ML Cheatsheet

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ABSTRACT: Everything I know about machine learning.

Contents

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1 Conventions

Math Notation

- $x \in \{0,1\}^r$: x is a vector of form *e.g.* $(0,1,1,0,\ldots,1,0)$ 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 (roman or greek) are matrices, *e.g.* $\mathbf{A} = \mathbf{U}\mathbf{\Lambda}\mathbf{V}^T$
- log is base e by default $\rightarrow$ entropy in nats.
- $\mathbb{E}_\theta$: Expectation value (with respect to some parameter θ. Parameter may be omitted if clear from context.)

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

BISHOP

- N : number of training examples in the dataset
- D : dimension of training examples
- M : number of basis functions
- Boldface lower-case letters (roman or greek) are *column* vectors, *e.g.* $d = \mathbf{x}^T \mathbf{A}\mathbf{x}$, or $\mathbf{y} = \mathbf{A}\mathbf{x}$.
- $\boldsymbol{\phi}$: M-dim basis function
- $\boldsymbol{\Phi} \in \mathbb{R}^{N \times M}$: Design matrix (basis functions 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 $m \times (n+1)$ design matrix

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

  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 $x^{(i)}$, $1 \leq i \leq m$, 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 logistic regressions. Each has two classes: the target class, and all the rest. New examples are classified by whichever of these k logistic regressions has highest score.

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

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

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 logistic regression 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

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

TODO: finish —

4.2 Naive Bayes (for text classification)

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

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

[1] the j^{th} entry is 1 if the example contains the j^{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 $x = (1, 1, 0)$.

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

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

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

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

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 comparison to find best value of hypers (on frequentist stats), versus using things like computing the evidence in Bayesian stats. ← **TODO: more detail here**

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***:

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

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 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: 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:

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

6.2 Regression

TODO: Write this section.

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 vectors along the directions of maximum variance, ordered by decreasing variance in their directions.

To calc:

- **via eigenvectors:** Principal components of *de-meaned* $m \times n$ design matrix $\mathbf{X}$ are the eigenvectors of the covariance matrix of $\mathbf{X}$, $\mathbf{C_X} = \frac{1}{m}\mathbf{X}^T\mathbf{X}$.
- **via SVD:** Define $\mathbf{Y} = \frac{1}{\sqrt{m}}\mathbf{X}$, 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.**

TODO: re-check everything in PCA section, as I have redefined the design matrix X.

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 Bishop's notation).

Let d be the number of ***basis functions*** $\vec{\phi}$, which are non-linear functions of the n-dim 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-dim 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 of basis functions is now $\mathbf{\Phi} \in \mathbb{R}^{m \times d}$, so the hypothesis evaluated on our training examples is an m-dim vector

$$\vec{y} = \mathbf{\Phi}\vec{w} \tag{10.3}$$

Each element of $\vec{y}$ is a 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 each element of $\vec{y}$ is a Gaussian. Then the vector $\vec{y}$ itself is a multivariate Gaussian, completely specified by its mean vector and covariance matrix.

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

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

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 t_i 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, $\vec{t}$, 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.11), analogous 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 t_{m+1}, based on the m training examples, we form the joint distribution over $m+1$ examples,

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

where $\vec{t}$ is now $(m+1)$-dim, and the $(m+1) \times (m+1)$ matrix $\mathbf{C}_{m+1}$ is 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 $p\left(t_{m+1}|\vec{t}\right)$ 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.7). ← **TODO: check to make sure this is the right eq.**

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 γ to minimize $KL\left[p(\vec{\theta}|\vec{y})||q(\vec{\theta}|\gamma)\right] \rightarrow$ complicated, since we don't know $p(\vec{\theta}|\vec{y})$. Eventually will use ***expectation propagation*** to solve.
- Adjust γ to minimize $KL\left[q(\vec{\theta}|\gamma)||p(\vec{\theta}|\vec{y})\right] \rightarrow$ simpler: ***variational Bayes***.
- **Variational Bayes**: minimizing $KL\left[q(\vec{\theta}|\gamma)||p(\vec{\theta}|\vec{y})\right] \iff$ 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 Matrix Identities

(NB More useful stuff in **BARBER** chapter 29.)

Trace Identities

- $\mathrm{Tr}(\mathbf{A}^T) = \mathrm{Tr}(\mathbf{A})$
- $\mathrm{Tr}(\mathbf{A} + \mathbf{B}) = \mathrm{Tr}(\mathbf{A}) + \mathrm{Tr}(\mathbf{B})$
- $\mathrm{Tr}(a\mathbf{A}) = a\mathrm{Tr}(\mathbf{A})$ (with a a scalar)
- $\mathrm{Tr}(\mathbf{AB}) = \mathrm{Tr}(\mathbf{BA})$
- $\mathrm{Tr}(\mathbf{ABC}) = \mathrm{Tr}(\mathbf{BCA}) = \mathrm{Tr}(\mathbf{CAB})$ (cyclicity of trace)

Transpose Identities

- $(\mathbf{AB})^T = \mathbf{B}^T\mathbf{A}^T$

Determinant Identities

- $|\mathbf{AB}| = |\mathbf{A}||\mathbf{B}|$
- $|\mathbf{A}^{-1}| = \frac{1}{|\mathbf{A}|}$
- $|\mathbf{A}^T| = |\mathbf{A}|$

Inverse Indentities

- $(\mathbf{AB})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1}$
- $(\mathbf{A}^T)^{-1} = (\mathbf{A}^{-1})^T$

A.1.2 Matrix derivatives

$$\frac{\partial}{\partial \vec{x}}\left(\vec{x}^T\vec{a}\right) = \frac{\partial}{\partial \vec{x}}\left(\vec{a}^T\vec{x}\right) = \vec{a}^{[2]} \tag{A.1}$$

For a matrix $\mathbf{A}(x)$ as a function of a scalar x (equivalently a component x_i of a vector $\vec{x}$)

$$\frac{\partial}{\partial x}\log|\mathbf{A}| = \mathrm{Tr}\left(\mathbf{A}^{-1}\frac{\partial \mathbf{A}}{\partial x}\right) \tag{A.2}$$

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

A.1.3 Partitioned Matrix Inversion

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

$$\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{pmatrix}^{-1} = \begin{pmatrix} \mathbf{M} & -\mathbf{M}\mathbf{B}\mathbf{D}^{-1} \\ -\mathbf{D}^{-1}\mathbf{C}\mathbf{M} & \mathbf{D}^{-1} + \mathbf{D}^{-1}\mathbf{C}\mathbf{M}\mathbf{B}\mathbf{D}^{-1} \end{pmatrix}, \tag{A.3}$$

where

$$\mathbf{M} = \left(\mathbf{A} - \mathbf{B}\mathbf{D}^{-1}\mathbf{C}\right)^{-1} \tag{A.4}$$

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

A.1.4 Symmetric Matrix Properties

TODO: Do this section.

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

$$\vec{x} = \begin{pmatrix} \vec{x}_a \\ \vec{x}_b \end{pmatrix}, \quad \vec{\mu} = \begin{pmatrix} \vec{\mu}_a \\ \vec{\mu}_b \end{pmatrix} \tag{A.5}$$

$$\mathbf{\Sigma} = \begin{pmatrix} \mathbf{\Sigma}_{aa} & \mathbf{\Sigma}_{ab} \\ \mathbf{\Sigma}_{ba} & \mathbf{\Sigma}_{bb} \end{pmatrix}, \quad \mathbf{\Lambda} = \begin{pmatrix} \mathbf{\Lambda}_{aa} & \mathbf{\Lambda}_{ab} \\ \mathbf{\Lambda}_{ba} & \mathbf{\Lambda}_{bb} \end{pmatrix}. \tag{A.6}$$

(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:

$$p(\vec{x}_a|\vec{x}_b) = \mathcal{N}(\vec{x}|\vec{\mu}_{a|b}, \mathbf{\Lambda}_{aa}^{-1}), \qquad \text{where} \quad \vec{\mu}_{a|b} \equiv \vec{\mu}_a - \mathbf{\Lambda}_{aa}^{-1}\mathbf{\Lambda}_{ab}(\vec{x}_b - \vec{\mu}_b). \tag{A.7}$$

The *marginal distribution* is:

$$p(\vec{x}_a) = \mathcal{N}(\vec{x}_a|\vec{\mu}_a, \mathbf{\Sigma}_{aa}) \tag{A.8}$$

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:

$$p(\vec{x}) = \mathcal{N}(\vec{x}|\vec{\mu}, \mathbf{\Lambda}^{-1}) \tag{A.9}$$

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

we have

$$p(\vec{y}) = \mathcal{N}(\vec{y}|\mathbf{A}\vec{\mu} + \vec{b}, \mathbf{L}^{-1} + \mathbf{A}\mathbf{\Lambda}^{-1}\mathbf{A}^T) \tag{A.11}$$

$$p(\vec{x}|\vec{y}) = \mathcal{N}(\vec{x}|\mathbf{\Sigma}\{\mathbf{A}^T\mathbf{L}(\vec{y} - \vec{b}) + \mathbf{\Lambda}\vec{\mu}\}, \mathbf{\Sigma}) \tag{A.12}$$

where

$$\mathbf{\Sigma} \equiv \left(\mathbf{\Lambda} + \mathbf{A}^T\mathbf{L}\mathbf{A}\right)^{-1}. \tag{A.13}$$

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 $\mathbf{A} = \mathbf{U}\mathbf{D}\mathbf{U}^{-1} = \mathbf{U}\mathbf{D}\mathbf{U}^T$, with $\mathbf{U}$ an orthogonal[3] matrix with columns $\vec{u}_i$ equal to $\mathbf{A}$'s eigenvectors, and $\mathbf{D}$ a diagonal matrix of $\mathbf{A}$'s eigenvalues, λ_i.

We can also write down the ***spectral decomposition*** of $\mathbf{A}$:

$$\mathbf{A} = \mathbf{U}\mathbf{D}\mathbf{U}^T = \sum_{i=1}^{N} \lambda_i \vec{u}_i \vec{u}_i^T. \tag{A.14}$$

A.3.2 Singular value decomposition

Using conventions of **PRESS**, section 2.6.

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 —

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 θ, β.

[3] An *orthogonal* matrix should really be called an *orthonormal* matrix, as its columns are not just linearly independent, but also normalized.

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?
- half-A: not sure if you can? You typically use the evidence approx (see "Full Bayesian", below) to find best values for β and α.. OTOH we found most likely β in previous section ("Maximum Likelihood"), so why can't we do it here? **← TODO: finish answering this.**

B.3 Full Bayesian (stationary prior)

Calculate posterior $p(\theta|y) = p(y|\theta;\beta)p(\theta;\alpha)/p(y;\alpha,\beta)$, where $p(y;\alpha,\beta) = \int_\theta p(y|\theta;\beta)p(\theta;\alpha)d\theta$ is the ***evidence***. Determine values of hypers α, β by maximizing evidence wrt them. 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)

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