

Linear Classifiers

f(x) = theta^T x - theta_0 = sum_{i=1}^d theta_i x_i + theta_0, y = { 1 if f(x) >= 0, -1 if f(x) < 0 }
Decision boundary H = { x in R^d : theta^T x + theta_0 = 0 }
Perceptron algorithm: Inputs (x_1, y_1), ..., (x_n, y_n) in R^d x {+1, -1}
Convergence Theorem: Given linearly separable data, for any choice of updates, algorithm terminates with all data correctly classified.

Since theta = sum_{i=1}^n y_i x_i, theta_0 = sum_{i=1}^n y_i x_i^T x = sum_{i=1}^n y_i (x_i^T x)
data in any inner product space
View as stochastic gradient descent, where J(theta) = sum_{i=1}^n (y_i (theta^T x_i))^2
Converges only if data linearly separable, time to converge depends on margin, solution depends on the starting point

Support Vector Machines

Optimize linear classification by choosing the classifier minimizing ||theta||
Find separating hyperplane theta^T x = 0 and scale theta by ||theta||
Support vectors are the points that satisfy constraints (compressed)
Hard Margin SVM: min ||theta|| s.t. y_i (theta^T x_i + theta_0) >= 1
Soft Margin SVM: Relax inequalities y_i (theta^T x_i) >= 1 by introducing slack variables epsilon_i

Feature Selection: Linear classifier: f(x) = theta^T x, quadratic: f(x) = ||x - c||^2 - r^2
Quadratic is simply the linear classifier with features phi(x)
Kernels: we can work in inner product space, so (x_i, x_j) = phi(x_i)^T phi(x_j)

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Quadratic is simply the linear classifier with features phi(x)
Kernels add modularity to classifier training since same optimization procedure can be used (K(x_i, x_j) needed)

Decision Theory

The Prediction Problem: Given a training set (x_1, y_1), ..., (x_n, y_n) choose a function f: X -> Y s.t. that for subset S of X, f(x) is a good predictor of y
Loss function L(y, y-hat) = R where L(y, y-hat) is cost of predicting y-hat for y
Can define identical or asymmetric loss functions

Risk in classification: Risk is misclassification probability: R(f) = E[1 - I(f(x) = y)] = P(f(x) != y)
Bayes Decision Rule: f*(x) = argmin_{y in Y} P(y = 1 | x)
Risk is minimized when f is Bayes optimal (Bayes) rule: R(f) = E[L(f(x), y)]
Error rate of decision rule can be quantified in terms of a certain distance from f*

Risk in regression: Risk is expected squared error: R(f) = E[(f(x) - y)^2] = E[E[(f(x) - y)^2 | x]]
Minimize the conditional expectation of the loss E[E[(f(x) - y)^2 | x]] by f*(x) = E[y | x]

Bayes-Variance Decomposition: R(f) = E[E[(f(x) - y)^2 | x]] = E[E[(f(x) - E[y | x])^2 | x]] + E[E[(E[y | x] - y)^2 | x]]
Minimizing R(f) is equivalent to minimizing E[E[(f(x) - E[y | x])^2 | x]] + E[E[(E[y | x] - y)^2 | x]]
Using random training data to choose f, we would like E[R(f)] to be small

Three approaches to choosing classifiers:
1) Estimate a generative model by P(x) and P(y|x), use Bayes theorem
2) Estimate a discriminative model by P(y|x) and use Bayes rule as actual P(y|x)
3) Cross a classifier (heuristic) based on optimization of criterion

Generative and Discriminative Models

Recall P(y) = E[P(y|x)] = E[E[y|x]] = E[E[y|x] * 1] = E[E[y|x] * P(x)] = E[E[y|x] * P(x)] = E[E[y|x] * P(x)]
For Gaussian class conditional densities: P(x_i | y) = N(x_i | mu_y, Sigma)
Suppose class conditional distributions are Gaussians: P(x_i | y) = N(x_i | mu_y, Sigma)

Consider the 2-dimensional case x = [x_1, x_2]^T, mu = [mu_1, mu_2]^T, Sigma = [[sigma_1^2, rho], [rho, sigma_2^2]]
(covariance matrix)
(covariance matrix)
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Inv-dimensions: theta = sum_{i=1}^d (mu_i - x_i) / sigma_i^2
The discriminant function minimizes Bayesian data overlap - log(P(x|y))
LDA: P(x|y) = 1 / (sqrt(2*pi)^d |Sigma|) exp(-1/2 (x - mu)^T Sigma^-1 (x - mu))

log b = -1/2 (x - mu)^T Sigma^-1 (x - mu) = -1/2 x^T x + 1/2 x^T mu + 1/2 mu^T x - 1/2 mu^T Sigma^-1 mu + log pi
S_k(x) = mu_k^T Sigma^-1 x - 1/2 mu_k^T Sigma^-1 mu_k + log pi_k (predict class k that maximizes S_k(x))
Assume class conditional distributions are Gaussian, common covariance
MLE estimate: mu-hat = P(x|y) = sum_{i=1}^n x_i / n, Sigma-hat = 1/n sum_{i=1}^n (x_i - mu-hat)(x_i - mu-hat)^T

Parameter Estimation Methods

We are interested in estimating Bernoulli and Gaussian parameters - distributions
Bernoulli Random Variable (biased coin)
Method of Moments: choose p such that distribution has same expectation as average of data
Maximum Likelihood: Count number of 1 outcomes and write l(p) = p^k (1-p)^(n-k) -> log-likelihood
Bayesian estimation: Model p as a random variable and belief about p captured by prior over possible values

Bayesian Random Variable: Model p as a random variable and belief about p captured by prior over possible values
Method of Moments: choose theta such that first moment (E[X]) and second moment (E[X^2]) of data
Maximum Likelihood: choose theta such that distribution gives observed data high prob
Bayesian Estimation: Prior: P(theta), Posterior: P(theta | x) proportional to likelihood times prior

Multivariate Normal Distribution

Review the Gaussian density function: p(x) = 1 / (sqrt(2*pi)^d |Sigma|) exp(-1/2 (x - mu)^T Sigma^-1 (x - mu))
Covariance Matrices: symmetric, positive semidefinite, invertible
Diagonal Covariance Matrices: consider X ~ N(mu, Sigma) where Sigma is diagonal

Non-Diagonal Covariance and Principalization: Start with a diagonal Sigma and consider transformed vector y = Ax + G(x - mu)
Eigenvalues and Eigenvectors: For a square matrix A, lambda is an eigenvalue and x is an eigenvector if Ax = lambda x

Spectral Theorem: For a symmetric real matrix A in R^n, we can find n orthonormal eigenvectors of A (v_1, ..., v_n) and eigenvalues (lambda_1, ..., lambda_n) are real
Covariance matrix Sigma is symmetric so Sigma = U Lambda U^T and positive semidefinite

Properties of Multivariate Gaussians: Probability: P(x) = 1 / (sqrt(2*pi)^d |Sigma|) exp(-1/2 (x - mu)^T Sigma^-1 (x - mu))
Covariance: Cov(x) = E[(x - mu)(x - mu)^T] = Sigma
Mean and variance of y evident from definition: y = Ax + G(x - mu)

Affine Transformations: Given d-dimensional Gaussian X ~ N(mu, Sigma), affine transformation Y = AX + B
Eigen decomposition: Eigen decomposition of Sigma = U Lambda U^T, Y = AX + B ~ N(mu_Y, Sigma_Y)

Bayesian view of Linear Regression: Given linear model P(y|x) = N(y | theta^T x, sigma^2)
MLE estimates beta-hat as mode of distribution
Quadratic regression with Bayesian prior, Lasso -> MAP Laplace prior

Laplace Regression: P(y|x) = 1 / (sqrt(2*pi)) exp(-1/2 (y - theta^T x)^2 / sigma^2)
First derivative: d/dtheta_j log P(y|x) = (y - theta^T x) / sigma^2
MLE yields beta-hat = (sum_{i=1}^n x_i x_i^T)^-1 (sum_{i=1}^n x_i y_i)

Gradient Ascent: beta-hat = argmax_{beta} P(beta) = beta-hat + eta sum_{i=1}^n (y_i - theta^T x_i) x_i
Stochastic Gradient Descent/Ascent: Instead compute approximations to gradient: beta-hat = (y + mu_i) / (1 + mu_i)

Newton's Method: Use 2nd-order Taylor approximation f(x) approx f(x_0) + f'(x_0)(x - x_0) + 1/2 f''(x_0)(x - x_0)^2
Solve for f(x) = 0: x_1 = x_0 - f'(x_0)/f''(x_0)
Solve beta-hat = 0 using x_{k+1} = x_k - [f''(x_k)]^-1 f'(x_k)

New MLEs minimizing log loss for beta-hat = (sum_{i=1}^n x_i x_i^T)^-1 (sum_{i=1}^n x_i y_i)
Define loss as L_n(beta-hat) = -log P(y|x) = -log pi - 1/2 sum_{i=1}^n (y_i - theta^T x_i)^2 / sigma^2
Write log loss as log pi + log(1 - exp(-y_i theta^T x_i / sigma^2))

One MLE corresponds to minimizing sample entropy: -log pi + log(1 + exp(-y_i theta^T x_i / sigma^2))
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Regression

Linear Regression: Recall quadratic loss function L(theta) = sum_{i=1}^n (y_i - theta^T x_i)^2 = E[(f(x) - y)^2]
Bayesian view of Linear Regression: Given linear model P(y|x) = N(y | theta^T x, sigma^2)
MLE estimates beta-hat as mode of distribution

Empirical Risk Minimization: Risk R(theta) = E[(f(x) - y)^2] is the expected squared error while
Empirical risk R-hat(theta) = 1/n sum_{i=1}^n (y_i - theta^T x_i)^2 is sample average of squared error

Optimal approximation in space spanned by columns of X: (y - y-hat)^T X = 0
Beta-hat = (X^T X)^-1 X^T y

Regularization in Regression: Bayesian view of Linear Regression: Given linear model P(y|x) = N(y | theta^T x, sigma^2)
MAP estimates beta-hat as mode of distribution

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Convex Optimization and SVMs

Recall hard margin SVM: $\min_x \|G\|^2$ s.t. $y_i G \cdot x_i \geq 1$

soft margin SVM: $\min_x \|G\|^2 + C \sum_{i=1}^n (1 - y_i G \cdot x_i)$

ASGP: hard margin SVM: $\min_x \|G\|^2$ s.t. $y_i G \cdot x_i \geq 1$

soft margin SVM: $\min_x \|G\|^2 + C \sum_{i=1}^n \xi_i$ s.t. $\xi_i \geq 0, \xi_i \geq 1 - y_i G \cdot x_i$

Convex sets are those in which it is possible to draw line all in set

Consider convex optimization problem $p^* = \min_x f_0(x)$ s.t. $f_i(x) \leq 0$ $\forall i \in \{1, \dots, m\}$

Writing constraints as penalties $p^* = \min_x f_0(x) + \begin{cases} 0 & \text{if all } f_i(x) \leq 0 \\ \infty & \text{otherwise} \end{cases}$

Replace constraint penalty with something smaller:

Introduce Lagrange multipliers (dual variables) $\lambda_1, \dots, \lambda_m \geq 0$ and define

Lagrangian $L: \mathbb{R}^n \times \mathbb{R}^m \rightarrow \mathbb{R}$ as $L(x, \lambda) = f_0(x) + \sum_{i=1}^m \lambda_i f_i(x)$

λ_i cost of violating constraint $f_i(x) \leq 0$

L defines saddle point game: one player (MIN) chooses x to minimize

L , the other player (MAX) chooses λ to maximize L . If MIN violates a

constraint, $f_i(x) > 0$, MAX can drive L to infinity.

Primal problem $p^* = \min_x \max_{\lambda \geq 0} L(x, \lambda)$ (infeasible $x \rightarrow \infty$, feasible $x \rightarrow \lambda_i f_i(x) = 0$)

Dual problem $d^* = \max_{\lambda \geq 0} g(\lambda) = \max_{\lambda \geq 0} \min_x L(x, \lambda)$ $g(\lambda) := \min_x L(x, \lambda)$

This is a zero sum game where better to play second:

$p^* = \min_x \max_{\lambda \geq 0} L(x, \lambda) \geq \max_{\lambda \geq 0} \min_x L(x, \lambda) = d^*$ (weak duality)

If there is saddle point (x^*, λ^*) so that for all x and $\lambda \geq 0$, $L(x^*, \lambda) \leq L(x^*, \lambda^*) \leq L(x, \lambda^*)$

then $p^* = \min_x \max_{\lambda \geq 0} L(x, \lambda) = \max_{\lambda \geq 0} \min_x L(x, \lambda) = d^*$ (strong duality)

Complementary Slackness

If $p^* = d^*$ and we have primal solution x^* and dual solution λ^*

then for i th constraint $(f_i(x^*) \leq 0)$, $\lambda_i^* f_i(x^*) = 0$.

$f_i(x^*) < 0 \Rightarrow \lambda_i = 0$, $\lambda_i > 0 \Rightarrow f_i(x^*) = 0$

As a result, every term in $\sum_{i=1}^m \lambda_i^* f_i(x^*) \geq 0 \approx 0$

Karush-Kuhn-Tucker Optimality Conditions

Suppose f_0, f_i are convex and differentiable. Then x and λ optimal if and only if:

① Primal feasibility: $f_i(x) \leq 0$ ② Dual feasibility: $\lambda_i \geq 0$

③ Complementary slackness: $\lambda_i f_i(x) = 0$ ④ Stationarity: $\nabla f_0(x) + \sum_{i=1}^m \lambda_i \nabla f_i(x) = 0$

SVMs

Hard Margin SVMs $\theta(w) = \min_x L(\theta; x)$

Write $\min_x \|G\|^2$ s.t. $y_i G \cdot x_i \geq 1$ as $L(\theta; x) = \frac{1}{2} \|G\|^2 + \sum_{i=1}^n \alpha_i (1 - y_i G \cdot x_i)$

$\nabla_x L(\theta; x) = G + (-1) \sum_{i=1}^n \alpha_i y_i x_i \rightarrow G^* = \sum_{i=1}^n \alpha_i y_i x_i$

$g(\theta) = \frac{1}{2} \theta^T \theta + \sum_{i=1}^n \alpha_i - \sum_{i=1}^n \alpha_i y_i G \cdot x_i = \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i,j=1}^n \alpha_i \alpha_j y_i y_j x_i^T x_j$

If \exists feasible $\theta \Rightarrow$ strong duality $\rightarrow \max_{\alpha_i \geq 0} \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i,j=1}^n \alpha_i \alpha_j y_i y_j x_i^T x_j$

$\alpha_i > 0 \Rightarrow y_i G^* \cdot x_i = 1$ and $y_i G^* \cdot x_i \leq 1 \Rightarrow \alpha_i = 0$

Express solution as kernel $\langle x, x \rangle = \text{sign}(\langle \theta, \theta(x) \rangle) = \text{sign}(\sum_{i=1}^n \alpha_i \langle x, x_i \rangle \langle \theta, x_i \rangle)$

where α solves dual problem $\max_{\alpha_i \geq 0} \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i,j=1}^n \alpha_i \alpha_j y_i y_j x_i^T x_j$

Soft Margin SVMs $\min_x \frac{1}{2} \|G\|^2 + C \sum_{i=1}^n (1 - y_i G \cdot x_i)$ as $\min_x \frac{1}{2} \|G\|^2 + \sum_{i=1}^n \xi_i$ s.t. $\xi_i \geq 1 - y_i G \cdot x_i$

$L(\theta, \xi, \alpha) = \frac{1}{2} \theta^T \theta + \sum_{i=1}^n \xi_i + \sum_{i=1}^n \alpha_i (1 - y_i G \cdot x_i - \xi_i) \rightarrow \sum_{i=1}^n \lambda_i \xi_i$

$\nabla_x L(\theta; x) = G + (-1) \sum_{i=1}^n \alpha_i y_i x_i \rightarrow G^* = \sum_{i=1}^n \alpha_i y_i x_i$

$\nabla_{\xi} L(\theta; \xi, \alpha) = \sum_{i=1}^n \alpha_i - \xi \rightarrow \alpha_i - \xi_i \rightarrow \alpha_i + \xi_i = C$ so $g(\theta; \lambda) = \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i,j=1}^n \alpha_i \alpha_j y_i y_j x_i^T x_j$

Dual problem given by $\max_{\alpha_i \geq 0} \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i,j=1}^n \alpha_i \alpha_j y_i y_j x_i^T x_j$

$\alpha_i \geq 0, x_i \geq 0, \alpha_i + \lambda_i = C/n$

Consequences of complementary slackness: $\alpha_i^* (1 - y_i x_i^T G^* - \xi_i^*) = 0$

$\alpha_i^* > 0 \Rightarrow y_i x_i^T G^* = 1 - \xi_i^* \leq 1$ 'support vector' $x_i^* \xi_i^* = 0$

ie in the wrong side of half space

If $y_i x_i^T G^* < 1$, $\xi_i^* > 0$ so $x_i^* = 0$ and $\alpha_i^* = C/n$ so

support vectors in open halfspace have $\alpha_i^* = C/n$