ML Cheatsheet

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Abstract: Everything I know about machine learning.

Contents

1   Conventions

Math Notation

- $x \in \{0,1\}^r$: x is a vector of form *e.g.* $(0,1,1,0,\ldots,1,0)$ 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.

- $\mathbf{I}_k$: $k \times k$ identity matrix

- Boldface capital letters are matrices, *e.g.* $\mathbf{A} = \mathbf{UWV}^T$

- log is base e by default $\rightarrow$ entropy in nats.

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- 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), $1 \le i \le m$

- $y^{(i)}$: i^{th} output (*column* vector), $1 \le i \le m$

- x_j : j^{th} component of a training example, $1 \le j \le n$.

- $\mathbf{X} \in \mathbb{R}^{n \times m}$: (input/design) matrix (training examples are *column* vectors)[1]

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[1]Note our non-conventional definition of the design matrix $\mathbf{X}$. The more conventional version is denoted $\mathbb{X}$.

- $\mathbb{X} \in \mathbb{R}^{m \times n}$: (input/design) matrix (training examples are *row* vectors)

2 Linear Regression

2.1 Basics

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

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

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

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

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 $x^{(i)}, \; 1 \le i \le m$, we have

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

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

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

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

with deriv

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

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

The log-likelihood is just the cross entropy

$$H(p, q) = -\sum_i p_i \log q_i \tag{3.6}$$

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

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

so that the final output layer has k units. The log-likelihood is

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

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

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

TODO: finish —

4.2 Naive Bayes (for text classification)

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

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

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[2]the jth entry is 1 if the example contains the jth 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 $x = (1, 1, 0)$.

Model is parameterized by

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

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

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

which has MLE values

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

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

$$p(y = 1|x) \propto p(x|y = 1)p(y = 1)$$
$$p(y = 0|x) \propto p(x|y = 0)p(y = 0) \tag{4.6}$$

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

$$\begin{pmatrix} TN & FP \\ FN & TP \end{pmatrix}, \tag{6.1}$$

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

$$\text{precision} = \frac{\text{TP}}{\text{TP} + \text{FP}}, \qquad \text{recall} = \frac{\text{TP}}{\text{TP} + \text{FN}}. \tag{6.2}$$

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 classifer 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: More on why the ROC is useful. Maybe a picture.

6.1.3   F1 Score

The F1 score is the *harmonic mean* of precision and recall. It's an ok one-number metric for evaluating effectiveness of different classifiers on problem:

$$\text{F1} = \frac{2}{\left(\frac{1}{\text{prec}} + \frac{1}{\text{rec}}\right)} \tag{6.3}$$

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 $\mathbf{X}$, $\mathbf{C_X} = \frac{1}{m}\mathbf{XX}^T$.
- **via SVD:** Define $\mathbf{Y} = \frac{1}{\sqrt{m}}\mathbf{X}^T$, and take its SVD A.3.2, which is $\mathbf{Y} = \mathbf{UWV}^T$. 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

10.1 Prior over functions, from basis functions

Following the treatment in section 6.4 of BISHOP (with different notation than above).

Let d be the number of *basis functions* $\vec{\phi}$, which are non-linear functions of the n dimensional training examples $\vec{x}$. We write the hypothesis as

$$y(\vec{x}) = \vec{w}^T \vec{\phi}(\vec{x}) \tag{10.1}$$

where $\vec{w}$ is a d dimensional vector of weights.

As in MAP and Bayesian linear regression, we introduce a isotropic Gaussian prior over the weights, with α its inverse variance:

$$p(\vec{w}) = \mathcal{N}(\vec{w}|\vec{0}, \alpha^{-1}\mathbf{I}_d) \tag{10.2}$$

The prior over $\vec{w}$ thus induces a prior over *functions* $y(\vec{x})$.

The design matrix is now $\mathbb{X} \in \mathbb{R}^{m \times d}$, so the hypothesis evaluated on our training examples is an m dim vector

$$\vec{y} = \mathbb{X}\vec{w} \tag{10.3}$$

Each element of $\vec{y}$ is linear combination of Gaussians (given by the $\vec{w}$ prior), where the weights in the linear combination come from elements of the design matrix. Thus the vector $\vec{y}$ itself is a multivariate Gaussian, completely specified by its mean vector and covariance matrix.

$$\mathbb{E}[\vec{y}] = \mathbb{X}\,\mathbb{E}[\vec{w}] = \vec{0} \tag{10.4}$$

$$\text{cov}[\vec{y}] = \mathbb{E}[\vec{y}\vec{y}^T] = \mathbb{X}\,\mathbb{E}[\vec{w}\vec{w}^T]\,\mathbb{X}^T = \alpha^{-1}\mathbb{X}\,\mathbb{X}^T \equiv \mathbf{K} \tag{10.5}$$

where $\mathbf{K}$ is the $m \times m$ *Gram matrix* with elements

$$\mathbf{K}_{ij} \equiv k(\vec{x}_i, \vec{x}_j) = \alpha^{-1}\vec{\phi}(\vec{x}_i)^T\,\vec{\phi}(\vec{x}_j). \tag{10.6}$$

Our prior over functions is then

$$p(\vec{y}) = \mathcal{N}(\vec{y}|\vec{0}, \mathbf{K}) \tag{10.7}$$

10.2   Basic Gaussian process regression

For regression, we assume our target variables are given by the hypothesis $\vec{y}$ with added Gaussian noise

$$p(t_i|y_i) = \mathcal{N}(t_i|y_i, \beta^{-1}) \qquad 1 \le i \le m \tag{10.8}$$

where β is the inverse variance of the Gaussian, and the noise is i.i.d for each training example. The m dim vector of target variables is then given by a multivariate Gaussian

$$p(\vec{t}|\vec{y}) = \mathcal{N}(\vec{t}|\vec{y}, \beta^{-1}\mathbf{I}_m) \tag{10.9}$$

To get the joint distribution $p(\vec{t})$ over all the target variables, we integrate out $\vec{y}$ via A.10, analagous to how we integrate out the weights $\vec{w}$ in Bayesian regression,

$$p(\vec{t}) = \int p(\vec{t}|\vec{y})p(\vec{y})d\vec{y} = \mathcal{N}(\vec{t}|\vec{0}, \mathbf{C}) \tag{10.10}$$

where $\mathbf{C}$ is $m \times m$ with elements $\mathbf{C}_{ij} = \mathbf{K}_{ij} + \beta^{-1}\delta_{ij}$.

To make a prediction based on the m training examples, we form the joint distribution over $m + 1$ examples,

$$\mathcal{N}(\vec{t}_{m+1}|\vec{0}, \mathbf{C}_{m+1}) \tag{10.11}$$

with the $(m + 1) \times (m + 1)$ matrix $\mathbf{C}_{m+1}$ partitioned as

$$\mathbf{C}_{m+1} = \begin{pmatrix} \mathbf{C}_m & \vec{k} \\ \vec{k}^T & c \end{pmatrix}, \tag{10.12}$$

where

- $\mathbf{C}_m$ is $m \times m$ with elements $\mathbf{C}_{ij} = \mathbf{K}_{ij} + \beta^{-1}\delta_{ij}$
- $\vec{k}$ has elements $k(\vec{x}_i, \vec{x}_{m+1})$ for $1 \le i \le m$

- $c = k(\vec{x}_{m+1}, \vec{x}_{m+1}) + \beta^{-1}$

The conditional distribution $p(t_{m+1}|\vec{t})$ is then given by a Gaussian with

$$m(\vec{x}_{m+1}) = \vec{k}^T \mathbf{C}_m^{-1} \vec{t} \tag{10.13}$$

$$\sigma^2(\vec{x}_{m+1}) = c - \vec{k}^T \mathbf{C}_m^{-1} \vec{k}. \tag{10.14}$$

which we obtain by using A.6.

TODO: check this to make sure it's the right eq.

11 Neural Networks

11.1 Hyperparameters

Hypers: learning rate, num iteractions, num hidden layers, num units in each layer, choice of activation function, amout 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 γ to minimize $KL\big[p(\vec{\theta}|\vec{y})||q(\vec{\theta}|\gamma)\big] \rightarrow$ complicated, since we don't know $p(\vec{\theta}|\vec{y})$. Eventually will use ***Expectation Propagation*** to solve.
- Adjust γ to minimize $KL\big[q(\vec{\theta}|\gamma)||p(\vec{\theta}|\vec{y})\big] \rightarrow$ simpler: ***Variational Bayes***.
- **Variational Bayes**: minimizing $KL\big[q(\vec{\theta}|\gamma)||p(\vec{\theta}|\vec{y})\big] \iff$ maximizing ELBO $\mathscr{L}$
- 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:

$$\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{pmatrix}^{-1} = \begin{pmatrix} \mathbf{M} & -\mathbf{MBD}^{-1} \\ -\mathbf{D}^{-1}\mathbf{CM} & \mathbf{D}^{-1} + \mathbf{D}^{-1}\mathbf{CMBD}^{-1} \end{pmatrix},$$

(A.1)

where

$$\mathbf{M} = \left(\mathbf{A} - \mathbf{BD}^{-1}\mathbf{C} \right)^{-1}$$

(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

$$\vec{x} = \begin{pmatrix} \vec{x}_a \\ \vec{x}_b \end{pmatrix}, \quad \vec{\mu} = \begin{pmatrix} \vec{\mu}_a \\ \vec{\mu}_b \end{pmatrix}$$

(A.3)

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

(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:

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

(A.5)

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

(A.6)

The *marginal distribution* is:

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

(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:

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

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

we have

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

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

where

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

A.3 Matrix Factorization

A.3.1 Diagonalization (Eigendecomposition)

A square $N \times N$ symmetric matrix $\mathbf{A}$ has real eigenvalues from its symmetricity, and N linearly independent eigenvectors. We can write $\mathbf{A} = \mathbf{O}\mathbf{D}\mathbf{O}^{-1} = \mathbf{O}\mathbf{D}\mathbf{O}^T$, with $\mathbf{O}$ an orthogonal[3] matrix with columns equal to $\mathbf{A}$'s eigenvectors, and $\mathbf{D}$ a diagonal matrix of $\mathbf{A}$'s eigenvalues.

A.3.2 Singular value decomposition

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

If $\mathbf{A}$ is square, the columns of $\mathbf{V}$ are its eigenvectors, and $\mathbf{D}$ 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

$$\frac{\partial}{\partial \vec{x}} \left(\vec{x}^T \vec{a} \right) = \frac{\partial}{\partial \vec{x}} \left(\vec{a}^T \vec{x} \right) = \vec{a} \tag{A.13}$$

TODO: review understanding of this (I recall this expression was 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.

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[3]An *orthogonal* matrix should really be called an *orthonormal* matrix, as its columns are linearly indepdendent, but also normalized.

B.1 Maximum likelihood

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

B.2 Maximum a posteriori

Introduce prior $p(\theta; \alpha) = \exp(-\alpha\theta^T\theta)$. Find θ by maximizing $p(y|\theta; \beta)p(\theta; \alpha)$ wrt θ.
Q: what is proper way to estimate β and α 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 α, β by maximizing evidence. This is difficult to do directly, as derivs wrt α, β are hard to compute, so use EM algorithm.

B.4 Variational Bayes (non-stationary prior)