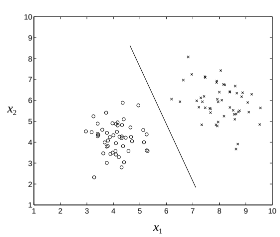
Lecture 6:

Classification Models

January 30, 2006

Reminder: Classification

- Given examples of a discrete *class label* y and some *features* $\mathbf{x}$.
- Goal: compute label (y) for new inputs $\mathbf{x}$.
- Two approaches:
  Generative: model $p(\mathbf{x}, y) = p(y)p(\mathbf{x}|y)$;
  use Bayes' rule to infer conditional $p(y|\mathbf{x})$.
  Discriminative: model discriminants $f(y|\mathbf{x})$ directly and take max.
- Generative approach is related to conditional *density estimation* while discriminative approach is closer to *regression*.

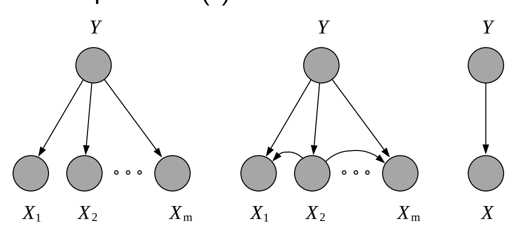


Probabilistic Classification: Bayes Classifiers

- Generative model: $p(\mathbf{x}, y) = p(y)p(\mathbf{x}|y)$.
  $p(y)$ are called class *priors*.
  $p(\mathbf{x}|y)$ are called *class conditional feature distributions*.
- For the prior we use a Bernoulli or multinomial:
  $p(y = k|\pi) = \pi_k$ with $\sum_k \pi_k = 1$.
- Classification rules:
  ML: $\operatorname{argmax}_y \, p(\mathbf{x}|y)$ (can behave badly if skewed priors)
  MAP: $\operatorname{argmax}_y \, p(y|\mathbf{x}) = \operatorname{argmax}_y \, \log p(\mathbf{x}|y) + \log p(y)$ (safer)
- Fitting: maximize $\sum_n \log p(\mathbf{x}^n, y^n) = \sum_n \log p(\mathbf{x}^n|y^n) + \log p(y^n)$
  1) Sort data into batches by class label.
  2) Estimate $p(y)$ by counting size of batches (plus regularization).
  3) Estimate $p(\mathbf{x}|y)$ separately within each batch using ML.
  (also with regularization).

Three Key Regularization Ideas

- To avoid overfitting, we can put *priors* on the parameters of the class and class conditional feature distributions.
- We can also *tie* some parameters together so that fewer of them are estimated using more data.
- Finally, we can make *factorization* or *independence* assumptions about the distributions. In particular, for the class conditional distributions we can assume the features are fully dependent, partly dependent, or independent (!).



(a) (b) (c)

Gaussian Class-Conditional Distributions 4

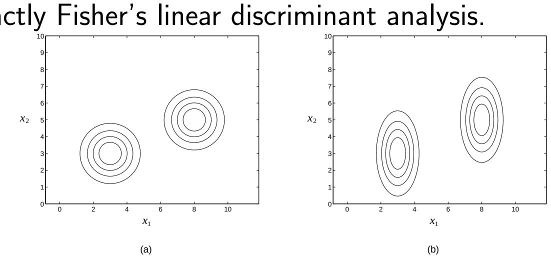
- If all features are continuous, a popular choice is a Gaussian class-conditional.

$$p(\mathbf{x}|y=k,\theta) = |2\pi\Sigma|^{-1/2} \exp\left\{-\frac{1}{2}(\mathbf{x}-\mu_k)\Sigma^{-1}(\mathbf{x}-\mu_k)\right\}$$

- Fitting: use the following amazing and useful fact.
  The maximum likelihood fit of a Gaussian to some data is the Gaussian whose mean is equal to the data mean and whose covariance is equal to the sample covariance.
  [Try to prove this as an exercise in understanding likelihood, algebra, and calculus all at once!]
- Seems easy. And works amazingly well.
  But we can do even better with some simple regularization...

Regularized Gaussians 5

- Idea 1: assume all the covariances are the same (tie parameters). This is exactly Fisher's linear discriminant analysis.



- Idea 2: Make independence assumptions to get diagonal or identity-multiple covariances. (Or sparse inverse covariances.) More on this in a few minutes...
- Idea 3: add a bit of the identity matrix to each sample covariance. This "fattens it up" in directions where there wasn't enough data. Equivalent to using a "Wishart prior" on the covariance matrix.

Gaussian Bayes Classifier 6

- Maximum likelihood estimates for parameters:
  priors π_k: use observed frequencies of classes (plus smoothing)
  means μ_k: use class means
  covariance Σ: use data from single class or pooled data $(\mathbf{x}^m - \mu_{y^m})$ to estimate full/diagonal covariances
- Compute the posterior via Bayes' rule:

$$\begin{aligned} p(y=k|\mathbf{x},\theta) &= \frac{p(\mathbf{x}|y=k,\theta)p(y=k|\pi)}{\sum_j p(\mathbf{x}|y=j,\theta)p(y=j|\pi)} \\ &= \frac{\exp\{\mu_k^\top\Sigma^{-1}\mathbf{x} - \mu_k^\top\Sigma^{-1}\mu_k/2 + \log\pi_k\}}{\sum_j \exp\{\mu_j^\top\Sigma^{-1}\mathbf{x} - \mu_j^\top\Sigma^{-1}\mu_j/2 + \log\pi_j\}} \\ &= e^{\beta_k^\top\mathbf{x}} / \sum_j e^{\beta_j^\top\mathbf{x}} = \exp\{\beta_k^\top\mathbf{x}\}/Z \end{aligned}$$

where $\beta_k = [\Sigma^{-1}\mu_k\,;\,(\mu_k^\top\Sigma^{-1}\mu_k + \log\pi_k)]$ and we have augmented $\mathbf{x}$ with a constant component always equal to 1 (bias term).

Softmax/Logit 7

- The squashing function is known as the *softmax* or *logit*:

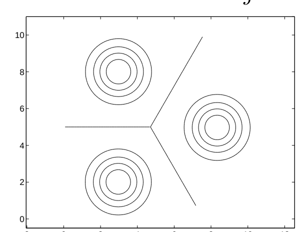
$$\phi_k(\mathbf{z}) \equiv \frac{e^{z_k}}{\sum_j e^{z_j}} \qquad g(\eta) = \frac{1}{1+e^{-\eta}}$$

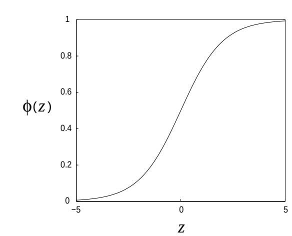
- It is invertible (up to a constant):

$$z_k = \log\phi_k + c \qquad \eta = \log(g/1-g)$$

- Derivative is easy:

$$\frac{\partial\phi_k}{\partial z_j} = \phi_k(\delta_{kj} - \phi_j) \qquad \frac{dg}{d\eta} = g(1-g)$$





Linear Geometry

- Taking the ratio of any two posteriors (the "odds") shows that the contours of equal pairwise probability are linear surfaces in the feature space:
$$\frac{p(y=k|\mathbf{x},\theta)}{p(y=j|\mathbf{x},\theta)} = \exp\left\{(\beta_k - \beta_j)^\top \mathbf{x}\right\}$$
- The pairwise discrimination contours $p(y_k) = p(y_j)$ are orthogonal to the differences of the means in feature space when $\Sigma = \sigma I$. For general Σ shared b/w all classes the same is true in the transformed feature space $\mathbf{w} = \Sigma^{-1}\mathbf{x}$.
- The priors do not change the geometry, they only shift the operating point on the logit by the log-odds $\log(\pi_k/\pi_j)$.
- Thus, for equal class-covariances, we obtain a *linear classifier*.
- If we use difference covariances, the decision surfaces are conic sections and we have a quadratic classifier.

Exponential Family Class-Conditionals

- Bayes Classifier has the same softmax form whenever the class-conditional densities are *any* exponential family density:
$$\begin{aligned} p(\mathbf{x}|y=k,\eta_k) &= h(\mathbf{x})\exp\{\eta_k^\top \mathbf{x} - a(\eta_k)\} \\ p(y=k|\mathbf{x},\eta) &= \frac{p(\mathbf{x}|y=k,\eta_k)p(y=k|\pi)}{\sum_j p(\mathbf{x}|y=j,\eta_j)p(y=j|\pi)} \\ &= \frac{\exp\{\eta_k^\top \mathbf{x} - a(\eta_k)\}}{\sum_j \exp\{\eta_j^\top \mathbf{x} - a(\eta_j)\}} \\ &= \frac{e^{\beta_k^\top \mathbf{x}}}{\sum_j e^{\beta_j^\top \mathbf{x}}} \end{aligned}$$
where $\beta_k = [\eta_k \, ; \, -a(\eta_k)]$ and we have augmented $\mathbf{x}$ with a constant component always equal to 1 (bias term).
- Resulting classifier is linear in the sufficient statistics.

Discrete Bayesian Classifier

- If the inputs are discrete (categorical), what should we do?
- The simplest class conditional model is a joint multinomial (table):
$$p(x_1 = a, x_2 = b, \ldots |y=c) = \eta^c_{ab\ldots}$$
- This is conceptually correct, but there's a big practical problem.
- Fitting: ML params are observed counts:
$$\eta^c_{ab\ldots} = \frac{\sum_n [y_n = c][x_1 = a][x_2 = b][\ldots][\ldots]}{\sum_n [y_n = c]}$$
- Consider the 16x16 digits at 256 gray levels.
- How many entries in the table? How many will be zero? What happens at test time? Doh!
- We obviously need some regularlization. Smoothing will not help much here. Unless we know about the relationships between inputs beforehand, sharing parameters is hard also. But what about independence?

Naive (Idiot's) Bayes Classifier

- Assumption: conditioned on class, attributes are independent.
$$p(\mathbf{x}|y) = \prod_i p(x_i|y)$$
- Sounds crazy right? Right! But it works.
- Algorithm: sort data cases into bins according to y_n. Compute marginal probabilities $p(y=c)$ using frequencies.
- For each class, estimate distribution of i^{th} variable: $p(x_i|y=c)$.
- At test time, compute $\mathrm{argmax}_c \; p(c|\mathbf{x})$ using
$$\begin{aligned} c(\mathbf{x}) = \mathrm{argmax}_c \; p(c|\mathbf{x}) &= \mathrm{argmax}_c \; [\log p(\mathbf{x}|c) + \log p(c)] \\ &= \mathrm{argmax}_c \; [\log p(c) + \sum_i \log p(x_i|c)] \end{aligned}$$

DISCRETE (MULTINOMIAL) NAIVE BAYES 12

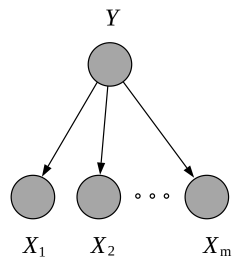
Discrete features x_i, assumed independent given the class label y.

$$p(x_i = j|y = k) = \eta_{ijk}$$
$$p(\mathbf{x}|y = k, \eta) = \prod_i \prod_j \eta_{ijk}^{[x_i=j]}$$

Classification rule:

$$p(y = k|\mathbf{x}, \eta) = \frac{\pi_k \prod_i \prod_j \eta_{ijk}^{[x_i=j]}}{\sum_q \pi_q \prod_i \prod_j \eta_{ijq}^{[x_i=j]}}$$
$$= \frac{e^{\beta_k^\top \mathbf{x}}}{\sum_q e^{\beta_q^\top \mathbf{x}}}$$

$\beta_k = \log[\eta_{11k} \ldots \eta_{1jk} \ldots \eta_{ijk} \ldots \log \pi_k]$
$\mathbf{x} = [x_1{=}1; x_1{=}2; \ldots; x_i{=}j; \ldots; 1]$



(a)

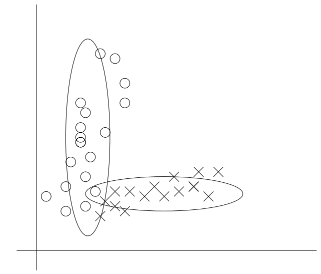
FITTING DISCRETE NAIVE BAYES 13

- ML parameters are class-conditional frequency counts:
$$\eta_{ijk}^* = \frac{\sum_m [x_i{}^m = j][y^m = k]}{\sum_m [y^m = k]}$$
- How do we know? Write down the likelihood:
$$\ell(\theta; \mathcal{D}) = \sum_m \log p(y^m|\pi) + \sum_{mi} \log p(x_i{}^m|y^m, \eta)$$
  and optimize it by setting its derivative to zero
  (careful! enforce normalization with Lagrange multipliers):

$$\ell(\eta; \mathcal{D}) = \sum_m \sum_{ijk} [x_i{}^m = j][y^m = k] \log \eta_{ijk} + \sum_{ik} \lambda_{ik}(1 - \textstyle\sum_j \eta_{ijk})$$
$$\frac{\partial \ell}{\partial \eta_{ijk}} = \frac{\sum_m [x_i{}^m = j][y^m = k]}{\eta_{ijk}} - \lambda_{ik}$$
$$\frac{\partial \ell}{\partial \eta_{ijk}} = 0 \quad \Rightarrow \lambda_{ik} = \sum_m [y^m = k] \quad \Rightarrow \eta_{ijk}^* = \text{above}$$

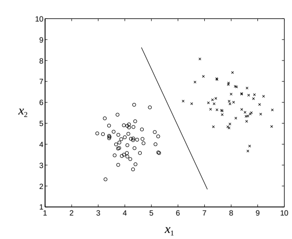
GAUSSIAN NAIVE BAYES 14

- This is just a Gaussian Bayes Classifier with a separate diagonal covariance matrix for each class.
- Equivalent to fitting a one-dimensional Gaussian to each input for each possible class.
- Decision surfaces are quadratics, not linear...



DISCRIMINATIVE MODELS 15

- Parametrize $p(y|\mathbf{x})$ directly, forget $p(\mathbf{x}, y)$ and Bayes' rule.
- As long as $p(y|\mathbf{x})$ or discriminants $f(y|\mathbf{x})$ are linear functions of $\mathbf{x}$ (or monotone transforms), decision surfaces will be piecewise linear.
- Don't need to model the density of the features.
  Some density models have lots of parameters.
  Many densities give same linear classifier.
  But we cannot generate new labeled data.
- Optimize the same cost function we use at test time.



Logistic/Softmax Regression 16

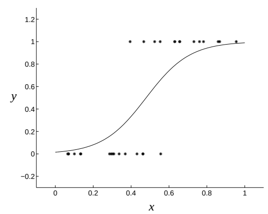
- Model: y is a multinomial random variable whose posterior is the softmax of linear functions of *any* feature vector.

$$p(y = k|\mathbf{x}, \theta) = \frac{e^{\theta_k^\top \mathbf{x}}}{\sum_j e^{\theta_j^\top \mathbf{x}}}$$

- Fitting: now we optimize the *conditional* likelihood:

$$\ell(\theta; \mathcal{D}) = \sum_{mk} [y^m = k] \log p(y = k|\mathbf{x}^m, \theta) = \sum_{mk} y_k^m \log p_k^m$$

$$\begin{aligned}\frac{\partial \ell}{\partial \theta_i} &= \sum_{mk} \frac{\partial \ell_k^m}{\partial p_k^m} \frac{\partial p_k^m}{\partial z_i^m} \frac{\partial z_i^m}{\partial \theta_i} \\ &= \sum_{mk} \frac{y_k^m}{p_k^m} p_k^m (\delta_{ik} - p_i^m) \mathbf{x}^m \\ &= \sum_m (y_k^m - p_k^m) \mathbf{x}^m\end{aligned}$$



More on Logistic Regression 17

- Hardest Part: picking the feature vector $\mathbf{x}$.
- Amazing fact: the conditional likelihood is (almost) convex in the parameters θ. Still no local minima!
- Gradient is easy to compute; so easy (if slow) to optimize using gradient descent or Newton-Raphson / IRLS.
- Why almost? Consider what happens if there are two features with identical classification patterns in our training data. Logistic Regression can only see the sum of the corresponding weights.
- Solution? Weight decay: add $\epsilon \sum \theta^2$ to the cost function, which subtracts $2\epsilon\theta$ from each gradient.
- Why is this method called logistic regression?
- It should really be called "softmax linear regression".
- Log odds (logit) between any two classes is linear in parameters.

Joint vs. Conditional Models 18

- Many of the methods we have seen so far have linear or piecewise linear decision surfaces in some space $\mathbf{x}$:
  LDA, perceptron, Gaussian Bayes, Naive Bayes, KNN,...
- But the criteria used to find this hyperplane is different:
- Naive Bayes is a joint model; it optimizes $p(\mathbf{x}, y) = p(\mathbf{x})p(y|\mathbf{x})$.
- Logistic Regression is conditional: optimizes $p(y|\mathbf{x})$ directly.

Other Models 19

- Noisy-OR (see slides)
- Classification via Regression (see slides)
- Non-parametric (e.g. K-nearest-neighbour).
- Semiparametric (e.g. kernel classifiers, support vector machines, Gaussian processes).
- Probit regression.
- Complementary log-log.
- Generalized linear models.
- Some return a value for y without a distribution.

Noisy-OR Classifier

- Many probabilistic models can be obtained as noisy versions of formulas from propositional logic.
- Noisy-OR: each input x_i activates output y w/some probability.

$$p(y=0|\mathbf{x},\alpha) = \prod_i \alpha_i^{x_i} = \exp\left\{\sum_i x_i \log \alpha_i\right\}$$

- Letting $\theta_i = -\log \alpha_i$ we get yet another linear classifier:

$$p(y=1|\mathbf{x},\theta) = 1 - e^{-\theta^\top \mathbf{x}}$$

Classification via Regression

- Binary case: $p(y=1|\mathbf{x})$ is also the conditional expectation.
- So we could forget that y was a discrete (categorical) random variable and just attempt to model $p(y|\mathbf{x})$ using regression.
- One idea: do regression to an *indicator matrix*.
- For two classes, this is equivalent* to LDA. For 3 or more, disaster...
- Very bad idea! Noise models (e.g. Gaussian) for regression are totally inappropriate, and fits are oversensitive to outliers. Furthermore, gives unreasonable predictions < 0 and > 1.