

Prepared for submission to JHEP

# ML Cheatsheet

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Abstract: Everything I know about machine learning.

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## 1 Conventions

### Math Notation

- $x \in \{0, 1\}^r$  :  $x$  is a vector of form *e.g.*  $(0, 1, 1, 0, \dots, 1, 0)$  of length  $r$ .
- $\sim$  : random variable drawn from a distribution
- $\propto$  : “proportional to”
- $\mathbf{1}(\cdot)$  : indicator function — 1 when arg is true, 0 when arg is false.
- Boldface capital letters are matrices, *e.g.*  $\mathbf{A} = \mathbf{U}\mathbf{W}\mathbf{V}^T$
- $\log$  is base  $e$  by default  $\rightarrow$  entropy in nats.

### Ng CS229 / DeepLearning.ai

- $m$  : number of training examples in the dataset
- $n$  : dimension of training examples
- $x^{(i)} \in \mathbb{R}^n$  :  $i^{th}$  training example (*column* vector),  $1 \leq i \leq m$
- $y^{(i)}$  :  $i^{th}$  output (*column* vector),  $1 \leq i \leq m$
- $x_j$  :  $j^{th}$  component of a training example,  $1 \leq j \leq n$ .
- $\mathbf{X} \in \mathbb{R}^{n \times m}$  : (input/design) matrix (training examples are *column* vectors)<sup>1</sup>
- $\mathbf{X} \in \mathbb{R}^{m \times n}$  : (input/design) matrix (training examples are *row* vectors)

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<sup>1</sup>Note our non-conventional definition of the design matrix  $\mathbf{X}$ . The more conventional version is denoted  $\mathbf{X}$ .

## 2 Linear Regression

### 2.1 Basics

- Hypothesis  $h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \dots = \sum_{j=0}^n \theta_j x_j \equiv \theta^T x$ , where  $x_0 = 1$ .
- Cost function

$$J(\theta) = \frac{1}{2} \sum_{i=1}^m (h_\theta(x^{(i)}) - y^{(i)})^2 \quad (2.1)$$

- Analytically solve via normal equations, where  $\mathbf{X}$  is the augmented  $(n+1) \times m$  design matrix

$$\vec{\theta} = (\mathbf{X}\mathbf{X}^T)^{-1} \mathbf{X} \vec{y} \quad (2.2)$$

where  $\vec{\theta}$  and  $\vec{y}$  are column vectors of the  $n+1$  weights and  $m$  outputs, respectively.

## 3 Logistic Regression

### 3.1 2 classes

With 2 labels  $y \in \{0, 1\}$  and  $m$  training examples  $x^{(i)}$ ,  $1 \leq i \leq m$ , we have

$$h_\theta(x) = \frac{1}{1 + e^{-\theta^T x}} \quad (3.1)$$

$$p(y|x; \theta) = (h_\theta(x))^y (1 - h_\theta(x))^{1-y} \quad (3.2)$$

$$L(\theta) = \prod_{i=1}^m (h_\theta(x^{(i)}))^{y^{(i)}} (1 - h_\theta(x^{(i)}))^{1-y^{(i)}} \quad (3.3)$$

$$l(\theta) = \log L(\theta) = \sum_{i=1}^m y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log(1 - h_\theta(x^{(i)})) \quad (3.4)$$

with deriv

$$\frac{\partial}{\partial \theta_j} l(\theta) = x_j^T (y - h_\theta(x)) \quad (3.5)$$

We can't minimize the log-likelihood analytically, so we must use numerical optimization.

The log-likelihood is just the cross entropy

$$H(p, q) = - \sum_i p_i \log q_i \quad (3.6)$$

with  $p$  the actual outputs, and  $q$  the hypothesis  $h_\theta(x)$

### 3.2 2+ classes

**One-versus-all:** For  $k$  classes, do  $k$  normal log regs. Each has two classes: the target class, and all the rest. New examples are classified by whichever of these  $k$  log regs. has highest score.

**Softmax regression:** Model classification cases as *multinomial* distribution. For  $k$  classes, hypothesis is  $k$ -dim vector

$$h_{\theta}(x) = \frac{1}{\sum_{l=1}^k \exp(\theta^{(l)T} x)} \times [\exp(\theta^{(1)T} x), \dots, \exp(\theta^{(k)T} x)] \quad (3.7)$$

The log-likelihood is

$$l(\theta) = - \sum_{i=1}^m \sum_{l=1}^k \mathbf{1}(y^{(i)} = l) \log \frac{\exp(\theta^{(l)T} x)}{\sum_{m=1}^k \exp(\theta^{(m)T} x)} \quad (3.8)$$

**TODO: show how 2-class log reg cost func can be written this way. write down deriv of cost func. clean up notation.**

## 4 Gaussian Discriminant Analysis (GDA) and Naive Bayes

**Generative algorithm:** Instead of modeling  $p(y|x)$ , model  $p(y)$  and  $p(x|y)$ , then get posterior  $p(y|x)$  via Bayes' theorem.

### 4.1 GDA

Can use GDA for classification problem when input features are continuous-val random vars. Models  $p(x|y)$  as multivariate Gaussian. Model is

$$\begin{aligned} y &\sim \text{Bernoulli}(\phi) \\ x|y = 0 &\sim \mathcal{N}(\mu_0, \Sigma) \\ x|y = 1 &\sim \mathcal{N}(\mu_1, \Sigma) \end{aligned} \quad (4.1)$$

**TODO: finish —**

### 4.2 Naive Bayes (for text classification)

For training examples  $x \in \{0, 1\}^n$  (a **vocabulary**<sup>2</sup> of length  $n$ ), assume the components of an example,  $x_j$ , are conditionally independent given  $y$  (**Naive Bayes assumption**).

$$p(x_1, \dots, x_n | y) = \prod_{i=1}^n p(x_i | y) \quad (4.2)$$

Model is parameterized by

$$\phi_y = p(y = 1), \quad \phi_{j|y=1} = p(x_j = 1 | y = 1), \quad \phi_{j|y=0} = p(x_j = 1 | y = 0) \quad (4.3)$$

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<sup>2</sup>the  $j^{\text{th}}$  entry is 1 if the example contains the  $j^{\text{th}}$  word in the vocabulary. **Example:** If the vocab is {cats, rats, bats}, then  $n = 3$ , and a training example that contains “cats”, “rats”, but not “bats”, would be  $x = (1, 1, 0)$ .

where  $j \in (1, n)$ , for a total of  $2n + 1$  parameters. Likelihood is

$$L(\phi_y, \{\phi_{j|y=1}, \phi_{j|y=0}\}_{j=1}^n) = \prod_{i=1}^m p(x^{(i)}, y^{(i)}) \quad (4.4)$$

which has MLE values

$$\begin{aligned} \phi_{j|y=1} &= \text{fraction of spam (y=1) in which word j appears} \\ \phi_{j|y=0} &= \text{fraction of non-spam (y=0) in which word j appears} \\ \phi_y &= \text{fraction of training examples that are spam} \end{aligned} \quad (4.5)$$

To make predictions, we don't need the evidence  $p(x)$ ; we just need to compare

$$\begin{aligned} p(y = 1|x) &\propto p(x|y = 1)p(y = 1) \\ p(y = 0|x) &\propto p(x|y = 0)p(y = 0) \end{aligned} \quad (4.6)$$

and pick the class that has the higher value (un-normalized posterior).

**TODO: finish — show how last two eqs are actually calculated**

## 5 Bias/Variance Tradeoff

- **High bias:** underfitting. high training error and test error.
- **High variance:** overfitting. *low* training error and *high* test error

Can't use the test set to decide on values of hypers (*e.g.* number of parameters in model) because “we could just tweak the values of the hypers until the estimator performs optimally [on the test set]”.

Cross-validation allows you to do model scoring (on frequentist stats, versus *e.g.* info criteria for Bayesian stats.. **TODO: verify i know what i'm talking about**).

Can average together multiple models with high capacity (low bias, but high variance). The result of combining is to *reduce* the variance of the combined model.

## 6 Model Assessment

### 6.1 Classification

#### 6.1.1 Precision/Recall

For 2 classes, with  $\{TN, FN, FP, TP\} = \{\text{true negatives, false negatives, false positives, true positives}\}$ , we have the *loss* or *confusion matrix*:

$$\begin{pmatrix} TN & FP \\ FN & TP \end{pmatrix}, \quad (6.1)$$

where the rows/columns are actual/predicted numbers of examples not-in-class (negative), or in-class (positive). We define the **precision** and **recall**:

$$\text{precision} = \frac{TP}{TP + FP}, \quad \text{recall} = \frac{TP}{TP + FN}. \quad (6.2)$$

**Precision** is ability of classifier to not classify actual negatives as positive (*i.e.* low false positives). So *e.g.* if positive is “person doesn’t have cancer”, we want *high precision*.

**Recall** is ability of classifier to find all positive samples.

### 6.1.2 Receiver operating characteristic curve (ROC)

**True Positive Rate (TPR)**: same as recall

**True Negative Rate (TNR)**: fraction of actual negatives that are classified as negative  $TN/(TN + FP)$

**False Positive Rate (FPR)**:  $1 - TNR$

ROC plots TPR versus FPR.

**TODO: F score**

## 6.2 Misc

$k$ : number of model parameters

- **Akaike Information Criteria (AIC)**:  $2k - 2 \ln L(\theta)$

**TODO: how to apply in practice**

## 7 K-means

- Setup: Select any  $K$  points from data to serve as initial centroids of the clusters.
- Repeat until (stopping criteria: *e.g.* no points change clusters, sum of distances is minimized, some total number of iterations..):
  1. Assign each datapoint to the cluster with closest centroid.
  2. Compute  $K$  new centroids, each the mean of the datapoints in its cluster.

## 8 PCA

PCA is unsupervised technique for finding directions of most variance in dataset. The **principal components** are a set of  $n$  orthonormal  $n$ -dim basis vects along the directions of maximum variance, ordered by decreasing variance in their directions.

To calc:

- **via eigenvectors:** Principal components of *de-meaned*  $n \times m$  design matrix  $\mathbf{X}$  are the eigenvectors of the covariance matrix of  $\mathbf{X}$ ,  $\mathbf{C}_\mathbf{X} = \frac{1}{m} \mathbf{X} \mathbf{X}^T$ .
- **via SVD:** Define  $\mathbf{Y} = \frac{1}{\sqrt{m}} \mathbf{X}^T$ , and take its SVD [A.3](#), which is  $\mathbf{Y} = \mathbf{U} \mathbf{W} \mathbf{V}^T$ . Then  $\mathbf{U}^T$  is  $n \times m$  matrix that projects  $\mathbf{X}$  onto its principal components,  $\mathbf{W}$  is the matrix of principal comp values, and  $\mathbf{V}$  is orthonormal matrix of the principal components. **TODO: Verify/fix statement on U projection.**

## 9 Time Series

### 9.1 Stationarity

**Definition 1 (Second Order Stationarity)** *is when correlation between sequential observations is only a function of the lag.*

- **Dickey-Fuller test:** tests for stationarity of AR model. Null hypothesis is “series is *non-stationary*”.

### 9.2 ARCH

- **Box-Jenkins:** systematic methodology for identifying and estimating models that can incorporate both AR and MA.

## 10 Gaussian Processes

## 11 Neural Networks

### 11.1 Hyperparameters

Hypers: learning rate, num iterations, num hidden layers, num units in each layer, choice of activation function, amount of momentum, minibatch size, regularization type and amount.

### 11.2 Bias/Variance

Bias/variance is less of a *tradeoff* in neural network training, since we have a number of methods to reduce both independently.

- **Reduce bias (train set perf):** Bigger network, train longer, (NN arch search)
- **Reduce variance (dev set perf):** More data, regularization.. (when changed go back and retune bias)



## 12 Variational Methods

### Preliminary section!

If our prior is not a conjugate prior to our likelihood, we can't compute posterior in closed form. Try:

- approximate intractable posterior  $p(\vec{\theta}|\vec{y})$  with tractable  $q(\vec{\theta}|\gamma)$ .
- Adjust  $\gamma$  to minimize  $KL[p(\vec{\theta}|\vec{y})||q(\vec{\theta}|\gamma)] \rightarrow$  complicated, since we don't know  $p(\vec{\theta}|\vec{y})$ . Eventually will use *Expectation Propagation* to solve.
- Adjust  $\gamma$  to minimize  $KL[q(\vec{\theta}|\gamma)||p(\vec{\theta}|\vec{y})] \rightarrow$  simpler: *Variational Bayes*.
- **Variational Bayes**: minimizing  $KL[q(\vec{\theta}|\gamma)||p(\vec{\theta}|\vec{y})] \iff$  maximizing ELBO  $\mathcal{L}$
- note the *latent/hidden variables* helping us are the  $\vec{\theta}$

## Appendix A Math Stuff

### A.1 Matrix Stuff

#### A.1.1 Partitioned Matrix Inversion

Given block decomposition of matrix into submatrices  $\mathbf{A}, \mathbf{B}, \mathbf{C}, \mathbf{D}$ , the inverse is:

$$\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{pmatrix}^{-1} = \begin{pmatrix} \mathbf{M} & -\mathbf{M}\mathbf{B}\mathbf{D}^{-1} \\ -\mathbf{D}^{-1}\mathbf{C}\mathbf{M} & \mathbf{D}^{-1} + \mathbf{D}^{-1}\mathbf{C}\mathbf{M}\mathbf{B}\mathbf{D}^{-1} \end{pmatrix}, \quad (\text{A.1})$$

where

$$\mathbf{M} = (\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C})^{-1} \quad (\text{A.2})$$

(NB compare with Matt Headrick's compendium inversion formula)

### A.2 Gaussians

#### A.2.1 Partitioned Gaussians: Conditional and Marginal Distributions

From BISHOP, sections 2.3.1 - 2.3.2.

Consider a joint Gaussian distribution,  $\mathcal{N}(\vec{x}|\vec{\mu}, \mathbf{\Sigma})$  with  $\mathbf{\Lambda} \equiv \mathbf{\Sigma}^{-1}$  and

$$\vec{x} = \begin{pmatrix} \vec{x}_a \\ \vec{x}_b \end{pmatrix}, \quad \vec{\mu} = \begin{pmatrix} \vec{\mu}_a \\ \vec{\mu}_b \end{pmatrix} \quad (\text{A.3})$$

$$\mathbf{\Sigma} = \begin{pmatrix} \mathbf{\Sigma}_{aa} & \mathbf{\Sigma}_{ab} \\ \mathbf{\Sigma}_{ba} & \mathbf{\Sigma}_{bb} \end{pmatrix}, \quad \mathbf{\Lambda} = \begin{pmatrix} \mathbf{\Lambda}_{aa} & \mathbf{\Lambda}_{ab} \\ \mathbf{\Lambda}_{ba} & \mathbf{\Lambda}_{bb} \end{pmatrix}. \quad (\text{A.4})$$

(That is, the vector  $\vec{x}$  is partitioned into  $\vec{x}_a$  and  $\vec{x}_b$ , which induces a block partitioning of the covariance matrix  $\mathbf{\Sigma}$ .)

The *conditional distribution* is:

$$p(\vec{x}_a|\vec{x}_b) = \mathcal{N}(\vec{x}|\vec{\mu}_{a|b}, \mathbf{\Lambda}_{aa}^{-1}) \quad (\text{A.5})$$

$$\vec{\mu}_{a|b} = \vec{\mu}_a - \mathbf{\Lambda}_{aa}^{-1}\mathbf{\Lambda}_{ab}(\vec{x}_b - \vec{\mu}_b) \quad (\text{A.6})$$

The *marginal distribution* is:

$$p(\vec{x}_a) = \mathcal{N}(\vec{x}_a|\vec{\mu}_a, \mathbf{\Sigma}_{aa}) \quad (\text{A.7})$$

#### A.2.2 Bayes' theorem for Gaussian variables

From BISHOP, section 2.3.3. NB This is known as a *linear Gaussian model*.

Given a marginal Gaussian distribution for  $\vec{x}$  and a conditional Gaussian distribution for  $\vec{y}$  given  $\vec{x}$  in the form:

$$p(\vec{x}) = \mathcal{N}(\vec{x}|\vec{\mu}, \Lambda^{-1}) \quad (\text{A.8})$$

$$p(\vec{y}|\vec{x}) = \mathcal{N}(\vec{y}|\mathbf{A}\vec{x} + \vec{b}, \mathbf{L}^{-1}), \quad (\text{A.9})$$

we have

$$p(\vec{y}) = \mathcal{N}(\vec{y}|\mathbf{A}\vec{\mu} + \vec{b}, \mathbf{L}^{-1} + \mathbf{A}\Lambda^{-1}\mathbf{A}^T) \quad (\text{A.10})$$

$$p(\vec{x}|\vec{y}) = \mathcal{N}(\vec{x}|\Sigma\{\mathbf{A}^T\mathbf{L}(\vec{y} - \vec{b}) + \Lambda\vec{\mu}\}, \Sigma) \quad (\text{A.11})$$

where

$$\Sigma \equiv (\Lambda + \mathbf{A}^T\mathbf{L}\mathbf{A})^{-1} \quad (\text{A.12})$$

### A.3 Singular value decomposition

An  $M \times N$  matrix  $\mathbf{A}$  can be written as  $\mathbf{U}\mathbf{W}\mathbf{V}^T$ , where  $\mathbf{U}$  is  $M \times N$ ,  $\mathbf{W}$  is  $N \times N$  and diagonal, and  $\mathbf{V}$  is  $N \times N$  and orthonormal.

If  $\mathbf{A}$  is square,  $\mathbf{V}$  are its eigenvectors, and  $\mathbf{W}$  are its eigenvalues...

Uses

- If  $M \geq N$ , cols of  $\mathbf{U}$  are an orthonormal basis for space spanned by cols of  $\mathbf{A}$

**TODO: finish —**

### A.4 Matrix derivatives

$$\frac{\partial}{\partial \vec{x}} (\vec{x}^T \vec{a}) = \frac{\partial}{\partial \vec{x}} (\vec{a}^T \vec{x}) = \vec{a} \quad (\text{A.13})$$

**TODO: review understanding of this (I recall this expression not enough to answer my questions on a formula derivation) and give examples.**

## Appendix B The Linear Regression Hierarchy

Linear regression starting from maximum likelihood, through variational Bayes.

### B.1 Maximum likelihood

Maximize likelihood  $p(y|\theta; \beta)$  wrt  $\theta, \beta$ .

### B.2 Maximum a posteriori

Introduce prior  $p(\theta; \alpha) = \exp(-\alpha\theta^T\theta)$ . Find  $\theta$  by maximizing  $p(y|\theta; \beta)p(\theta; \alpha)$  wrt  $\theta$ .

Q: what is proper way to estimate  $\beta$  and  $\alpha$  here?

### B.3 Full Bayesian (stationary prior)

Calc posterior  $p(\theta|y) = p(y|\theta; \beta)p(\theta; \alpha)/p(y; \alpha, \beta)$ , where  $p(y; \alpha, \beta) = \int_{\theta} p(y|\theta; \beta)p(\theta; \alpha)$  is the evidence. Determine values of hypers  $\alpha, \beta$  by maximizing evidence. This is difficult to do directly, as derivs wrt  $\alpha, \beta$  are hard to compute, so use EM algorithm.

### B.4 Variational Bayes (non-stationary prior)