1 - g_\theta(x) & \text{if } y = 0 \end{cases}, \quad \text{where } g_\theta(x) = \frac{1}{1 + e^{-\theta^T x}}$$

- **Log-likelihood function:**

$$\begin{aligned} \ell(\theta) &= \sum_{i=1}^{n} \log p(y^{(i)} \mid x^{(i)}; \theta) \\ &= \sum_{i=1}^{n} \left[y^{(i)} \log g_\theta(x^{(i)}) + (1 - y^{(i)}) \log(1 - g_\theta(x^{(i)})) \right] \end{aligned}$$

- Find parameters through **maximizing log-likelihood**, $\text{argmax}_\theta\, \ell(\theta)$ (in Pset1).

Sigmoid and Softmax

- **Sigmoid**: The sigmoid function (also known as logistic function) is given by:

$$g(z) = \frac{1}{1 + e^{-z}}$$

- **Softmax regression**: Also called as multi-class logistic regression, it generalizes logistic regression to multi-class cases

$$p(y = k | x; \theta) = \frac{\exp \theta_k^T x}{\sum_j \exp \theta_j^T x}$$

Outline

Exponential Family

Definition

Probability distribution with **natural or canonical parameter** η, **sufficient statistic** $T(y)$ and a **log-partition** function $a(\eta)$ whose density (or mass function) can be written as

$$p(y; \eta) = b(y) \exp\left(\eta^T T(y) - a(\eta)\right)$$

- Oftentimes, $T(y) = y$
- In many cases, $\exp(-a(\eta))$ can be considered as a normalization term that makes the probabilities sum to one

Common Exponential Distributions

Bernoulli distribution:

$$p\left(y;\phi\right)=\phi^{y}\left(1-\phi\right)^{1-y}=\exp\left(\left(\log\left(\frac{\phi}{1-\phi}\right)\right)y+\log\left(1-\phi\right)\right)$$

$$\implies b\left(y\right)=1,\quad T\left(y\right)=y,\quad \eta=\log\left(\frac{\phi}{1-\phi}\right),\quad a\left(\eta\right)=\log\left(1+e^{\eta}\right)$$

More examples:

Categorical distribution, Poisson distribution, Multivariate normal distribution, etc

Common Exponential Distributions

Distribution	η	$T(y)$	$a(\eta)$	$b(y)$
Bernoulli	$\log\left(\frac{\phi}{1-\phi}\right)$	y	$\log(1+\exp(\eta))$	1
Gaussian	μ	y	$\frac{\eta^2}{2}$	$\frac{1}{\sqrt{2\pi}}\exp\left(-\frac{y^2}{2}\right)$
Poisson	$\log(\lambda)$	y	e^{η}	$\dfrac{1}{y!}$
Geometric	$\log(1-\phi)$	y	$\log\left(\frac{e^{\eta}}{1-e^{\eta}}\right)$	1

Properties

- $\mathbb{E}\left[T\left(Y\right);\eta\right]=\nabla_{\eta}a\left(\eta\right)$
- $\mathrm{Var}\left(T\left(Y\right);\eta\right)=\nabla_{\eta}^{2}a\left(\eta\right)$

Non-exponential Family Distribution

Uniform distribution over interval $[a, b]$:

$$p\left(y;a,b\right)=\frac{1}{b-a}\cdot 1_{\{a\leq y\leq b\}}$$

Reason: $b\left(y\right)$ cannot depend on parameter η.

Outline

Generalized Linear Model (GLM)

Generalized Linear Models (GLM) aim at predicting a random variable y as a function of x and rely on the following components:

Assumed model:

$$p\left(y \mid x;\theta\right) \sim \mathrm{ExponentialFamily}\left(\eta\right)$$

- $\eta = \theta^T x$
- Predictor: $h\left(x\right) = \mathbb{E}\left[T\left(Y\right);\eta\right] = \nabla_\eta a\left(\eta\right)$.
- Fitting through maximum likelihood:

$$\max_\theta \ell\left(\theta\right) = \max_\theta \sum_{i=1}^{n} p(y^{(i)} \mid x^{(i)};\eta)$$

Generalized Linear Model (GLM)

Examples

- GLM under Bernoulli distribution: Logistic regression
- GLM under Poisson distribution: Poisson regression (in Pset1)
- GLM under Normal distribution: Linear regression
- GLM under Categorical distribution: Softmax regression

Outline

Gaussian Discriminant Analysis (GDA)

Generative Algorithm for Classification

- Learn $p(x \mid y)$ and $p(y)$
- Classify through Bayes rule: $\text{argmax}_y\, p(y \mid x) = \text{argmax}_y\, p(x \mid y)\, p(y)$

GDA Formulation

- Assume $p(x \mid y) \sim \mathcal{N}(\mu_y, \Sigma)$ for some $\mu_y \in \mathbb{R}^d$ and $\Sigma \in \mathbb{R}^{d \times d}$
- Estimate μ_y, Σ and $p(y)$ through maximum likelihood, which is

$$\text{argmax} \sum_{i=1}^{n} \left[\log p(x^{(i)} \mid y^{(i)}) + \log p(y^{(i)}) \right]$$

$$p(y) = \frac{\sum_{i=1}^{n} 1_{\{y^{(i)}=y\}}}{n}, \mu_y = \frac{\sum_{i=1}^{n} 1_{\{y^{(i)}=y\}} x^{(i)}}{\sum_{i=1}^{n} 1_{\{y^{(i)}=y\}}}, \Sigma = \frac{1}{n} \sum_{i=1}^{n} (x^{(i)} - \mu_{y^{(i)}})(x^{(i)} - \mu_{y^{(i)}})^T$$

Naive Bayes

Formulation

- Assume $p(x \mid y) = \prod_{j=1}^{d} p(x_j \mid y)$
- Estimate $p(x_j \mid y)$ and $p(y)$ through maximum likelihood, which gives

$$p(x_j \mid y) = \frac{\sum_{i=1}^{n} 1_{\left\{x_j^{(i)}=x_j, y^{(i)}=y\right\}}}{\sum_{i=1}^{n} 1_{\left\{y^{(i)}=y\right\}}}, \quad p(y) = \frac{\sum_{i=1}^{n} 1_{\left\{y^{(i)}=y\right\}}}{n}$$

Laplace Smoothing

Assume x_j takes value in $\{1, 2, \ldots, k\}$, the corresponding modified estimator is

$$p(x_j \mid y) = \frac{1 + \sum_{i=1}^{n} 1_{\left\{x_j^{(i)}=x_j, y^{(i)}=y\right\}}}{k + \sum_{i=1}^{n} 1_{\left\{y^{(i)}=y\right\}}}$$

Outline

Kernel

- Core idea: reparametrize parameter θ as a linear combination of featurized vectors
- Feature map: $\phi : \mathbb{R}^d \mapsto \mathbb{R}^p$
- Fitting linear model with gradient descent gives us

$$\theta = \sum_{i=1}^{n} \beta_i \phi(x^{(i)})$$

- Predict a new example z:

$$h_\theta(z) = \sum_{i=1}^{n} \beta_i \phi(x^{(i)})^T \phi(z) = \sum_{i=1}^{n} \beta_i K(x^{(i)}, z)$$

- It brings nonlinearity without much sacrifice in efficiency as long as $K(\cdot, \cdot)$ can be computed efficiently

Kernel

- Given a feature mapping ϕ, we define the kernel K as follows:

$$K(x, z) = \phi(x)^T \phi(z)$$

- "Kernel trick" to compute the cost function using the kernel because we actually don't need to know the explicit mapping ϕ, which is often very complicated
- Instead, only the values $K(x, z)$ are needed
- Suppose $K(x^{(i)}, x^{(j)}) = \mathrm{K}_{ij}$
- If $\mathrm{K} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$ then is K a valid kernel function?
- If $\mathrm{K} = \begin{bmatrix} 3 & 5 \\ 5 & 3 \end{bmatrix}$ then is K a valid kernel function?

Kernel

Theorem

$K(x, z)$ is a valid kernel if and only if for any set of $\{x^{(1)}, \dots, x^{(n)}\}$, its Gram matrix, defined as

$$G = \begin{bmatrix} K(x^{(1)}, x^{(1)}) & \dots & K(x^{(1)}, x^{(n)}) \\ \vdots & \ddots & \vdots \\ K(x^{(n)}, x^{(1)}) & \dots & K(x^{(n)}, x^{(n)}) \end{bmatrix} \in \mathbb{R}^{n \times n}$$

is positive semi-definite.

Examples

- Polynomial kernels: $K(x, z) = (x^T z + c)^d$, $\forall\ c \geq 0$ and $d \in \mathbb{N}$
- Gaussian kernels: $K(x, z) = \exp\left(-\frac{\|x-z\|_2^2}{2\sigma^2}\right)$, $\forall\ \sigma^2 > 0$

Support Vector Machine (SVM)

Goal: find the line that maximizes the minimum distance to the line
The optimal margin classifier h with $(y \in \{-1, 1\})$ is such that:

$$h(x) = \mathrm{sign}(w^T x - b)$$

$$\begin{array}{ll} \min_{\{w,b\}} & \frac{1}{2}\|w\|_2^2 \\ \text{subject to} & y^{(i)}(w^T x^{(i)} + b) \geq 1, \quad \forall\, i \in \{1, \dots, n\} \end{array}$$

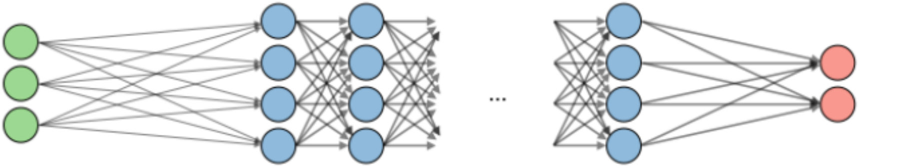
Properties

- The optimal solution has the form $w^\star = \sum_{i=1}^n \alpha_i y^{(i)} x^{(i)}$ and thus can be kernelized.
- The soft-SVM can be treated as a minimization over hinge loss plus ℓ_2 regularization:

$$\min_{\{w,b\}} \sum_{i=1}^{n} \max\left\{0, 1 - y^{(i)}(w^T x^{(i)} + b)\right\} + \lambda \|w\|_2^2$$

Outline

Neural Networks



By noting i the i^{th} layer of the network and j the j^{th} hidden unit of the layer, we have:

$$\boxed{z_j^{[i]} = {w_j^{[i]}}^T x + b_j^{[i]}}$$

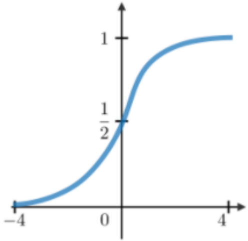
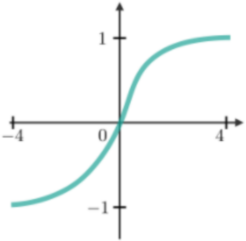
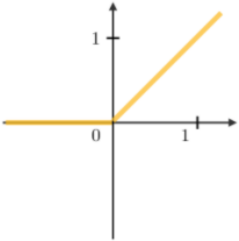
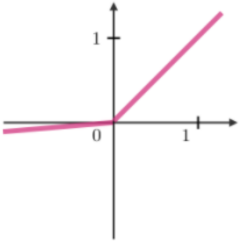
where we note w, b, z the weight, bias and output respectively.

Neural Networks

Multi-layer Fully-connected Neural Networks (with Activation Function f)

$$
\begin{aligned}
a^{[1]} &= f\left(W^{[1]}x + b^{[1]}\right) \\
a^{[2]} &= f\left(W^{[2]}a^{[1]} + b^{[2]}\right) \\
&\cdots \\
a^{[r-1]} &= f\left(W^{[r-1]}a^{[r-2]} + b^{[r-1]}\right) \\
h_\theta(x) = a^{[r]} &= W^{[r]}a^{[r-1]} + b^{[r]}
\end{aligned}
$$

Activation Functions

Sigmoid	Tanh	ReLU	Leaky ReLU
$g(z) = \frac{1}{1+e^{-z}}$	$g(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$	$g(z) = \max(0, z)$	$g(z) = \max(\epsilon z, z)$ with $\epsilon \ll 1$
			

Updating Weights

- Step 1: Take a batch of training data
- Step 2: Perform forward propagation to obtain the corresponding loss
- Step 3: Backpropagate the loss to get the gradients
- Step 4: Use the gradients to update the weights of the network

Backpropagation

Let J be the loss function and $z^{[k]} = W^{[k]}a^{[k-1]} + b^{[k]}$. By chain rule, we have

$$\frac{\partial J}{\partial W_{ij}^{[r]}} = \frac{\partial J}{\partial z_i^{[r]}} \frac{\partial z_i^{[r]}}{\partial W_{ij}^{[r]}} = \frac{\partial J}{\partial z_i^{[r]}} a_j^{[r-1]} \implies \frac{\partial J}{\partial W^{[r]}} = \frac{\partial J}{\partial z^{[r]}} a^{[r-1]T}, \quad \frac{\partial J}{\partial b^{[r]}} = \frac{\partial J}{\partial z^{[r]}}$$

$$\frac{\partial J}{\partial a_i^{[r-1]}} = \sum_{j=1}^{d_r} \frac{\partial J}{\partial z_j^{[r]}} \frac{\partial z_j^{[r]}}{\partial a_i^{[r-1]}} = \sum_{j=1}^{d_r} \frac{\partial J}{\partial z_j^{[r]}} W_{ji}^{[r]} \implies \frac{\partial J}{\partial a^{[r-1]}} = W^{[r]T} \frac{\partial J}{\partial z^{[r]}}$$

$$\frac{\partial J}{\partial z^{[r]}} := \delta^{[r]} \implies \frac{\partial J}{\partial z^{[r-1]}} = \left(W^{[r]T}\delta^{[r]}\right) \odot f'\left(z^{[r-1]}\right) := \delta^{[r-1]}$$

$$\implies \frac{\partial J}{\partial W^{[r-1]}} = \delta^{[r-1]} a^{[r-2]T}, \quad \frac{\partial J}{\partial b^{[r-1]}} = \delta^{[r-1]}$$

Continue for layers $r-2, \ldots, 1$.

Tips

- Practice, practice, practice
- For proofs, give reasoning and show how you go from one step to the next
- Prepare a cheat sheet – easy to run out of time in open book exams
- Pay attention to notation and indices. "Silly mistakes" can completely change the meaning of your reasoning
- Think in vector terms!

All the best :)