7 Gaussian Discriminant Analysis (including QDA and LDA)

GAUSSIAN DISCRIMINANT ANALYSIS

Fundamental assumption: each class comes from normal distribution (Gaussian).

$$X \sim N(\mu, \sigma^2) : P(x) = \frac{1}{(\sqrt{2\pi}\sigma)^d} \exp\left(-\frac{|x-\mu|^2}{2\sigma^2}\right) \qquad [\mu \ \& \ x = \text{vectors; } \sigma = \text{scalar; } d = \text{dimension}]$$

For each class C, suppose we estimate mean μ_C, variance σ_C^2, and prior $\pi_C = P(Y = C)$.

Given x, Bayes decision rule $r^*(x)$ returns class C that maximizes $P(X = x|Y = C)\,\pi_C$.

$\ln \omega$ is monotonically increasing for $\omega > 0$, so it is equivalent to maximize

$$Q_C(x) = \ln\left((\sqrt{2\pi})^d P(x)\,\pi_C\right) = -\frac{|x-\mu_C|^2}{2\sigma_C^2} - d\ln\sigma_C + \ln\pi_C$$

↑ quadratic in x. ↑ normal distribution, estimates $P(X = x|Y = C)$

[In a 2-class problem, you can also incorporate an asymmetrical loss function the same way we incorporate the prior π_C. In a multi-class problem, it gets a bit more complicated, because the penalty for guessing wrong might depend not just on the true class, but also on the wrong guess.]

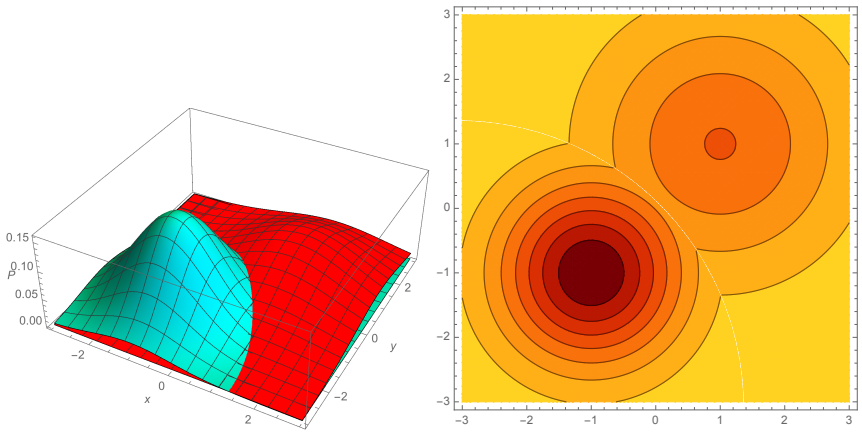
Quadratic Discriminant Analysis (QDA)

Suppose only 2 classes C, D. Then

$$r^*(x) = \begin{cases} C & \text{if } Q_C(x) - Q_D(x) > 0, \\ D & \text{otherwise} \end{cases}$$

Decision fn is quadratic in x. Bayes decision boundary is $Q_C(x) - Q_D(x) = 0$.

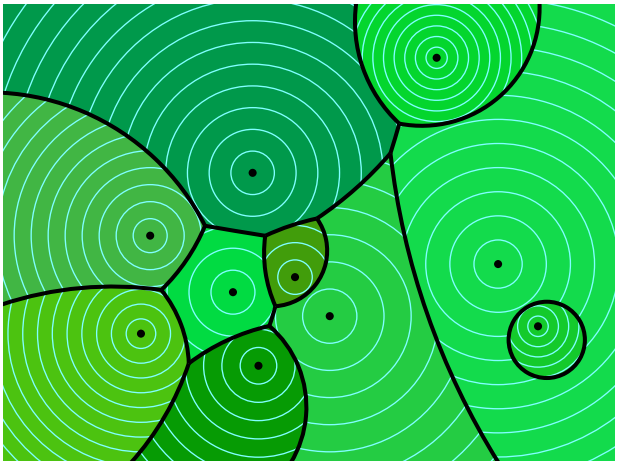
- In 1D, B.d.b. may have 1 or 2 points. [Solutions to a quadratic equation]
- In d-D, B.d.b. is a quadric. [In 2D, that's a conic section]



qda3d.pdf, qdacontour.pdf [The same example I showed during the last lecture.]

[You're probably familiar with the Gaussian distribution where x and μ are scalars, but as I've written it, it applies equally well to a multi-dimensional feature space with isotropic, spherical Gaussians. Then x and μ are vectors, but the variance σ is still a scalar. Next lecture we'll look at anisotropic Gaussians where the variance is different along different directions.]

[QDA works very nicely with more than 2 classes.]



multiplicative.pdf [The feature space gets partitioned into regions. In two or more dimensions, you typically wind up with multiple decision boundaries that adjoin each other at joints. It looks like a sort of Voronoi diagram. In fact, it's a special kind of Voronoi diagram called a multiplicatively, additively weighted Voronoi diagram.]

[You might not be satisfied with just knowing how each point is classified. One of the great things about QDA is that you can also determine the probability that your classification is correct. Let's work that out.]

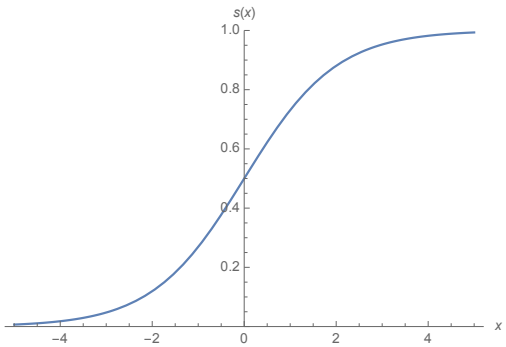
To recover posterior probabilities in 2-class case, use Bayes:

$$P(Y = \mathrm{C}|X) = \frac{P(X|Y = \mathrm{C})\,\pi_\mathrm{C}}{P(X|Y = \mathrm{C})\,\pi_\mathrm{C} + P(X|Y = \mathrm{D})\,\pi_\mathrm{D}}$$

recall $e^{Q_\mathrm{C}(x)} = (\sqrt{2\pi})^d\, P(x)\,\pi_\mathrm{C}$ [by definition of Q_C]

$$\begin{aligned} P(Y = \mathrm{C}|X = x) &= \frac{e^{Q_\mathrm{C}(x)}}{e^{Q_\mathrm{C}(x)} + e^{Q_\mathrm{D}(x)}} = \frac{1}{1 + e^{Q_\mathrm{D}(x) - Q_\mathrm{C}(x)}} \\ &= s(Q_\mathrm{C}(x) - Q_\mathrm{D}(x)), \quad \text{where} \end{aligned}$$

$$s(\gamma) = \frac{1}{1 + e^{-\gamma}} \quad \Leftarrow \text{logistic fn aka sigmoid fn}$$



logistic.pdf [The logistic function. Write beside it:] $s(0) = \frac{1}{2}$, $s(\infty) \to 1$, $s(-\infty) \to 0$, monotonically increasing.

[We interpret $s(0) = \frac{1}{2}$ as saying that on the decision boundary, there's a 50% chance of class C and a 50% chance of class D.]

Linear Discriminant Analysis (LDA)

[LDA is a variant of QDA with linear decision boundaries. It's less likely to overfit than QDA.]

Fundamental assumption: all the Gaussians have same variance σ.
[The equations simplify nicely in this case.]

$$Q_C(x) - Q_D(x) = \underbrace{\frac{(\mu_C - \mu_D) \cdot x}{\sigma^2}}_{w \cdot x} \underbrace{- \frac{|\mu_C|^2 - |\mu_D|^2}{2\sigma^2} + \ln \pi_C - \ln \pi_D}_{+\alpha}$$

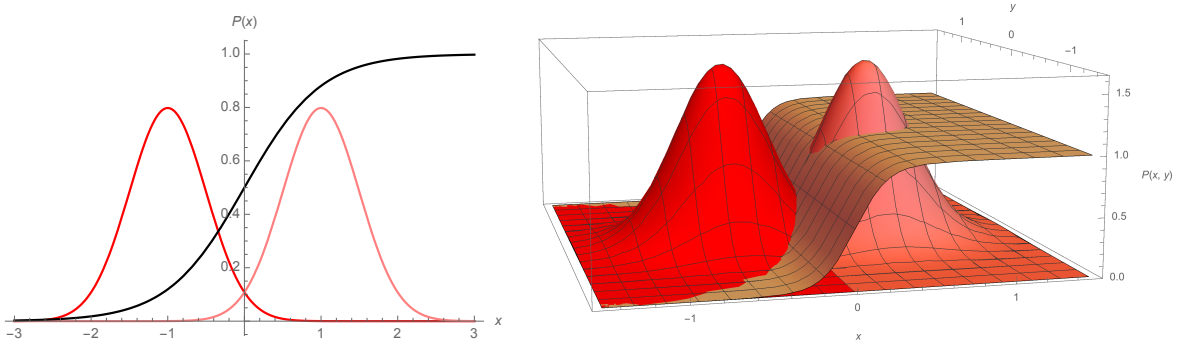
[The quadratic terms in Q_C and Q_D cancelled each other out!]

Now it's a linear classifier! Choose C that maximizes linear discriminant fn

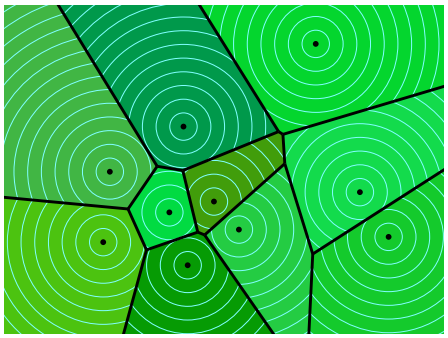
$$\frac{\mu_C \cdot x}{\sigma^2} - \frac{|\mu_C|^2}{2\sigma^2} + \ln \pi_C \qquad \text{[this works for any number of classes]}$$

In 2-class case: decision boundary is $w \cdot x + \alpha = 0$
Bayes posterior is $P(Y = C|X = x) = s(w \cdot x + \alpha)$

[The effect of "$w \cdot x + \alpha$" is to scale and translate the logistic fn in x-space. It's a linear transformation.]



lda1d.pdf [Two Gaussians (red) and the logistic function (black). The logistic function arises as the right Gaussian divided by the sum of the Gaussians. Observe that even when the Gaussians are 2D, the logistic function still looks 1D.]



voronoi.pdf [When you have many classes, their LDA decision boundaries form a classical Voronoi diagram if the priors π_C are equal. All the Gaussians here have the same width.]

$$\text{If } \pi_C = \pi_D = \frac{1}{2} \quad \Rightarrow \quad (\mu_C - \mu_D) \cdot x - (\mu_C - \mu_D) \cdot \left(\frac{\mu_C + \mu_D}{2} \right) = 0$$

This is the centroid method!

MAXIMUM LIKELIHOOD ESTIMATION OF PARAMETERS (Ronald Fisher, circa 1912)

[To use Gaussian discriminant analysis, we must first fit Gaussians to the sample points and estimate the class prior probabilities. We'll do priors first—they're easier, because they involve a discrete distribution. Then we'll fit the Gaussians—they're less intuitive, because they're continuous distributions.]

Let's flip biased coins! Heads with probability p; tails w/prob. $1 - p$.

10 flips, 8 heads, 2 tails. [Let me ask you a weird question.] What is the most likely value of p?

Binomial distribution: $X \sim B(n, p)$

$$P[X = x] = \binom{n}{x} p^x (1-p)^{n-x} \qquad \text{[this is the probability of getting exactly } x \text{ heads in } n \text{ coin flips]}$$

Our example: $n = 10$,

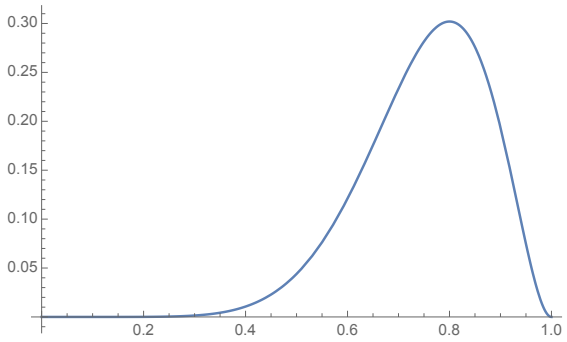
$$P[X = 8] = 45p^8 (1-p)^2 \qquad \stackrel{\text{def}}{=} \mathcal{L}(p)$$

Probability of 8 heads in 10 flips:
written as a fn $\mathcal{L}(p)$ of distribution parameter(s), this is the likelihood fn.

Maximum likelihood estimation (MLE): A method of estimating the parameters of a statistical model by picking the params that maximize [the likelihood function] $\mathcal{L}$.
. . . is one method of density estimation: estimating a PDF [probability density function] from data.

[Let's phrase it as an optimization problem.]

Find p that maximizes $\mathcal{L}(p)$.



binomlikelihood.pdf [Graph of $\mathcal{L}(p)$ for this example.]

Solve this example by setting derivative = 0:

$$\frac{\mathrm{d}\mathcal{L}}{\mathrm{d}p} = 360p^7(1-p)^2 - 90p^8(1-p) = 0$$

$$\Rightarrow \quad 4(1-p) - p = 0 \quad \Rightarrow \quad p = 0.8$$

[It shouldn't seem surprising that a coin that comes up heads 80% of the time is the coin most likely to produce 8 heads in 10 flips.]

[Note: $\frac{\mathrm{d}^2\mathcal{L}}{\mathrm{d}p^2} \doteq -18.9 < 0$ at $p = 0.8$, confirming it's a maximum.]

[Here's how this applies to prior probabilities. Suppose our data set is 10 sample points, and 8 of them are of class C and 2 are not. Then our estimated prior for class C will be $\pi_C = 0.8$.]

Likelihood of a Gaussian

Given sample points $X_1, X_2, \ldots, X_n$, find best-fit Gaussian.

[Let's do this with a normal distribution instead of a binomial distribution. If you generate a random point from a normal distribution, what is the probability that it will be exactly at the mean of the Gaussian?]

[Zero. So it might seem like we have a problem here. With a continuous distribution, the probability of generating any particular point is zero. But we're just going to ignore that and do "likelihood" anyway.]

Likelihood of generating these points is

$$\mathcal{L}(\mu, \sigma; X_1, \ldots, X_n) = P(X_1)\, P(X_2) \cdots P(X_n)$$ [How do we maximize this?]

The log likelihood $\ell(\cdot)$ is the ln of the likelihood $\mathcal{L}(\cdot)$.
Maximizing likelihood $\Leftrightarrow$ maximizing log likelihood.

$$\begin{aligned} \ell(\mu, \sigma; X_1, ..., X_n) &= \ln P(X_1) + \ln P(X_2) + ... + \ln P(X_n) \\ &= \sum_{i=1}^{n} \underbrace{\left(-\frac{|X_i - \mu|^2}{2\sigma^2} - d \ln \sqrt{2\pi} - d \ln \sigma \right)}_{\text{ln of normal distribution}} \end{aligned}$$

Want to set $\nabla_\mu \ell = 0$, $\dfrac{\partial \ell}{\partial \sigma} = 0$

$$\nabla_\mu \ell = \sum_{i=1}^{n} \frac{X_i - \mu}{\sigma^2} = 0 \quad \Rightarrow \quad \hat{\mu} = \frac{1}{n} \sum_{i=1}^{n} X_i$$ [The hats ˆ mean "estimated"]

$$\frac{\partial \ell}{\partial \sigma} = \sum_{i=1}^{n} \frac{|X_i - \mu|^2 - d\sigma^2}{\sigma^3} = 0 \quad \Rightarrow \quad \hat{\sigma}^2 = \frac{1}{dn} \sum_{i=1}^{n} |X_i - \mu|^2$$

We don't know μ exactly, so substitute $\hat{\mu}$ for μ to compute $\hat{\sigma}$.

I.e. we use mean & variance of points in class C to estimate mean & variance of Gaussian for class C.

For QDA: estimate conditional mean $\hat{\mu}_C$ & conditional variance $\hat{\sigma}_C^2$ of **each class C separately** [as above] & estimate the priors:

$$\hat{\pi}_C = \frac{n_C}{\sum_D n_D} \quad \Leftarrow \quad \text{total sample points in all classes}$$ [$\hat{\pi}_C$ is the coin flip parameter]

For LDA: same means & priors; one variance for all classes:

$$\hat{\sigma}^2 = \frac{1}{dn} \sum_{C} \sum_{\{i : y_i = C\}} |X_i - \mu_C|^2 \quad \Leftarrow \text{ pooled within-class variance}$$

[Notice that although we're computing one variance for all the data, each sample point contributes with respect to *its own class's mean*. This gives a very different result than if you simply use the global mean! It's usually smaller than the global variance. We say "within-class" because we use each point's distance from its class's mean, but "pooled" because we then pool all the classes together.]