Classification

k-Nearest Neighbors

kNNs are bounded by $\leq$ 2x the Bayes optimal error, $N, k \to \infty, k/N \to 0$.

Edge Case	2 pts w/ same features but diff classes.
Robustness	Generalizes better to test data.
Fit	Better training classification.
Validation	Hold back data subset as validation set. Train multiple times w/ diff hyperparams. Choose what is best on validation set.
Training Set	Used to learn model weights.
Validation Set	Tunes hyperparameters (ex. $k \in k$NN).
Test Set	used as FINAL evaluation of model.
Isocontour of f	$L_c = \{x \mid f(x) = c\}$, with isovalue c.
Isotropic Gaussian	Same var in ea dir: $\Sigma = cI$.
Anisotropic Gaussian	Allows diff amnts of var along diff dirs, $\Sigma \succ 0$.

Perceptron

Model/rule: 1 if $\vec{X_i} \cdot \vec{w} \geq 0$ elif $\vec{X_i} \cdot \vec{w} \leq 0 \implies$ -1.
Loss: $L(z, y_i) = 0$ if $y_i z \geq 0$ else $-y_i z$, (z=pred, y_i=true ans).

$$R(w) = \sum_{i=1}^{n} L\left(X_i \cdot w, y_i\right) = \sum_{i \in V} -y_i X_i \cdot w$$

Gives some linear boundary; if data is linearly separable, correctly classifies all data in at most $O\left(\frac{r^2}{\gamma^2}\right)$ iterations.

Support Vector Machines

Hard-Margin: $\min_{\vec{w},b} \|\vec{w}\|_2^2$, s.t. $y_i(\vec{w}^\top \vec{x_i} - b) \geq 1 \ \forall i$

Fails w/ non-linearly sep. data. Margin size = $\frac{1}{\|w\|}$, Slab size = $\frac{2}{\|w\|}$

Hyperplane	$H = \{x : w \cdot x = -\alpha\}$ flat, infinite, $\dim(d-1)$ plane
$x, y \in H$	$\vec{w} \cdot (y - x) = 0, \vec{w}$ is normal vec of H.
Support Vectors	Examples needed to find $f(\mathbf{x}) \in$ SVM. Examples with non-0 weight $\alpha_k \in$ SVM.

Soft-Margin

Allows misclassifications: $\min_{\vec{w},b,\xi_i} \frac{1}{2}\|\vec{w}\|^2 + C\sum_{i=1}^{n} \xi_i$ s.t.

$$y_i(\vec{w}^\top \vec{x_i} - b) \geq 1 - \xi_i, \quad \forall i; \quad \xi_i \geq 0, \quad \forall i$$

Small C: maximize margin, underfitting, less sensitive, more flat.
Big C: minimize margin, overfitting, very sensitive, more sinuous.
$C \to \infty \implies$ Soft-Margin $\to$ Hard-Margin. Note $C \geq 0$.

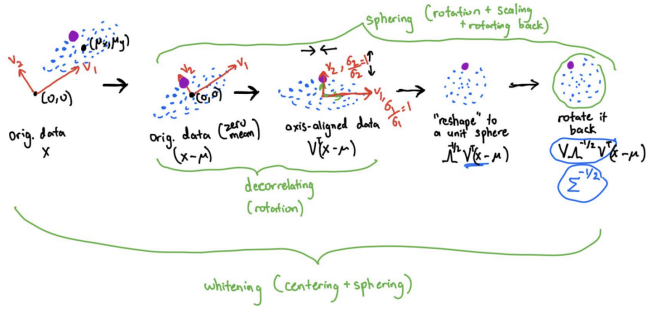
Generative

Want to learn **everything** about data before you classify:
the **priors** $\hat{\pi}_i = \Pr(Y = C_i)$ and **cond. dist** $\mathbb{P}(X|Y = C_i)$.
Posterior: $\mathbb{P}(Y = C_i|X) = \frac{\mathbb{P}(X|Y=C_i)\cdot\mathbb{P}(Y=C_i)}{\mathbb{P}(X)}$

Logistic Function:	$\frac{1}{1+e^{-h(x)}}$, where $h(x)$ is **linear** in terms of features. True in LDA but not QDA (where $h(x)$ is quadratic).
GDA:	Assumes each class models a Gaussian distribution.
QDA:	Works with any number of classes; $\frac{d(d+3)}{2} + 1$ params.
LDA:	when variances are equal; $d + 1$ params.

Isotropic:
QDA: $\widehat{\sigma}^2 = \frac{1}{dn}\sum_{i:y_i=C} \|x_i - \widehat{\mu_C}\|^2$
LDA: $\widehat{\sigma}^2 = \frac{1}{dn}\sum_{C}\sum_{i:y_i=C} \|x_i - \widehat{\mu_C}\|^2$
Anisotropic:
QDA: $\widehat{\Sigma}_c = \frac{1}{n_c}\sum_{i:y_i=C}(X_i - \widehat{\mu_C})(X_i - \widehat{\mu_C})^\top$
LDA: $\widehat{\Sigma} = \frac{1}{n}\sum_{C}\sum_{i:y_i=C}(X_i - \widehat{\mu_C})(X_i - \widehat{\mu_C})^T$

Choose C to maximize discriminant:
QDA: $Q_C = -\frac{1}{2}(x - \mu_C)^\top \Sigma_C^{-1}(x - \mu_C) - \frac{1}{2}\ln|\Sigma_C| + \ln \pi_C$
LDA: $Q_C = \mu_C^\top \Sigma^{-1} x - \frac{\mu_C^\top \Sigma^{-1} \mu_C}{2} + \ln \pi_C$

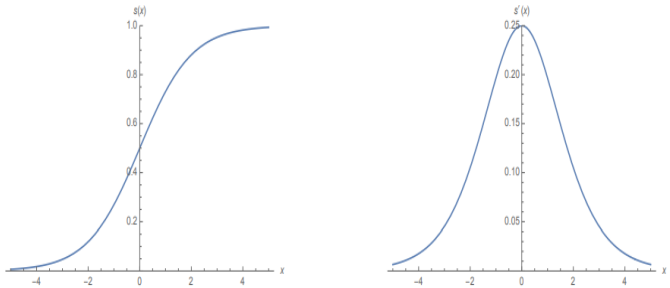


Discriminative

Want to learn a *few* things before trying to classify.
Only tries to model $\mathbb{P}(Y|X)$ from training data.
Logistic Reg (2 classes): For a training point, $P(Y = y_i \mid x) = p^{y_i}(1-p)^{1-y_i}$. Note that $p = s\left(w^T x\right)$ as given by our model of the posterior $P(Y = 1 \mid x)$. MLE on this leads to the cross entropy loss function (which is convex!), namely

$$L(w) = -\sum \Big(y_i \ln p_i + (1 - y_i)\ln(1 - p_i)\Big)$$

Note: $P(Y = 1 \mid x) = \frac{1}{1+\exp(-w^T x)}$; $s'(\gamma) = s(\gamma)(1 - s(\gamma))$
Sigmoid Function: $s(\gamma) = \frac{1}{1+e^{-\gamma}}$



Decision Boundary: of the form $w^T x > c_1$ thus must be linear.
Though probability predictions are non-linear, actual boundary is linear. Log Reg always separates linearly separable points.
Softmax Reg: logistic regression for multiple classes

Probability

Multivariate Gaussian PDF:
$f_{\mathbf{X}}(x_1, \ldots, x_k) = \frac{\exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\mathrm{T}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right)}{\sqrt{(2\pi)^k|\boldsymbol{\Sigma}|}}$

MLE (Maximum Likelihood Estimate)

We have A, B, C, D. $P(A \mid B) > P(A \mid C) > P(A \mid D)$
$\implies B$ is the MLE of A. MLE Estimate of Anisotropic can be PSD.
$\hat{\theta}_{MLE}(x) = \arg\max_{\theta} \Pi f(x \mid \theta) = \arg\max_{\theta} \ln \mathcal{L}(\theta; x)$
Mean is unbiased; Variance is biased (usually underestimate)
Predicts parameter which max the probability of the data.
Implicitly assumes uniform prior

MAP (Maximum a Posteriori)

We have A, B, C, D. $\mathbb{P}(A \mid B) > \mathbb{P}(C \mid B) > \mathbb{P}(D \mid B)$
$\implies A$ is the MAP of B.

$\hat{\theta}_{MAP} = \arg\max_{\theta} f(\theta \mid x) = \arg\max_{\theta} f(x \mid \theta) \cdot g(\theta)$
Predicts the parameter which maximizes the conditional probability of the parameter given the data.
Should be used when you have the prior probabilities.

MLE = MAP when all parameters have equal prior probability.
The axis lengths of Gaussian Isocontours are σ_i s.t. $\sigma^2(X) = \mathrm{Var}(X)$. Independent $\iff$ uncorrelated (only for MVGs).

Bayesian Risk

L (loss function) is symmetric: pick class with max posterior prob.
L is asymmetric: minimize $\mathbb{E}[L(\text{true class}, \text{prediction}) \mid \text{data}]$ or pick max loss-weighted posterior prob.
The risk for r is the expected loss over all values of x, y. Equals to 0 when class distros don't overlap or prior prob for one class is 1. Let C be the set of classes Y can take.

$$\begin{aligned} R(r) &= \mathbb{E}[L(r(X), Y)] \\ &= \sum_x \left(\sum_{c \in C} L(r(x), c) P(Y = c \mid X = x)\right) P(X = x) \\ &= \sum_{c \in C} \left(P(Y = c) \sum_x L(r(x), c) P(X = x \mid Y = c)\right) \\ &= R(\hat{y} = i \mid x) = \sum_{j=1}^{n} \lambda_{ij} P(Y = j \mid x) \end{aligned}$$

The Bayes decision rule aka Bayes classifier is the fn r^* that minimizes functional $R(r)$. Assuming $L(z, y) = 0$ for $z = y$:

$$r^*(x) = \begin{cases} 1 \text{ if } L(-1,1)P(Y = 1 \mid X = x) > L(1,-1)P(Y = -1 \mid X = x) \\ -1 \text{ otherwise} \end{cases}$$

Regression Methods

Model: $y = Xw$, Loss Function: least squares, $n \in N(X)$

Name	Objective	Solution
OLS	$\frac{1}{n}\|Y - Xw\|_2^2$	$w^* = (X^\top X)^\dagger X^\top y \in X^\dagger y + n$
Ridge: Assumes Gaussian Priors	$\frac{1}{n}\|Y - Xw\|_2^2 + \lambda\|w\|_2^2$	$w^* = (X^\top X + n\lambda I)^{-1} X^\top y$
LASSO	$\frac{1}{n}\|Y - Xw\|_2^2 + \lambda\|w\|_1$	No closed form

Linear Algebra

Matrix Calculus

$\nabla_{\vec{x}} \vec{w}^\top \vec{x} = \left(\frac{\partial \vec{w}^\top \vec{x}}{\partial \vec{x}}\right)^\top = \vec{w}$ $\quad$ $\nabla_{\vec{x}} (\vec{w}^\top A \vec{x}) = A^\top \vec{w}$

$\nabla_A \vec{w}^\top A \vec{x} = \vec{w}\vec{x}^\top$ $\quad$ $\nabla_{\vec{x}} (\vec{x}^\top A \vec{x}) = (A + A^\top)\vec{x}$

$\nabla^2_{\vec{x}} (\vec{x}^\top A \vec{x}) = A + A^\top$ $\quad$ $\nabla_{\vec{x}} (\alpha \vec{y}) = (\nabla_{\vec{x}} \alpha)\vec{y}^\top + \alpha \nabla_{\vec{x}} \vec{y}$

$\nabla_{\vec{x}} \vec{f}(\vec{y}) = (\nabla_{\vec{x}} \vec{y})(\nabla_{\vec{y}} \vec{f}(\vec{y}))$ $\quad$ $\nabla_{\vec{x}} (\vec{y} \cdot \vec{z}) = (\nabla_{\vec{x}} \vec{y})\vec{z} + (\nabla_{\vec{x}} \vec{z})\vec{y}$

$\nabla_{\vec{x}} C\vec{y}(\vec{x}) = (\nabla_{\vec{x}} \vec{y}(\vec{x}))C^\top$ $\quad$ $\frac{\partial \|\vec{x}\|_2^2}{\partial \vec{x}} = \frac{\partial (\vec{x}^\top \vec{x})}{\partial \vec{x}} = 2\vec{x}$

$$\nabla_{\vec{y}} (\vec{y} - A\vec{x})^\top W (\vec{y} - A\vec{x}) = 2W(\vec{y} - A\vec{x})$$

$$\nabla_{\vec{x}} (\vec{y} - A\vec{x})^\top W (\vec{y} - A\vec{x}) = -2A^\top W (\vec{y} - A\vec{x})$$

$$\nabla_{\vec{w}} \left(\|X\vec{w} - \vec{y}\|_2^2 + \lambda \|\vec{w}\|_2^2 \right) = 2X^\top X\vec{w} - 2X^\top \vec{y} + 2\lambda \vec{w}$$

Matrix A is Positive Semi-Definite iff

(a) $\forall \vec{x} \neq \vec{0} \in \mathbb{R}^n, \vec{x}^\top A \vec{x} \geq 0$. Symmetric.

(b) All eigenvalues of A are non-negative ($\lambda_i \geq 0$).

(c) $\exists$ unique matrix $L \in \mathbb{R}^{n \times n}$ such that $A = LL^\top$ (Cholesky decomposition).

PSD Example: $A = \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}$, with $\lambda = 3, 1$. $L = \begin{bmatrix} 1 & 0 \\ -1 & 1 \end{bmatrix}$.
All diagonal entries of A are non-negative and $\text{Tr}(A) \geq 0$.
Sum of all the entries ≥ 0. $\text{Var}(Mx) = M \,\text{Var}(x) M^T$, M is constant. $M \succ 0, N \succ 0, M - N \succeq 0 \implies N^{-1} - M^{-1} \succeq 0$
$M \succeq 0, N \succeq 0 \implies M - N \succeq 0 \iff \lambda_{\min}(M) > \lambda_{\max}(N)$.
$A = A^{\frac{1}{2}} A^{\frac{1}{2}} = U\Lambda^{\frac{1}{2}} \Lambda^{\frac{1}{2}} U^\top$, $A^{\frac{1}{2}} = U\Lambda^{\frac{1}{2}} U^\top$
A function is convex iff Hessian is PSD. Strict Convexity:
$(\forall 0 < t < 1), f(tx_1 + (1-t)x_2) < tf(x_1) + (1-t)f(x_2)$

Covariance Matrix

$$\Sigma = \frac{1}{n} \hat{X}^\top X = \begin{bmatrix} \text{Var}(X_1) & \text{Cov}(X_1, X_2) & \cdots & \text{Cov}(X_1, X_d) \\ \text{Cov}(X_2, X_1) & \text{Var}(X_2) & \cdots & \text{Cov}(X_2, X_d) \\ \vdots & \vdots & \ddots & \vdots \\ \text{Cov}(X_d, X_1) & \text{Cov}(X_d, X_2) & \cdots & \text{Var}(X_d) \end{bmatrix}$$

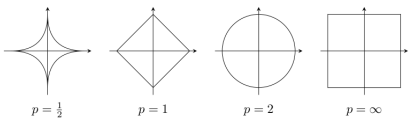
$= \mathbb{E}[(X - \mu)^\top (X - \mu)]$ where $X \in \mathbb{R}^{n \times d}$, all diag entries > 0

Symmetric, PSD $\implies \exists \Sigma = V\Lambda V^\top$ by Spectral Theorem. PD $\implies$ symmetric in this class. Eigenvectors are orthogonal directions along which points are uncorrelated. $\Sigma^{-1} = V\Lambda^{-1}V^\top = \sum_i \frac{1}{\Lambda_{ii}} v_i v_i^\top$

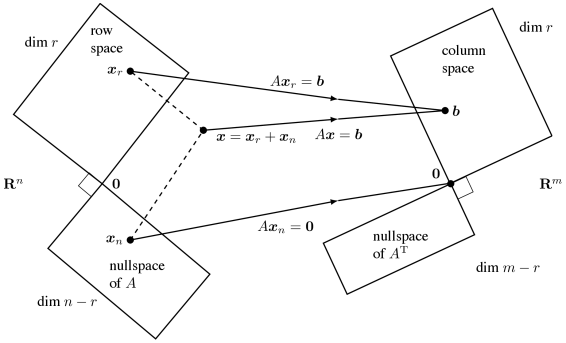
Spectral Theorem: $A = V\Lambda V^\top$. All real+symmetric $n \times n$ matrices have real eigenvalues and n eigenvectors that are mutually orthogonal: $v_i^\top v_j = 0 \quad \forall i \neq j$.

Norm Ball

ℓ_0 and ℓ_1 encourage sparsity (more than ℓ_2).



Fundamental Theorem of Linear Algebra



$(N(A)^\perp = R(A^\top)) \oplus (N(A^\top A) = N(A) = R(A^\top)^\perp) = \mathbb{R}^n$
$(N(A^\top)^\perp = R(A)) \oplus (N(A^\top) = R(A)^\perp) = \mathbb{R}^m$
Rank-nullity Theorem: $\dim(R(A)) + \dim(N(A)) = n$
Jensen's Inequality: If $f(x)$ is strictly convex, $\mathbb{E}[f(x)] > f(\mathbb{E}[x])$.
$\dim(\text{Row}(X)) = \dim(R(X^\top)) = \text{rank}(X^\top) = \text{rank}(X)$.
$\text{Row}(X^\top X) = R(X^\top X) = \text{Row}(X) = R(X^\top)$

Update Rule

Gradient Descent: $w^{(t+1)} \leftarrow w^{(t)} - \eta \nabla_w J(w^{(t)})$
Logistic Reg: $w^{(t+1)} \leftarrow w^{(t)} + \epsilon X^\top \left(y - s(Xw^{(t)})\right)$

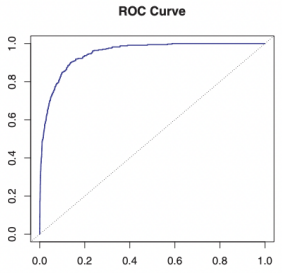
Newton's Method: $w^{(t+1)} \leftarrow w^{(t)} - (\nabla_w^2 J(w^{(t)}))^{-1} \nabla_w J(w^{(t)})$
*** Note: If J quadratic, Newton's method only needs one step to find exact solution. Newton's Method doesn't work for most nonsmooth functions, and is generally faster than BGD/SGD.

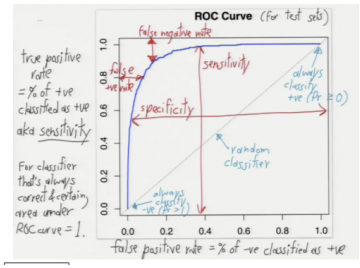
Stochastic GD: $w \leftarrow w - \epsilon \nabla_w J(w)_i$ for some $i \in U([1, \ldots, n])$
Logistic Reg: $w \leftarrow w + \epsilon(y_i - s(X_i \cdot w))X_i$

Cost Functions

$y_i = f(X_i) + \epsilon_i$: ϵ_i from Gaussian, all ϵ_i same mean, all y_i same var
General: $J = \sum_{i=1}^n L(X_i \cdot w, y_i)$
Linear: $J = \sum_{i=1}^n (X_i \cdot w + \alpha - y_i)^2 = \|Xw - y\|_2^2$
Logistic: $J = -\sum_{i=1}^n (y_i \ln s(X_i \cdot w) + (1 - y_i) \ln(1 - s(X_i \cdot w)))$
Weight LS: $J = \sum_{i=1}^n w_i (X_i \cdot w - y_i)^2 = (Xw - y)^\top \Omega (Xw - y)$

ROC Curve





Design Matrix

Centering: subtracting $\mu^\top$ from each row of X: $X \to \dot{X}$
Decorrelating: Applying rotation $Z = \dot{X}V$ where $\text{Var}(X) = V\Lambda V^\top$. Covariance matrix of Z is Λ (diagonal)
Sphering: $W = \dot{X}\,\text{Var}(X)^{-1/2}$ ($\Sigma^{-1/2}$:ellipsoid to sphere)
Whitening: Perform centering, and then sphering

Bias-Variance Tradeoff

Statistical Bias: $\mathbb{E}[\hat{\theta} - \theta] = \mathbb{E}[\hat{\theta}] - \theta$.

Bias: error due to inability of hypothesis h to fit g perfectly e.g., fitting quadratic g with a linear h
Variance: error due to fitting random noise in data e.g., we fit linear g with a linear h, yet $h \neq g$.

Overfitting: Low Bias, High Variance
Underfitting: High Bias, Low Variance.

Adding a feature usually increases variance [don't add a feature unless it reduces bias more]. Adding a feature results in a non-increasing bias.

Forward/Backward stepwise selection aren't guaranteed to find optimal features. Backward stepwise selection looks at $d' - 1$ features at a time, where d' is current num of features (one at a time). Use Forward selection if we think few features important, Backward selection if many features important.

higher residuals $\implies$ higher bias
higher complexity $\implies$ higher variance

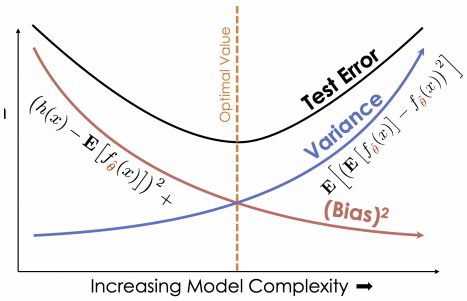
$\text{Var}(h(z)) = E\left[(h(z) - E[h(z)])^2\right] \approx \sigma^2 \frac{d}{n}$

Bias-Variance Decomposition:
Model Risk $= \mathbb{E}[L(h(z), \gamma)] = \mathbb{E}[(h(z) - \gamma)^2]$

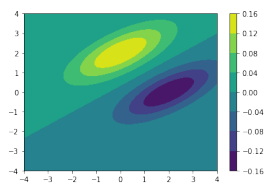
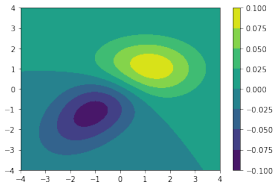
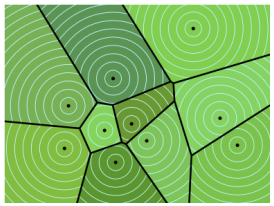
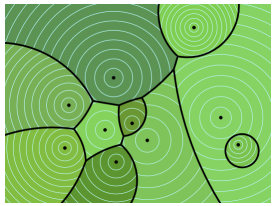
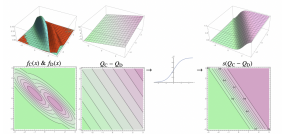
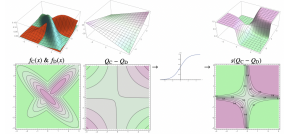
$$= \underbrace{(\mathrm{E}[h(z)] - g(z))^2}_{\text{bias}^2 \text{ of method}} + \underbrace{\text{Var}(h(z))}_{\text{variance of method}} + \underbrace{\text{Var}(\epsilon)}_{\text{irreducible error}}$$

where $\mathrm{E}[\gamma] = g(z)$; $\text{Var}(\gamma) = \text{Var}(\epsilon)$.

Note: the model determines Bias-Variance Tradeoff, not the algorithm used to solve the model/optimization problem.



Isocontour/Voronoi Diagrams

LDA: same variance; decision boundary is linear

QDA: different variance; decision boundary is curved towards class(es) w/ lower variance

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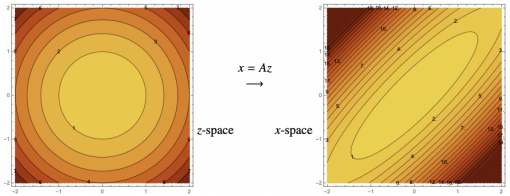

Quadratic Form: $x^\top A^{-2} x = \|A^{-1}x\|_2^2$ is an ellipsoid with axes $v_1, v_2, \ldots v_n$ (eigenvectors of A) and radii $\lambda_1, \lambda_2, \ldots, \lambda_n$ (eigenvalues of A). Note that $A > 0$.

Gaussian with covariance matrix $\Sigma = \frac{1}{n}\hat{X}^\top \hat{X}$ isocontours with radii of length $\sqrt{\lambda_i(\Sigma)} = \sigma_i(X)$

Decision Trees

Tree with each node denoting a split over some feature. Leaf node specifies class. deep decision tree = overfit = high variance

Calculate entropy (2 classes C, D): $H(S) = -\sum_C p_C \log_2 p_C$

$p_C = \frac{|\{i \in S : y_i = C\}|}{|S|}$.

Choose split that maximizes information gain

$H(S) - H_{\text{after}} = H(S) - \frac{|S_l| H(S_l) + |S_r| H(S_r)}{|S_l| + |S_r|}$.

Classification: worst case $O(depth)$, often $O(\log n)$

Training: $O(nd)$, at each split point try $O(d)$ splits.

Regression: Leaf stores label $\mu_S = \frac{1}{|S|}\sum_{i \in S} y_i$

Cost $J(S) = \text{Var}(\{y_i : i \in S\}) = \frac{1}{|S|}\sum_{i \in S}(y_i - \mu_S)^2$

Stop early: reasons: speed, pure leaves (i.e. complete alg) overfits. use: check node and use majority (mean for regression).

Pruning: greedily remove split whose removal improves validation performance. more reliable than stopping.

Bagging: run learning algorithm on random subsamples of training set (weak learner). regression: take average, class: take majority. Minimize bias as much as possible - averaging reduces variance/overfit. Bagging worse for kNN.

Random Forests

At each node, take rnd sample of m features (out of d).

Classification: $m_{\text{init}} \approx \sqrt{d}$

Regression: $m_{\text{init}} \approx \frac{d}{3}$

Smaller m = less features = less complex model = more bias

Kernels

Can speedup algorithms such as SVMs, kNN, Regression (linear & logistic), k-means, etc.

$w = X^\top a = \sum_{i=1}^n a_i X_i$ Substitute this into the algorithm so we have to optimize n weights a instead of d weights w

Kernel Ridge Regression: Center X and y so means are 0, $X_{i,d+1} = 1$. Solve normal equations: $(X^\top X + \lambda I)w = X^\top y$

If a is a solution to $(X^\top X + \lambda I)a = y$,

$X^\top y = X^\top X X^\top a + \lambda X^\top a = (X^\top X + \lambda I) X^\top a \implies w = X^\top a$

The dual: $\min \|XX^\top a - y\|^2 + \lambda \|X^\top a\|^2$

Test phase: $h(z) = w^\top z = a^\top X z = \sum_{i=1}^n a_i (X_i^\top z)$, if $X_i^\top z$ are precomputed, it takes $O(n)$ time to evaluate h vs $O(d)$ time for primal method.

kernel fn: $k(x, z) = x^\top z$, kernel mtx: $K = XX^\top$ $(K_{ij} = k(X_i, X_j))$

kernel matrix must be PSD + symmetric

Solve $(K + \lambda I)a = y$ $O(n^3)$, test $h(z) = \sum a_i k(X_i, z)$ $O(nd)$ time

Dual: $O(n^3 + n^2 d)$, Primal: $O(d^3 + d^2 n)$, dual is better when $d > n$.

Kernel Trick: Polynomial kernel = $k(x, z) = (x^\top z + 1)^p$

Gaussian kernel = $k(x, z) = \exp\left(-\frac{\|x - z\|^2}{2\sigma^2}\right)$

Can compute $k(x, z) = \Phi(x)^\top \Phi(z)$ in $O(d)$ time instead of $O(d^p)$

Enables us to implicitly handle polynomial features efficiently

Kernel Perceptrons:

$w \leftarrow y_1 \Phi(X_1)$: while some $y_i \Phi(X_i) \cdot w < 0$, $w \leftarrow w + \epsilon y_i \Phi(X_i)$

for each test pt z, $h(z) \leftarrow w \cdot \Phi(z)$

Let $\Phi(X)$ be $x \times D$ matrix with rows $\Phi(X_i)^\top$

Dualize with $w = \Phi(X)^\top a$, $a_i \leftarrow a_i + \epsilon y_i$,

$h(z) = \sum_{i=1}^n a_j + k(X_{ij}, z)$

$\Phi(X_i) \cdot w = (\Phi(X) w)_i = (\Phi(X)\Phi(X)^\top a)_i = (Ka)_i$

$a \leftarrow \begin{bmatrix} y_1 & 0 & \cdots & 0 \end{bmatrix}^\top$: while some $y_i (Ka)_i < 0$, $a_i \leftarrow a_i + \epsilon y_i$

$O(n^2 d)$ to kernel mtx $O(1)$ to update a, $O(n)$ to update Ka

Learning Theory

Range Space (P, H): P = set of all possible train/test pts (ex. $\mathbb{R}^d$) H = set of all possible hypotheses Dichotomy: split of input data into two separate classes, not necessarily linear decision boundary.

Shatter Function: $\Pi_H(X) = |\{X \cap h : h \in H\}|$ = maximum number of dichotomies hypothesis class H can produce in particular set of points X. $\Pi_H(n) = \max_{|X|=n, X \subseteq P} \Pi_H(X)$= maximum number of dichotomies hypothesis class H can produce amongst a set of n data points and is only ever 2^n (known as shattering) or polynomial in n.

VC Dimension = the largest number of points D s.t. $\Pi_H(D) = 2^n$. Basically largest number of points a hypothesis class can produce all dichotomies of. Can be infinite, can be 0. A linear perceptron classifier with d parameters (d-dimensional weight vectors) has a VC dimension of d. For example, $2d$ linear perceptron (three weights - one for each dimension and one fictitious dimension = bias) has VC dimension of 3.

AdaBoost

Ensemble method that trains multiple learns on weighted sample points and weights learner. (misclassified points = increased weights, accurate learners = increased weights). Find classifier G_T and coefficient β_T to minimize

Risk $= \frac{1}{n}\sum_{i=1}^n L(M(X_i), y_i)$ with $M(X_i) = \sum_{t=1}^T \beta_t G_t(X_i)$

AdaBoost metalearner uses $L(\rho, \ell) = e^{-\rho \ell}$

$w_i^{(T+1)} = w_i^{(T)} \exp(-\beta_T y_i G_T(X_i))$, $\beta_T = \frac{1}{2}\ln\left(\frac{1 - \text{err}_T}{\text{err}_T}\right)$

$\text{err}_T = \frac{\sum_{y_i \neq G_T(X_i)} w_i^{(T)}}{\sum_{i=1}^n w_i^{(T)}}$. metalearner: $h(z) = \text{sign}(\sum_{t=1}^T \beta_t G_t(z))$

AdaBoost reduces bias, but effect on variance is hard to figure out (may sometimes overfit).

Neural Nets

Multi-layered perceptron, each layer puts outputs of previous layer linear function and then activation function. Minimize loss via gradient descent

Naive: $O(e^2)$, Backprop: $O(e)$.

Solve vanishing gradient problem: use ReLU activation

$r(\gamma) = \max\{0, \gamma\}$ Softmax activation:

$z_i(t) = \frac{e^{t_i}}{\sum_{j=1}^k e^{t_j}}; z_i \in (0, 1); \sum_{i=1}^k z_i = 1$

Use cross entropy instead of squared loss; k-class softmax output, cross-entropy: $L(z, y) = -\sum_{i=1}^k y_i \ln z_i$

$\nabla_W L = (z - y)h^\top$, $\nabla_h L = W^\top (z - y)$

CNNs: local connectivity and filter - perform convolution of small patches of image.

Principal Component Analysis

Goal: find directions with highest variance

Sol: Use SVD to decompose matrix and find eigenvectors for greatest singular values; same as finding Rayleigh quotients.

Low-rank approximation is lossy feature selection: you lose lower variance components yet select out low-singular values (often "noise" components)

Clustering

NP-hard: find $\text{argmin}_y \sum_{i=1}^k \sum_{y_j = i} ||X_j - \mu_i||^2$

K-means: alternate between fixed y_j's update μ_i's and vice versa. Halt when step 2 changes no assignments. Both steps decrease objective fn unless they change nothing; alg must terminate.

Initialization: Forgy method (choose k random points to be centroids). Can also use the (worse) random partitions - randomly assign each point to a cluster. K-medioids: K-means, but instead of using mean, use medioid, sample point minimizing total distance to other points in cluster.

Hierarchical clustering: creates a tree, every subtree is a cluster. Bottom-up (agglomerative) start with each point a cluster; repeatedly fuse pairs minimizing $d(A, B)$. Linkage functions:

complete: $d(A, B) = \max\{d(w, x) : w \in A, x \in B\}$

single: $d(A, B) = \min\{d(w, x) : w \in A, x \in B\}$

average: $d(A, B) = \frac{1}{|A||B|}\sum_{w \in A}\sum_{x \in B} dist(w, x)$

centroid: $d(A, B) = dist(\mu_A, \mu_B)$

Top-down (divisive) starts with single cluster, repeatedly splits

Miscellaneous

NP-Hard to find optimal linear classifier

Bayes vs. GDA	Bayes uses true mean/variance, while GDA uses sample mean/variance. True mean/variance equal $\not\Rightarrow$ Sample mean/variance equal
Cauchy-Schwarz	$\|\langle x, y\rangle| \leq \|x\| \cdot \|y\|$
Unique Optimum	Only ridge regression has one unique optimum (not Least Squares, Lasso, or Logistic).
Training Data:	Training on less data can improve train acc, training on more data can improve val/test acc.

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