Basics

Fundamental Assumption

Data is iid for unknown P: $(x_i,y_i)\sim P(X,Y)$

True risk and estimated error

True risk: $R(w)=\int P(x,y)(y-w^Tx)^2\partial x\partial y=\mathbb{E}_{x,y}[(y-w^Tx)^2]$

Est. error: $\hat{R}_D(w)=\frac{1}{|D|}\sum_{(x,y)\in D}(y-w^Tx)^2$

Standardization

Centered data with unit variance: $\tilde{x}_i=\frac{x_i-\hat{\mu}}{\hat{\sigma}}$

$\hat{\mu}=\frac{1}{n}\sum_{i=1}^n x_i$, $\hat{\sigma}^2=\frac{1}{n}\sum_{i=1}^n(x_i-\hat{\mu})^2$

Cross-Validation

For all models m, for all $i\in\{1,...,k\}$ do:

1. Split data: $D=D_{train}^{(i)}\uplus D_{test}^{(i)}$ (Monte-Carlo or k-Fold)
2. Train model: $\hat{w}_{i,m}=\operatorname*{argmin}_w \hat{R}_{train}^{(i)}(w)$
3. Estimate error: $\hat{R}_m^{(i)}=\hat{R}_{test}^{(i)}(\hat{w}_{i,m})$

Select best model: $\hat{m}=\operatorname*{argmin}_m \frac{1}{k}\sum_{i=1}^k\hat{R}_m^{(i)}$

Parametric vs. Nonparametric models

Parametric: have finite set of parameters. e.g. linear regression, linear perceptron

Nonparametric: grow in complexity with the size of the data, more expressive. e.g. k-NN

Gradient Descent

1. Pick arbitrary $w_0\in\mathbb{R}^d$
2. $w_{t+1}=w_t-\eta_t\nabla\hat{R}(w_t)$

Stochastic Gradient Descent (SGD)

1. Pick arbitrary $w_0\in\mathbb{R}^d$
2. $w_{t+1}=w_t-\eta_t\nabla_w l(w_t;x',y')$, with u.a.r. data point $(x',y')\in D$

Regression

Solve $w^*=\operatorname*{argmin}_w \hat{R}(w)+\lambda C(w)$

Linear Regression

$\hat{R}(w)=\sum_{i=1}^n(y_i-w^Tx_i)^2=||Xw-y||_2^2$

$\nabla_w\hat{R}(w)=-2\sum_{i=1}^n(y_i-w^Tx_i)\cdot x_i$

$w^*=(X^TX)^{-1}X^Ty$

Ridge regression

$\hat{R}(w)=\sum_{i=1}^n(y_i-w^Tx_i)^2+\lambda||w||_2^2$

$\nabla_w\hat{R}(w)=-2\sum_{i=1}^n(y_i-w^Tx_i)\cdot x_i+2\lambda w$

$w^*=(X^TX+\lambda I)^{-1}X^Ty$

L1-regularized regression (Lasso)

$\hat{R}(w)=\sum_{i=1}^n(y_i-w^Tx_i)^2+\lambda||w||_1$

Classification

Solve $w^*=\operatorname*{argmin}_w l(w;x_i,y_i)$; loss function l

0/1 loss

$l_{0/1}(w;y_i,x_i)=1$ if $y_i\neq\operatorname{sign}(w^Tx_i)$ else 0

Perceptron algorithm

Use $l_P(w;y_i,x_i)=\max(0,-y_iw^Tx_i)$ and SGD

$$\nabla_w l_P(w;y_i,x_i)=\begin{cases}0 & \text{if } y_iw^Tx_i\geq 0\\ -y_ix_i & \text{otherwise}\end{cases}$$

Data lin. separable $\Leftrightarrow$ obtains a lin. separator (not necessarily optimal)

Support Vector Machine (SVM)

Hinge loss: $l_H(w;x_i,y_i)=\max(0,1-y_iw^Tx_i)$

$$\nabla_w l_H(w;y,x)=\begin{cases}0 & \text{if } y_iw^Tx_i\geq 1\\ -y_ix_i & \text{otherwise}\end{cases}$$

$w^*=\operatorname*{argmin}_w l_H(w;x_i,y_i)+\lambda||w||_2^2$

Kernels

efficient, implicit inner products

Properties of kernel

$k:\mathcal{X}\times\mathcal{X}\to\mathbb{R}$, k must be some inner product (symmetric, positive-definite, linear) for some space $\mathcal{V}$. i.e. $k(\mathbf{x},\mathbf{x}')=\langle\varphi(\mathbf{x}),\varphi(\mathbf{x}')\rangle_{\mathcal{V}}\overset{Eucl.}{=}\varphi(\mathbf{x})^T\varphi(\mathbf{x}')$ and $k(\mathbf{x},\mathbf{x}')=k(\mathbf{x}',\mathbf{x})$

Kernel matrix

$$K=\begin{bmatrix}k(x_1,x_1) & \dots & k(x_1,x_n)\\ \vdots & \ddots & \vdots\\ k(x_n,x_1) & \dots & k(x_n,x_n)\end{bmatrix}$$

Positive semi-definite matrices $\Leftrightarrow$ kernels k

Important kernels

Linear: $k(x,y)=x^Ty$

Polynomial: $k(x,y)=(x^Ty+1)^d$

Gaussian: $k(x,y)=exp(-||x-y||_2^2/(2h^2))$

Laplacian: $k(x,y)=exp(-||x-y||_1/h)$

Composition rules

Valid kernels k_1,k_2, also valid kernels: k_1+k_2; $k_1\cdot k_2$; $c\cdot k_1$, $c>0$; $f(k_1)$ if f polynomial with pos. coeffs. or exponential

Reformulating the perceptron

Ansatz: $w^*\in\operatorname{span}(X)\Rightarrow w=\sum_{j=1}^n\alpha_jy_jx_j$

$\alpha^*=\operatorname*{argmin}_{\alpha\in\mathbb{R}^n}\sum_{i=1}^n\max(0,-\sum_{j=1}^n\alpha_jy_iy_jx_i^Tx_j)$

Kernelized perceptron and SVM

Use α^Tk_i instead of w^Tx_i,

use $\alpha^TD_yKD_y\alpha$ instead of $||w||_2^2$

$k_i=[y_1k(x_i,x_1),...,y_nk(x_i,x_n)]$, $D_y=\operatorname{diag}(y)$

Prediction: $\hat{y}=\operatorname{sign}(\sum_{i=1}^n\alpha_iy_ik(x_i,\hat{x}))$ SGD update: $\alpha_{t+1}=\alpha_t$, if mispredicted: $\alpha_{t+1,i}=\alpha_{t,i}+\eta_t$ (c.f. updating weights towards mispredicted point)

Kernelized linear regression (KLR)

Ansatz: $w^*=\sum_{i=1}^n\alpha_ix$

$\alpha^*=\operatorname*{argmin}_\alpha||\alpha^TK-y||_2^2+\lambda\alpha^TK\alpha$

$=(K+\lambda I)^{-1}y$

Prediction: $\hat{y}=\sum_{i=1}^n\alpha_ik(x_i,\hat{x})$

k-NN

$y=\operatorname{sign}\left(\sum_{i=1}^n y_i[x_i\text{ among }k\text{ nearest neighbours of }x]\right)$ – No weights $\Rightarrow$ no training! But depends on all data :(

Imbalance

up-/downsampling

Cost-Sensitive Classification

Scale loss by cost: $l_{CS}(w;x,y)=c_\pm l(w;x,y)$

Metrics

$n=n_++n_-$, $n_+=TP+FN$, $n_-=TN+FP$

Accuracy: $\frac{TP+TN}{n}$, Precision: $\frac{TP}{TP+FP}$

Recall/TPR: $\frac{TP}{n_+}$, FPR: $\frac{FP}{n_-}$

F1 score: $\frac{2TP}{2TP+FP+FN}=\frac{2}{\frac{1}{prec}+\frac{1}{rec}}$

ROC Curve: y=TPR, x=FPR

TP	FP
FN	FP

Multi-class

one-vs-all (c), one-vs-one ($\frac{c(c-1)}{2}$), encoding

Multi-class Hinge loss

$l_{MC-H}(w^{(1)},...,w^{(c)};x,y)=\max(0,1+\max_{j\in\{1,\cdots,y-1,y+1,\cdots,c\}}w^{(j)T}x-w^{(y)T}x)$

Neural networks

Parameterize feature map with θ: $\phi(x,\theta)=\varphi(\theta^Tx)=\varphi(z)$ (activation function φ)

$\Rightarrow w^*=\operatorname*{argmin}_{w,\theta}\sum_{i=1}^n l(y_i;\sum_{j=1}^m w_j\phi(x_i,\theta_j))$

$f(x;w,\theta_{1:d})=\sum_{j=1}^m w_j\varphi(\theta_j^Tx)=w^T\varphi(\Theta x)$

Activation functions

Sigmoid: $\frac{1}{1+exp(-z)}$, $\varphi'(z)=(1-\varphi(z))\cdot\varphi(z)$

tanh: $\varphi(z)=tanh(z)=\frac{exp(z)-exp(-z)}{exp(z)+exp(-z)}$

ReLU: $\varphi(z)=\max(z,0)$

Predict: forward propagation

$v^{(0)}=x$; for $l=1,...,L-1$:

$v^{(l)}=\varphi(z^{(l)})$, $z^{(l)}=W^{(l)}v^{(l-1)}$

$f=W^{(L)}v^{(L-1)}$

Predict f for regression, $\operatorname{sign}(f)$ for class.

Compute gradient: backpropagation

Output layer: $\delta_j=l_j'(f_j)$, $\frac{\partial}{\partial w_{j,i}}=\delta_jv_i$

Hidden layer $l=L-1,...,1$:

$\delta_j=\varphi'(z_j)\cdot\sum_{i\in Layer_{l+1}}w_{i,j}\delta_i$, $\frac{\partial}{\partial w_{j,i}}=\delta_jv_i$

Learning with momentum

$a\leftarrow m\cdot a+\eta_t\nabla_W l(W;y,x)$; $W_{t+1}\leftarrow W_t-a$

Clustering

k-mean

$\hat{R}(\mu)=\sum_{i=1}^n\min_{j\in\{1,...k\}}||x_i-\mu_j||_2^2$

$\hat{\mu}=\operatorname*{argmin}_\mu \hat{R}(\mu)$ ...non-convex, NP-hard

Algorithm (Lloyd's heuristic): Choose starting centers, assign points to closest center, update centers to mean of each cluster, repeat

Dimension reduction

PCA

$D=x_1,...,x_n\subset\mathbb{R}^d$, $\Sigma=\frac{1}{n}\sum_{i=1}^n x_ix_i^T$, $\mu=0$

$(W,z_1,...,z_n)=\operatorname{argmin}\sum_{i=1}^n||Wz_i-x_i||_2^2$,

$W=(v_1|...|v_k)\in\mathbb{R}^{d\times k}$, orthogonal; $z_i=W^Tx_i$

v_i are the eigen vectors of Σ

Kernel PCA

Kernel PC: $\alpha^{(1)},...,\alpha^{(k)}\in\mathbb{R}^n$, $\alpha^{(i)}=\frac{1}{\sqrt{\lambda_i}}v_i$,

$K=\sum_{i=1}^n\lambda_iv_iv_i^T$, $\lambda_1\geq...\geq\lambda_d\geq 0$

New point: $\hat{z}=f(\hat{x})=\sum_{j=1}^n\alpha_j^{(i)}k(\hat{x},x_j)$

Autoencoders

Find identity function: $x\approx f(x;\theta)$

$f(x;\theta)=f_{decode}(f_{encode}(x;\theta_{encode});\theta_{decode})$

Probability modeling

Find $h:X\to Y$ that min. pred. error: $R(h)=\int P(x,y)l(y;h(x))\partial y\partial x\partial y=\mathbb{E}_{x,y}[l(y;h(x))]$

For least squares regression

Best h: $h^*(x)=\mathbb{E}[Y|X=x]$

Pred.: $\hat{y}=\hat{\mathbb{E}}[Y|X=\hat{x}]=\int\hat{P}(y|X=\hat{x})y\partial y$

Maximum Likelihood Estimation (MLE)

$\theta^*=\operatorname*{argmax}_\theta \hat{P}(y_1,...,y_n|x_1,...,x_n,\theta)$

E.g. lin. + Gauss: $y_i=w^Tx_i+\varepsilon_i,\varepsilon_i\sim\mathcal{N}(0,\sigma^2)$ i.e. $y_i\sim\mathcal{N}(w^Tx_i,\sigma^2)$, With MLE (use argmin $-\log$): $w^*=\operatorname*{argmin}_w\sum(y_i-w^Tx_i)^2$

Bias/Variance/Noise

Prediction error $=Bias^2+Variance+Noise$

Maximum a posteriori estimate (MAP)

Introduce bias o reduce variance. The small weight assumption is a Gaussian prior $w_i\in\mathcal{N}(0,\beta^2)$

Bay.: $P(w|x,y)=\frac{P(w|x)P(y|x,w)}{P(y|x)}=\frac{P(w)P(y|x,w)}{P(y|x)}$

Now we want to find MAP for w:

$$\hat{w} = argmax_w p(w|\bar{x},\bar{y})$$
$$= argmin_w - \log \frac{p(w) \cdot p(y|x,w)}{p(y|w)}$$
$$= argmin_w \frac{\sigma^2}{\beta^2}||w||_2^2 + \sum_{i=1}^{n}(y_i - w^T x_i)^2$$

Regularization can be understood as MAP inference, with different priors (= regularizers) and likelihoods (= loss functions).

Logistic regression

Link func.: $\sigma(w^T x) = \frac{1}{1+\exp(-w^T x)}$ (Sigmoid)
$P(y|x, w) = Ber(y; \sigma(w^T x)) = \frac{1}{1+\exp(-yw^T x)}$
Classification: Use $P(y|x,w)$, predict most likely class label.
MLE: $\underset{w}{\text{argmax}}\ P(y_{1:n}|w,x_{1:n})$
$\Rightarrow w^* = \underset{w}{\text{argmin}} \sum_{i=1}^n \log(1+\exp(-y_i w^T x_i))$
SGD update: $w = w + \eta_t y x \hat{P}(Y=-y|w,x)$
$\hat{P}(Y=-y|w,x) = \frac{1}{1+\exp(yw^T x)}$
MAP: Gauss. prior $\Rightarrow ||w||_2^2$, Lap. p. $\Rightarrow ||w||_1$
SGD: $w = w(1-2\lambda\eta_t) + \eta_t y x \hat{P}(Y=-y|w,x)$

Bayesian decision theory

- Conditional distribution over labels $P(y|x)$
- Set of actions $\mathcal{A}$
- Cost function $C: Y \times \mathcal{A} \to \mathbb{R}$

$a^* = \underset{a\in\mathcal{A}}{\text{argmin}}\ \mathbb{E}[C(y,a)|x]$
Calculate $\mathbb{E}$ via sum/integral.
Classification: $C(y,a) = [y \neq a]$; asymmetric:

$$C(y,a) = \begin{cases} c_{FP}, \text{ if } y=-1, a=+1 \\ c_{FN}, \text{ if } y=+1, a=-1 \\ 0, \text{ otherwise} \end{cases}$$

Regression: $C(y,a) = (y-a)^2$; asymmetric: $C(y,a) = c_1 \max(y-a,0) + c_2 \max(a-y,0)$
E.g. $y \in \{-1,+1\}$, predict $+$ if $c_+ < c_-$, $c_+ = \mathbb{E}(C(y,+1)|x) = P(y=1|x)\cdot 0 + P(y=-1|x)\cdot c_{FP}$, c_- likewise

Discriminative / generative modeling

Discr. estimate $P(y|x)$, generative $P(y,x)$
Approach (generative): $P(x,y) = P(x|y)\cdot P(y)$ -
Estimate prior on labels $P(y)$
- Estimate cond. distr. $P(x|y)$ for each class y
- Pred. using Bayes: $P(y|x) = \frac{P(y)P(x|y)}{P(x)}$

$P(x) = \sum_y P(x,y)$

Examples

MLE for $P(y) = p = \frac{n_+}{n}$
MLE for $P(x_i|y) = \mathcal{N}(x_i; \mu_{i,y}, \sigma_{i,y}^2)$:
$\hat{\mu}_{i,y} = \frac{1}{n_y}\sum_{x\in D_{x_i|y}} x$
$\hat{\sigma}_{i,y}^2 = \frac{1}{n_y}\sum_{x\in D_{x_i|y}} (x-\hat{\mu}_{i,y})^2$
MLE for Poi.: $\lambda = \text{avg}(x_i)$
$\mathbb{R}^d$: $P(X=x|Y=y) = \prod_{i=1}^d Pois(\lambda_y^{(i)}, x^{(i)})$

Deriving decision rule

$P(y|x) = \frac{1}{Z}P(y)P(x|y)$, $Z = \sum_y P(y)P(x|y)$
$y^* = \underset{y}{\text{amax}}\ P(y|x) = \underset{y}{\text{amax}}\ P(y)\prod_{i=1}^d P(x_i|y)$

Gaussian Bayes Classifier

$\hat{P}(x|y) = \mathcal{N}(x; \hat{\mu}_y, \hat{\Sigma}_y)$
$\hat{P}(Y=y) = \hat{p}_y = \frac{n_y}{n}$
$\hat{\mu}_y = \frac{1}{n_y}\sum_{i:y_i=y} x_i \in \mathbb{R}^d$
$\hat{\Sigma}_y = \frac{1}{n_y}\sum_{i:y_i=y}(x_i - \hat{\mu}_y)(x_i-\hat{\mu}_y)^T \in \mathbb{R}^{d\times d}$

Fisher's lin. discrim. analysis (LDA, c=2)

Assume: $p=0.5$; $\hat{\Sigma}_- = \hat{\Sigma}_+ = \hat{\Sigma}$
discriminant function: $f(x) = \log\frac{p}{1-p} + \frac{1}{2}[\log\frac{|\hat{\Sigma}_-|}{|\hat{\Sigma}_+|} + \left((x-\hat{\mu}_-)^T \hat{\Sigma}_-^{-1}(x-\hat{\mu}_-)\right) - \left((x-\hat{\mu}_+)^T\hat{\Sigma}_+^{-1}(x-\hat{\mu}_+)\right)]$
Predict: $y = \text{sign}(f(x)) = \text{sign}(w^T x + w_0)$
$w = \hat{\Sigma}^{-1}(\hat{\mu}_+ - \hat{\mu}_-)$;
$w_0 = \frac{1}{2}(\hat{\mu}_-^T\hat{\Sigma}^{-1}\hat{\mu}_- - \hat{\mu}_+^T\hat{\Sigma}^{-1}\hat{\mu}_+)$

Outlier Detection

$P(x) \le \tau$

Categorical Naive Bayes Classifier

MLE for feature distr.: $\hat{P}(X_i = c|Y=y) = \theta_{c|y}^{(i)}$
$\theta_{c|y}^{(i)} = \frac{Count(X_i=c, Y=y)}{Count(Y=y)}$
Prediction: $y^* = \underset{y}{argmax}\hat{P}(y|x)$

Missing data

Mixture modeling

Model each c. as probability distr. $P(x|\theta_j)$
$P(D|\theta) = \prod_{i=1}^n \sum_{j=1}^k w_j P(x_i|\theta_j)$
$L(w,\theta) = -\sum_{i=1}^n \log\sum_{j=1}^k w_j P(x_i|\theta_j)$

Gaussian-Mixture Bayes classifiers

Estimate prior $P(y)$; Est. cond. distr. for each class: $P(x|y) = \sum_{j=1}^{k_y} w_j^{(y)} \mathcal{N}(x; \mu_j^{(y)}, \Sigma_j^{(y)})$

Hard-EM algorithm

Initialize parameters $\theta^{(0)}$
E-step: Predict most likely class for each point:
$z_i^{(t)} = \underset{z}{\text{argmax}}\ P(z|x_i, \theta^{(t-1)})$
$= \underset{z}{\text{argmax}}\ P(z|\theta^{(t-1)})P(x_i|z,\theta^{(t-1)})$;
M-step: Compute the MLE: $\theta^{(t)} = \underset{\theta}{\text{argmax}} P(D^{(t)}|\theta)$, i.e. $\mu_j^{(t)} = \frac{1}{n_j}\sum_{i:z_i=j} x_i$

Soft-EM algorithm

E-step: Calc p for each point and cls.: $\gamma_j^{(t)}(x_i)$
M-step: Fit clusters to weighted data points:
$w_j^{(t)} = \frac{1}{n}\sum_{i=1}^n \gamma_j^{(t)}(x_i)$; $\mu_j^{(t)} = \frac{\sum_{i=1}^n \gamma_j^{(t)}(x_i) x_i}{\sum_{i=1}^n \gamma_j^{(t)}(x_i)}$
$\sigma_j^{(t)} = \frac{\sum_{i=1}^n \gamma_j^{(t)}(x_i)(x_i-\mu_j^{(t)})^T(x_i-\mu_j^{(t)})}{\sum_{i=1}^n \gamma_j^{(t)}(x_i)}$

Soft-EM for semi-supervised learning

labeled y_i: $\gamma_j^{(t)}(x_i) = [j = y_i]$, unlabeled:
$\gamma_j^{(t)}(x_i) = P(Z=j|x_i, \mu^{(t-1)}, \Sigma^{(t-1)}, w^{(t-1)})$

Useful math

Probabilities

$$\mathbb{E}_x[X] = \begin{cases} \int x \cdot p(x)\partial x & \text{if continuous} \\ \sum_x x\cdot p(x) & \text{otherwise} \end{cases}$$

$\text{Var}[X] = \mathbb{E}[(X-\mu_X)^2] = \mathbb{E}[X^2] - \mathbb{E}[X]^2$
$P(A|B) = \frac{P(B|A)\cdot P(A)}{P(B)}$; $p(Z|X,\theta) = \frac{p(X,Z|\theta)}{p(X|\theta)}$
$P(x,y) = P(y|x)\cdot P(x) = P(x|y)\cdot P(y)$

Bayes Rule

$P(A|B) = \frac{P(B|A)\cdot P(A)}{P(B)}$

P-Norm

$||x||_p = (\sum_{i=1}^n |x_i|^p)^{\frac{1}{p}}$, $1 \le p < \infty$

Some gradients

$\nabla_x ||x||_2^2 = 2x$
$f(x) = x^T A x$; $\nabla_x f(x) = (A+A^T)x$
E.g. $\nabla_w \log(1+\exp(\text{-yw}^\text{T}\text{x})) = \frac{1}{1+\exp(-yw^T x)}\cdot\exp(-yw^T x)\cdot(-yx) = \frac{1}{1+\exp(yw^T x)}\cdot(-yx)$

Convex / Jensen's inequality

g(x) convex $\Leftrightarrow g''(x) > 0 \Leftrightarrow x_1, x_2 \in \mathbb{R}, \lambda \in [0,1]$:
$g(\lambda x_1 + (1-\lambda)x_2) \le \lambda g(x_1) + (1-\lambda) g(x_2)$

Gaussian / Normal Distribution

$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} exp(-\frac{(x-\mu)^2}{2\sigma^2})$

Multivariate Gaussian

$\Sigma =$ covariance matrix, μ = mean
$f(x) = \frac{1}{2\pi\sqrt{|\Sigma|}} e^{-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)}$

Empirical: $\hat{\Sigma} = \frac{1}{n}\sum_{i=1}^n x_i x_i^T$ (needs centered data points)

Positive semi-definite matrices

$M \in \mathbb{R}^{n\times n}$ is psd $\Leftrightarrow$
$\forall x \in \mathbb{R}^n : x^T M x \ge 0 \Leftrightarrow$
all eigenvalues of M are positive: $\lambda_i \ge 0$