1 Regression

1.1 Linear Regression

Simple $y_n \approx f(\mathbf{x_n}) := w_0 + w_1 x_{n1}$
Multiple $y_n \approx f(\mathbf{x_n}) := w_0 + \sum_{j=1}^{D} w_j x_{nj} = \tilde{\mathbf{x}}_n^T \mathbf{w}$ If $D > N$ the task is under-determined (more dimensions than data) $\rightarrow$ regularization.

2 Cost functions

MSE $= \frac{1}{N}\sum_{n=1}^{N}[y_n - f(\mathbf{x_n})]^2$ Not good with outliers. MAE $= \frac{1}{N}\sum_{n=1}^{N}|y_n - f(\mathbf{x_n})|$ Error $e_n = y_n - f(\mathbf{x_n})$

2.1 Convexity

A line joining two points never intersects with the function anywhere else. $f(\lambda \mathbf{u} + (1-\lambda)\mathbf{v}) \leq \lambda f(\mathbf{u}) + (1-\lambda) f(\mathbf{v})$ with $\lambda \in [0;1]$. A strictly convex function has a unique global minimum w^*. Sums of convex functions are convex.
A function must always lie above its linearisation $\mathcal{L}(u) \geq \mathcal{L}(w) + \nabla\mathcal{L}(w)^T(u-w) \forall u, w$.
A set is convex iff the line segment between any two points of $\mathcal{C}$ lies in $\mathcal{C}$: $\theta u + (1-\theta)v \in \mathcal{C}$

3 Optimisation

Find $\mathbf{w}^* \in \mathcal{R}^D$ which $min \mathcal{L}(\mathbf{w})$. Gradient $\nabla\mathcal{L} := \left[\frac{\partial\mathcal{L}(\mathbf{w})}{\partial w_1} \quad \dots \quad \frac{\partial\mathcal{L}(\mathbf{w})}{\partial w_D}\right]$

3.1 Gradient descent

$\mathbf{w^{(t+1)}} = \mathbf{w^{(t)}} - \gamma\nabla\mathcal{L}(\mathbf{w^{(t)}})$. Very sensitive to ill-conditioning.
GD - Linear Reg
$\mathcal{L}(\mathbf{w}) = \frac{1}{2N}(\mathbf{y} - X\mathbf{w})^T(\mathbf{y} - X\mathbf{w}) \rightarrow \nabla\mathcal{L}(\mathbf{w}) = -\frac{1}{N}X^T(\mathbf{y} - X\mathbf{w})$.
Cost : $O_{error}(N*D) = 2N*D+N$ and $O_{weights} = 2N*D+D$.

3.2 SGD

$\mathcal{L} = \frac{1}{N}\sum\mathcal{L}_n(\mathbf{w})$ with update $\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \gamma\nabla\mathcal{L}_n(\mathbf{w}^{(t)})$.

3.3 Mini-batch SGD

$\mathbf{g} = \frac{1}{|B|}\sum_{n\in B}\nabla\mathcal{L}_n(\mathbf{w}^{(t)})$ with update $\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \gamma\mathbf{g}$.

3.4 Subgradient at w

$\mathbf{g} \in \mathbb{R}^D$ such that $\mathcal{L}(u) \geq \mathcal{L}(w) + \mathbf{g}^T(u-w)$. Example subgradient for MAE : $h(e) = |e| \rightarrow g(e) = sgn(e)$ if $e \neq 0, \lambda$ otherwise . We get the gradient : $\nabla\mathcal{L}_{MAE} = -\frac{1}{N}\sum_n sgn(x_n)\nabla f(x_n)$.

3.5 Projected SGD

$\mathbf{w}^{(t+1)} = \mathcal{P}_{\mathcal{C}}[\mathbf{w}^{(t)} - \gamma\nabla\mathcal{L}(\mathbf{w}^{(t)})]$

3.6 Newton's method

Second order (more expensive $O(ND^2 + D^3)$ but faster convergence).
$w^{(t+1)} = w^{(t)} - \gamma^{(t)}(H^{(t)})^{-1}\nabla\mathcal{L}(w^{(t)})$

3.7 Optimality conditions

Necessary : $\nabla\mathcal{L}(\mathbf{w}^*) = 0$ Sufficient : Hessian PSD $\mathbf{H}(\mathbf{w}^*) := \frac{\partial^2\mathcal{L}(\mathbf{w}^*)}{\partial w \partial w^T}$

4 Least Squares

4.1 Normal Equation

$X^T(\mathbf{y} - X\mathbf{w}) = 0 \Rightarrow \mathbf{w}^* = (XX^T)^{-1}X^T\mathbf{y}$ and $\hat{\mathbf{y}}_\mathbf{m} = \mathbf{x_m}^T\mathbf{w}^*$ Gram matrix invertible iff rank(X) = D (use SVD $X = USV^T$ if this is not the case to get pseudo-inverse $\mathbf{w}^* = V\tilde{S}U^T$ with $\tilde{S}$ pseudo-inverse of S).

5 Likelihood

Probabilistic model $y_n = \mathbf{x_n}^T\mathbf{w} + \epsilon_n$. Probability of observing the data given a set of parameters and inputs : $p(\mathbf{y}|X, \mathbf{w}) = \prod p(y_n|\mathbf{x_n}, \mathbf{w}) = \prod\mathcal{N}(y_n|\mathbf{x_n}^T\mathbf{w}, \sigma^2)$
Best model maximises log-likelihood $\mathcal{L}_{LL} = -\frac{1}{2\sigma^2}\sum(y_n - x_n^T w)^2 + cst$.

6 Regularization

6.1 Ridge Regression

$\mathcal{L}(\mathbf{w}) = \frac{1}{2}(\mathbf{y} - X\mathbf{w})^T(\mathbf{y} - X\mathbf{w}) + \frac{\lambda}{2}\|\mathbf{w}\|_2^2 \rightarrow \mathbf{w}^*_{\mathbf{ridge}} = (XX^T + \lambda I_D)^{-1}X^T\mathbf{y} = X^T(XX^T + \lambda I_N)^{-1}\mathbf{y}$
Can be considered a MAP estimator : $\mathbf{w}^*_{\mathbf{ridge}} = argmin_w - log(p(w|X, y))$

6.2 Lasso

Sparse solution. $\mathcal{L}(w) = \frac{1}{2N}(y - Xw)^T(y - Xw) + \lambda\|w\|_1$

7 Model Selection

7.1 Bias-Variance decomposition

Small dimensions : large bias, small variance. Large dimensions : small bias, large variance. Error for the val set compared to the emp distr of the data goes down like $\frac{1}{\sqrt{|\text{validation points}|}}$ and goes up like $\sqrt{ln(|\text{hyper parameters}|)}$

8 Classification

8.1 Optimal

$\hat{y}(\mathbf{x}) = argmax_{y\in\mathcal{Y}} p(y|\mathbf{x})$

8.2 Logistic regression

$\sigma(z) = \frac{e^z}{1+e^z}$ to limit the predicted values $y \in [0;1]$ ($p(1|\mathbf{x}) = \sigma(\mathbf{x}^T\mathbf{w})$ and $p(0|\mathbf{x}) = 1 - \sigma(\mathbf{x}^T\mathbf{w})$). We decide with respect to 0.5
Likelihood
$p(y|X, w) = \prod p(y_n|x_n) = \prod_{n:y_n=0} p(y_n = 0|x_n) \dots \prod_{n:y_n=K} p(y_n = K|x_n) = \prod_k^K\prod_n^N[p(y_n = k|x_n, w)]^{\tilde{y}_{nk}}$
where $tildey_{nk} = 1$ if $y_n = k$.
For binary classification
$p(y|X, w) = \prod p(y_n|x_n) = \prod_{n:y_n=0} p(y_n = 0|x_n)\prod_{n:y_n=1} p(y_n = 1|x_n) = \prod_n^N \sigma(x_n^T w)^{y_n}[1 - \sigma(x_n^T w)]^{1-y_n}$
Loss
$\mathcal{L}(w) = \sum_{n=1}^N ln(1 + exp(x_n^T w)) - y_n x_n^T w$ which is convex in w.
Gradient
$\nabla\mathcal{L}(w) = \sum_{n=1}^N x_n(\sigma(x_n^T w) - y_n) = X^T[\sigma(Xw) - y]$ (no closed form solution).
Hessian
$H(w) = X^T S X$ with $S_{nn} = \sigma(x_n^T w)[1 - \sigma(x_n^T w)]$

8.3 Exponential family

General form
$p(y|\eta) = h(y)exp[\eta^T\psi(y) - A(\eta)]$ where
Cumulant
$A(\eta) = ln[\int_y h(y)exp[\eta^T\psi(y)]dy]$
$\nabla A(\eta) = \mathbb{E}[\psi(y)]$
$\nabla^2 A(\eta) = \mathbb{E}[\psi\psi^T] - \mathbb{E}[\psi]\mathbb{E}[\psi^T]$
Link function
$\eta = g^{-1}(\mu) \Leftrightarrow \mu = g(\eta)$

- $\eta_{gaussian} = (\mu/\sigma^2, -1/2\sigma^2)$
- $\eta_{poisson} = ln(\mu)$
- $\eta_{bernoulli} = ln(\mu/1 - \mu)$
- $\eta_{general} = g^{-1}(\frac{1}{N}\sum_{n=1}^N\psi(y_n))$

8.4 Nearest Neighbor Models

Performs best in low dimensions.

8.4.1 k-NN

$f_{S^{t,k}}(x) = \frac{1}{k}\sum_{n:x_n\in ngbh_{S_{t,k}(x)}} y_n$ Pick odd k so there is a clear winner. Large $k \rightarrow$ large bias small variance (inv.)

8.4.2 Error bound

$\mathbb{E}[\mathcal{L}_{S^t}] \leq 2\mathcal{L}_{f^*} + 4c\sqrt{d}N^{-1/d+1}$

8.5 Support Vector Machines (SVM)

Logistic regression with hinge loss : $min_w\sum_{n=1}^N[1 - y_n x_n^T w]_+ + \frac{\lambda}{2}\|w\|^2$ where $y \in [-1;1]$ is the label and $hinge(x) = max\{0, x\}$. Convex but not differentiable so need subgradient.
We can also use duality : $\mathcal{L}(w) = max_\alpha G(w, \alpha)$. For SVM $min_w max_{\alpha\in[0,1]^N}\sum\alpha_n(1 - y_n x_n^T w) + \frac{\lambda}{2}\|w\|^2$ differentiable and convex.
Can switch max and min when convex in w and concave in α. This can make the formulation simpler:
$w(\alpha) = \frac{1}{\lambda}\sum\alpha_n y_n x_n = \frac{1}{\lambda}X^T diag(y)\alpha$ which yields the optimisation problem: $max_{\alpha\in[0,1]^N}\alpha^T\mathbf{1} - \frac{1}{2\lambda}\alpha^T YXX^TY\alpha$ The solution is sparse (α_n is the slope of the lines that are lower bounds to the hingle loss).

8.6 Kernel Ridge Regression

From duality $w^* := X^T\alpha^*$ where $\alpha^* := (K + \lambda I_N)^{-1}y$ and $K = XX^T = \phi^T(x)\phi(x) = \kappa(x, x')$ (needs to be PSD and symmetric).

9 Unsupervised Learning

9.1 K-means clustering

$min\mathcal{L}(z, \mu) = \sum_n^N\sum_k^K z_{nk}\|x_n - \mu_k\|_2^2$ with $z_{nk} \in \{0, 1\}$ (unique assignments: $\sum_k z_{nk} = 1$).
Algorithm (Coordinate Descent)

1. $\forall n$ compute $z_n = \begin{cases} 1 \text{ if } k = argmin_j\|x_n - \mu\|^2 \\ 0 \text{ otherwise} \end{cases}$
2. $\forall k$ compute $\mu_k = \frac{\sum_n z_{nk}x_n}{\sum_n z_{nk}}$

Issues

1. Heavy computation
2. Spherical clusters
3. Hard clusters

Probabilistic model $p(X|\mu, z) = \prod_n^N\mathcal{N}(x_n|\mu_k, I) = \prod_n^N\prod_k^K\mathcal{N}(x_n|\mu_k, I)^{z_{nk}}$

9.2 Gaussian Mixture Models

$p(X|\mu, z) = \prod_n^N p(x_n|z_n, \mu_k, \Sigma_k)p(z_n|\pi) = \prod_n^N\prod_k^K[\mathcal{N}(x_n|\mu_k, \Sigma_k)]^{z_{nk}}\prod_k^K[\pi_k]^{z_{nk}}$
where $pi_k = p(z_n = k)$
Marginal likelihood: z_n are latent variables so they can be factored out from the likelihood $p(x_n|\theta) = \sum\pi_k\mathcal{N}(x_n|\mu_k, \Sigma_k)$. (number of parameters reduced from $O(N)$ to $O(D^2K)$.

9.3 EM

9.3.1 GMM

Intialize $\mu^{(1)}, \Sigma^{(1)}, \pi^{(1)}$.

1. E-step: Compute the assignments. $q_{kn}^{(t)} := \frac{\pi_k^{(t)}\mathcal{N}(x_n|\mu_k^{(t)}, \Sigma_k^{(t)})}{\sum_k^K\pi_k^{(t)}\mathcal{N}(x_n|\mu_k^{(t)}, \Sigma_k^{(t)})}$
2. Compute Marginal Likelihood
3. M-step: Update
$\mu^{(t+1)} = \frac{\sum_n q_{kn}^{(t)}x_n}{\sum_n q_{kn}^{(t)}}$
$\Sigma^{(t+1)} = \frac{\sum_n q_{kn}^{(t)}(x_n - \mu^{(t+1)})(x_n - \mu^{(t+1)})^T}{\sum_n q_{kn}^{(t)}}$
$\pi^{(t+1)} = \frac{1}{N}\sum_n q_{kn}^{(t)}$

9.3.2 General

$\theta^{(t+1)} := argmax_\theta\sum_n^N\mathbb{E}_{p(z_n|x_n, \theta^{(t)})}[log\ p$

10 Quick maff

Chain rule $h = f(g(w)) \rightarrow \partial h(w) = \partial f(g(w))\nabla g(w)$
Gaussian $\mathcal{N}(y|\mu, \sigma^2)\frac{1}{\sqrt{2\pi\sigma^2}}exp(-\frac{(y-\mu)^2}{\sigma^2}$
Multivariate Gaussian $\mathcal{N}(y|\mu, \sigma^2)\frac{1}{\sqrt{(2\pi)^D det(\Sigma)}}exp(-\frac{1}{2}(y - \mu)^T\Sigma^{-1}(y - \mu))$
Bayes rule $p(x|y) = \frac{p(y|x)p(x)}{p(y)}$
Logit $\sigma(x) = \frac{\partial ln[1+e^x]}{\partial x}$
Naming Joint distribution $p(x, y) = p(x|y)p(y) = p(y|x)p(x)$ where

- $p(x|y) \rightarrow$ likelihood
- $p(y) \rightarrow$ prior
- $p(y|x) \rightarrow$ posterior
- $p(x) \rightarrow$ marginal likelihood

Marginal Likelihood
$p(\mathbb{X}|\alpha) = \int_\theta p(\mathbb{X}|\theta)p(\theta|\alpha)\ d\theta$
Posterior probability $\propto$ Likelihood $\times$ Prior
Maximising over a Gaussian is equivalent to minimising MSE:

$\beta^*_{MAP} = argmax_\beta p(y|X,\beta)p(\beta) \Leftrightarrow \beta^* = argmin_\beta \mathcal{L}(\beta)$

Identifiable model $\theta_1 = \theta_2 \rightarrow P_{\theta_1} = P_{\theta_2}$

10.1 Algebra

$(PQ + I_N)^{-1}P = P(QP + I_M)^{-1}$

$\sum_n (y_n - \beta^T \mathbf{x_n})^2 = (\mathbf{y} - \mathbf{X}\beta)^T(\mathbf{y} - \mathbf{X}\beta)$

$\sum_j \beta^2 = \beta^T\beta$

11 Mock Exam Notes

11.1 Normal equation

Unique if convex.

$\frac{1}{\sigma_k^2}X(X^T w_k - y_k) + w_k = 0 \Leftrightarrow$

$w_k^* = (\frac{1}{\sigma_k^2}XX^T + I_D)^{-1}\frac{1}{\sigma_k^2}Xy_k$

11.2 MAP solution

$\mathcal{L}(w) = \sum_k \sum_n \frac{1}{2\sigma_k^2}(y_{nk} - x_n^T w_k)^2 + \frac{1}{2}\sum_k \|w_k\|_2^2 \rightarrow$ Likelihood $p(y|X,w) = \prod_n \prod_k \mathcal{N}(y_{nk}|w_k^T x_n, \sigma_k^2)$ and prior $p(w) = \prod_k \mathcal{N}(w_k|0, I_D)$

11.3 Convexity

$ln[\sum_k^K e^{t_k}]$ is convex. Linear sum of parameters is convex.

11.4 Deriving marginal distribution

$p(y_n|x_n, r_n = k, \beta) = \mathcal{N}(y_n|\beta_k^T\tilde{x}_n, 1)$ Assume r_n follows a multinomial $p(r_n = k|\pi)$. Derive the marginal $p(y_n|x_n,\beta,\pi)$. $p(y_n|x_n, r_n = k,\beta) = \sum_k^K p(y_n, r_n = k|x_n,\beta,\pi) = \sum_k^K p(y_n|r_n = k, x_n, \beta, \pi)\cdot\pi_k = \sum_k^K \mathcal{N}(y_n|\beta_k^T\tilde{x}_n, \sigma^2)\cdot\pi_k$

11.5 MF

$\hat{r}_{um} = \langle \mathbf{v}_u, \mathbf{w}_m\rangle + b_u + b_m$ $\mathcal{L} = \frac{1}{2}\sum_{u\ m}(\hat{r}_{um} - r_{um}) + \frac{\lambda}{2}\left[\sum_u (b_u^2 + \|\mathbf{v}_u\|^2) + \sum_m (b_m^2 + \|\mathbf{w}_m\|^2)\right]$. The optimal value for b_u for a particular user u': $\sum_{u'\ m}(\hat{r}_{u'm} - r_{u'm}) + \lambda b_{u'} = 0$.

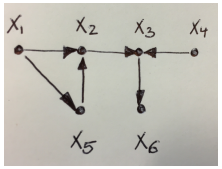
Problem jointly convex? Compute $H(\hat{r}(v,w)) = \begin{bmatrix} 2w^2 & 4vw - 2r \\ 4vw - 2r & 2v^2 \end{bmatrix}$ which is not PSD in general.

12 Multiple Choice Notes

12.1 True statements

- Regularisation term sometimes renders the min. problem into a strictly concave/convex problem.
- k-NN can be applied even if the data cannot be linearly separated.
- $max\{0,x\} = max_{\alpha\in[0,1]}\alpha x$
- $min\{0,x\} = min_{\alpha\in[0,1]}\alpha x$
- $g(x) = min_y f(x,y) \Rightarrow g(x) \leq f(x,y)$
- $max_x g(x) \leq max_x f(x,y)$
- $max_x min_y f(x,y) \leq min_y max_x f(x,y)$
- $\nabla_W(\mathbf{x}^T\mathbf{W}\mathbf{x}) = \mathbf{x}\mathbf{x}^T$
- $\nabla_x(\mathbf{x}^T\mathbf{W}\mathbf{x}) = (\mathbf{W} + \mathbf{W}^T)\mathbf{x}$
- If we initialize the K-means algorithm with optimal clusters then it will find in one step optimal representation points.
- If we initialize the K-means algorithm with optimal representation points then it will find in one step optimal clusters.
- Logistic loss is typically preferred over L_2 loss in classification tasks.
- For optimizing a matrix factorization of a $D\times N$ matrix, for large D, N : *per iteration, ALS has an increased computational cost over SGD* and *per iteration, SGD cost is independent of D, N.*
- A neural net with one hidden layer and an arbitrary number of hidden nodes with sigmoid activation functions can approximate any "sufficiently smooth" function on a bounded domain.
- The complexity of the backpropagation algorithm for a neural net with L layers and K nodes per layer is $O(K^2L)$
- Consider a convolutional net where the data is laid out in a one-dimensional fashion and the filter/kernel has M nonzero terms. Ignoring the bias terms, there are M parameters.

12.2 Bayes nets



- X_1 and X_4 are independent.
- X_1 and X_4 are **not** independent given X_6.
- X_1 and X_4 are independent given X_2.
- X_1 and X_4 are independent given X_2 and X_3.
- X_1 and X_4 are independent given X_5.

12.3 Convex functions

- $f(x) = x^\alpha, x \in \mathbb{R}^+, \forall\alpha \geq 1 or \leq 0$
- $f(x) = -x^3, x \in [-1, 0]$
- $f(x) = e^{ax}, \forall x, a \in \mathbb{R}$
- $f(x) = ln(1/x), x \in \mathbb{R}^+$
- $f(x) = g(h(x)), x \in \mathbb{R}, g, h$ convex and increasing over $\mathbb{R}$
- $f(x) = ax + b, x \in \mathbb{R}, \forall a, b \in \mathbb{R}$
- $f(x) = |x|^p, x \in \mathbb{R}, p \geq 1$
- $f(x) = xlog(x), x \in \mathbb{R}^+$

12.4 Non-convex functions

- $f(x) = x^3, x \in [-1, 1]$
- $f(x) = e^{-x/2}, x \in \mathbb{R}$
- $\sum \mathcal{N}$
- $sin(x) \forall x \in \mathbb{R}$