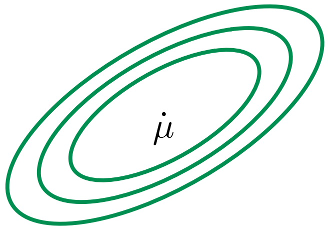
Multivariate generative modeling

The multivariate Gaussian

1. Functional form of the density
2. Special case: diagonal Gaussian
3. Special case: spherical Gaussian
4. Fitting a Gaussian to data

The multivariate Gaussian



$N(\mu, \Sigma)$: Gaussian in $\mathbb{R}^d$

- mean: $\mu \in \mathbb{R}^d$
- covariance: $d \times d$ matrix Σ

Generates points $X = (X_1, X_2, \ldots, X_d)$.

- μ is the vector of coordinate-wise means:

$$\mu_1 = \mathbb{E}X_1, \ \mu_2 = \mathbb{E}X_2, \ldots, \ \mu_d = \mathbb{E}X_d.$$

- Σ is a matrix containing all pairwise covariances:

$$\begin{aligned} \Sigma_{ij} = \Sigma_{ji} &= \text{cov}(X_i, X_j) \quad \text{if } i \neq j \\ \Sigma_{ii} &= \text{var}(X_i) \end{aligned}$$

Density $\quad p(x) = \dfrac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \exp\left(-\dfrac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu)\right)$

Special case: independent features

Suppose the X_i are independent, and $\text{var}(X_i) = \sigma_i^2$.

What is the covariance matrix Σ, and what is its inverse Σ^{-1}?

Diagonal Gaussian

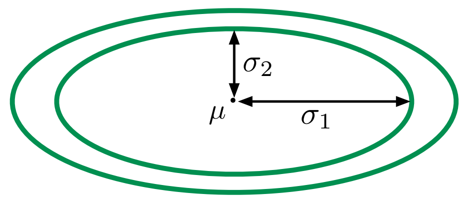
Diagonal Gaussian: the X_i are independent, with variances σ_i^2. Thus

$$\Sigma = \text{diag}(\sigma_1^2, \ldots, \sigma_d^2) \quad \text{(off-diagonal elements zero)}$$

Each X_i is an independent one-dimensional Gaussian $N(\mu_i, \sigma_i^2)$:

$$\Pr(x) = \Pr(x_1)\Pr(x_2)\cdots\Pr(x_d) = \frac{1}{(2\pi)^{d/2}\sigma_1\cdots\sigma_d} \exp\left(-\sum_{i=1}^{d} \frac{(x_i-\mu_i)^2}{2\sigma_i^2}\right)$$

Contours of equal density are **axis-aligned ellipsoids** centered at μ:



Even more special case: spherical Gaussian

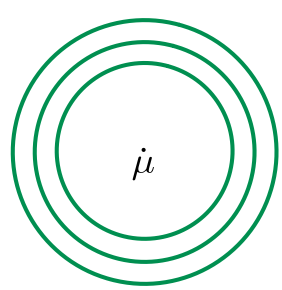
The X_i are independent and all have the same variance σ^2.

$$\Sigma = \sigma^2 I_d = \text{diag}(\sigma^2, \sigma^2, \ldots, \sigma^2) \quad \text{(diagonal elements } \sigma^2\text{, rest zero)}$$

Each X_i is an independent univariate Gaussian $N(\mu_i, \sigma^2)$:

$$\Pr(x) = \Pr(x_1)\Pr(x_2)\cdots\Pr(x_d) = \frac{1}{(2\pi)^{d/2}\sigma^d} \exp\left(-\frac{\|x-\mu\|^2}{2\sigma^2}\right)$$

Density at a point depends only on its distance from μ:



How to fit a Gaussian to data

Fit a Gaussian to data points $x^{(1)}, \ldots, x^{(m)} \in \mathbb{R}^d$.

- Empirical mean

$$\mu = \frac{1}{m}\left(x^{(1)} + \cdots + x^{(m)}\right)$$

- Empirical covariance matrix has i, j entry:

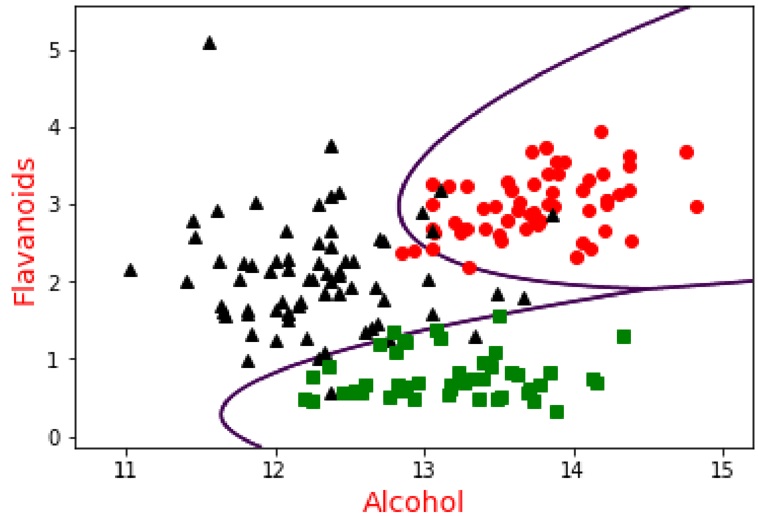
$$\Sigma_{ij} = \left(\frac{1}{m}\sum_{k=1}^{m} x_i^{(k)} x_j^{(k)}\right) - \mu_i \mu_j$$

Gaussian generative models

1. Classification using multivariate Gaussian generative modeling
2. The form of the decision boundaries

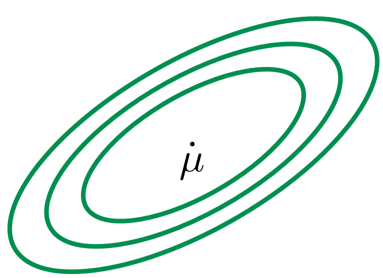
Back to the winery data

Go from 1 to 2 features: test error goes from 29% to 8%.



With all 13 features: test error rate goes to zero.

The multivariate Gaussian



$N(\mu, \Sigma)$: Gaussian in $\mathbb{R}^d$

- mean: $\mu \in \mathbb{R}^d$
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Density $\quad p(x) = \dfrac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \exp\left(-\dfrac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right)$

If we write $S = \Sigma^{-1}$ then S is a $d \times d$ matrix and

$$(x-\mu)^T\Sigma^{-1}(x-\mu) \;=\; \sum_{i,j} S_{ij}(x_i-\mu_i)(x_j-\mu_j),$$

a **quadratic function** of x.

Binary classification with Gaussian generative model

- Estimate class probabilities π_1, π_2
- Fit a Gaussian to each class: $P_1 = N(\mu_1, \Sigma_1)$, $P_2 = N(\mu_2, \Sigma_2)$

Given a new point x, predict class 1 if

$$\pi_1 P_1(x) > \pi_2 P_2(x) \quad \Leftrightarrow \quad x^T M x + 2w^T x \geq \theta,$$

where:

$$M = \frac{1}{2}(\Sigma_2^{-1} - \Sigma_1^{-1})$$
$$w = \Sigma_1^{-1}\mu_1 - \Sigma_2^{-1}\mu_2$$

and θ is a threshold depending on the various parameters.

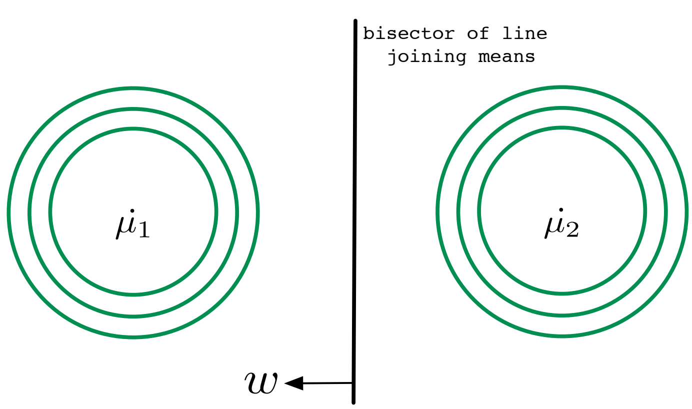
Linear or **quadratic** decision boundary.

Common covariance: $\Sigma_1 = \Sigma_2 = \Sigma$

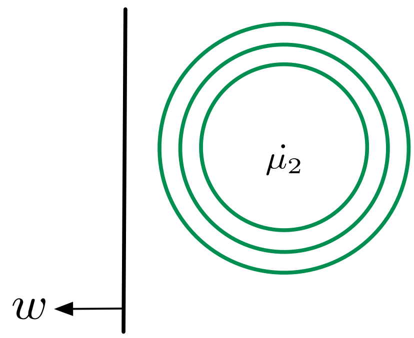
Linear decision boundary: choose class 1 if

$$x \cdot \underbrace{\Sigma^{-1}(\mu_1 - \mu_2)}_{w} \geq \theta.$$

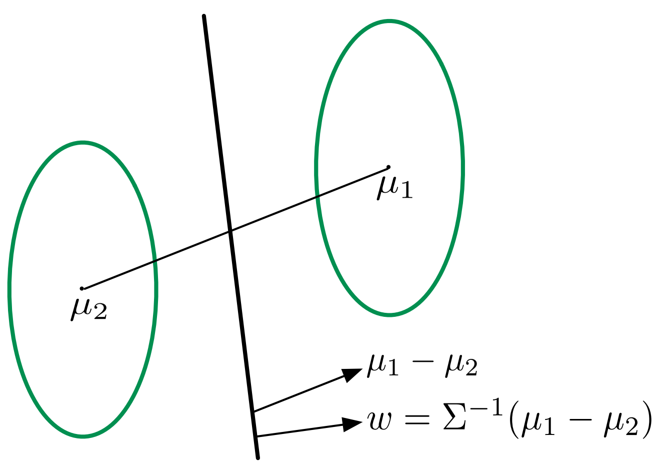
Example 1: Spherical Gaussians with $\Sigma = I_d$ and $\pi_1 = \pi_2$.



Example 2: Again spherical, but now $\pi_1 > \pi_2$.



Example 3: Non-spherical.



Classification rule: $w \cdot x \geq \theta$

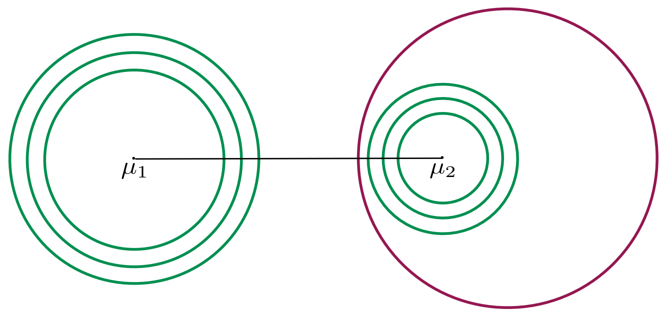
- Choose w as above
- Common practice: fit θ to minimize training or validation error

Different covariances: $\Sigma_1 \neq \Sigma_2$

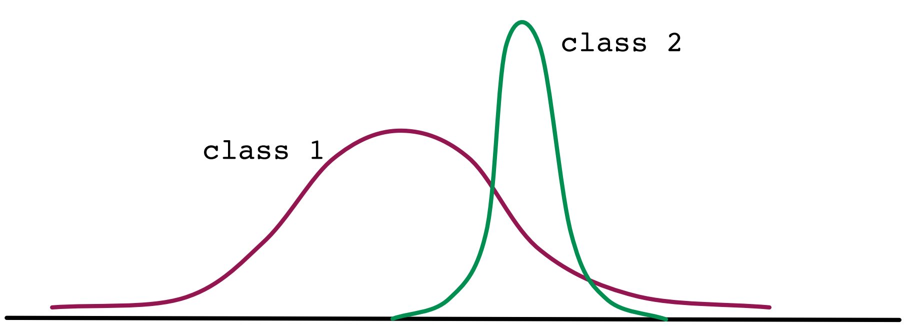
Quadratic boundary: choose class 1 if $x^T M x + 2w^T x \geq \theta$, where:

$$M = \frac{1}{2}(\Sigma_2^{-1} - \Sigma_1^{-1})$$
$$w = \Sigma_1^{-1}\mu_1 - \Sigma_2^{-1}\mu_2$$

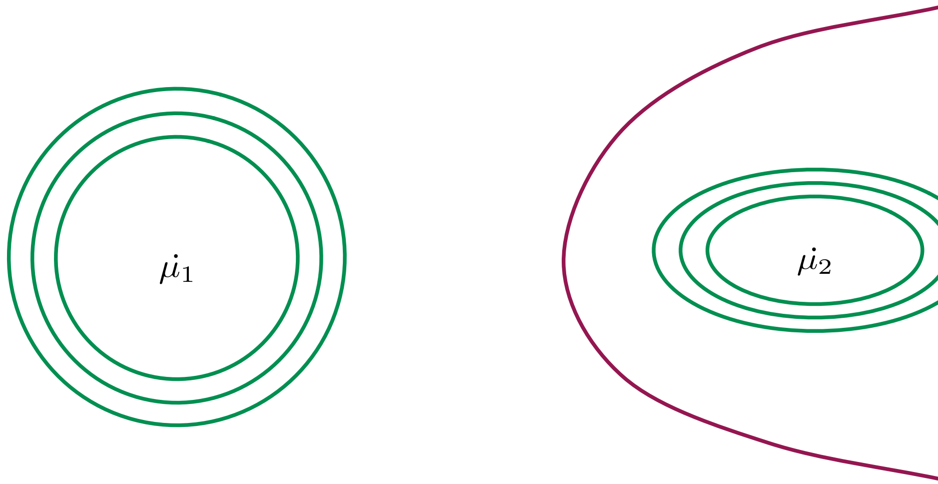
Example 1: $\Sigma_1 = \sigma_1^2 I_d$ and $\Sigma_2 = \sigma_2^2 I_d$ with $\sigma_1 > \sigma_2$



Example 2: Same thing in 1-d. $\mathcal{X} = \mathbb{R}$.



Example 3: A parabolic boundary.



Multiclass discriminant analysis

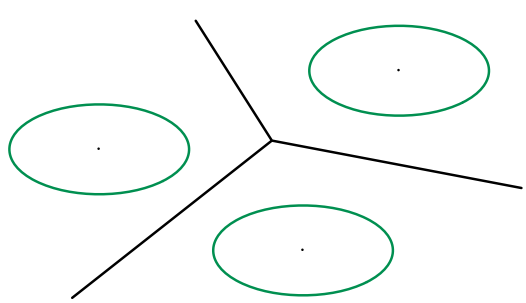
k classes: weights π_j, class-conditional densities $P_j = N(\mu_j, \Sigma_j)$.

Each class has an associated **quadratic** function

$$f_j(x) = \log\left(\pi_j \, P_j(x)\right)$$

To classify point x, pick $\arg\max_j f_j(x)$.

If $\Sigma_1 = \cdots = \Sigma_k$, the boundaries are **linear**.



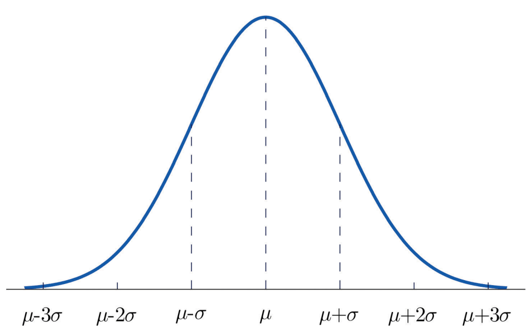
More generative modeling

1. Beyond Gaussians
2. A variety of univariate distributions
3. Moving to higher dimension

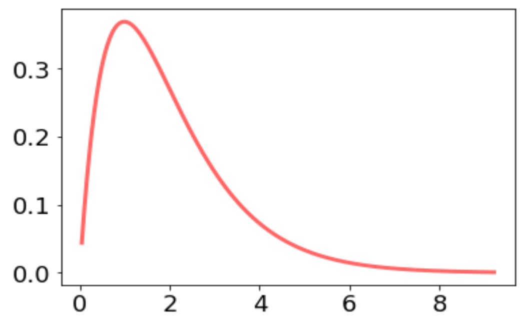
Classification with generative models

- Fit a **distribution** to each class separately
- Use Bayes' rule to classify new data

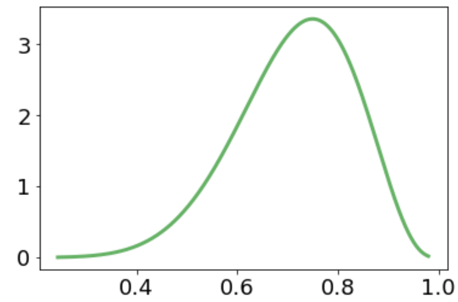
What distribution to use? Are Gaussians enough?



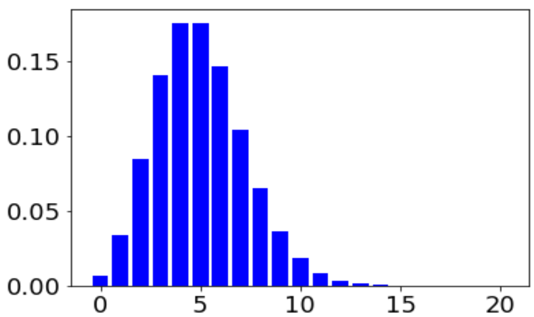
Exponential families of distributions



GAMMA



BETA



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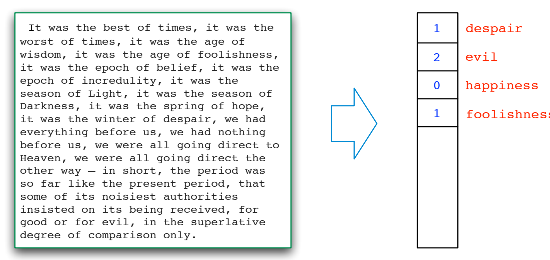

CATEGORICAL

Multivariate distributions

We've described a variety of distributions for **one-dimensional** data.
What about higher dimensions?

1. **Naive Bayes**: Treat coordinates as independent.
   For $x = (x_1, \ldots, x_d)$, fit separate models $\Pr_i$ to each x_i, and assume

$$\Pr(x_1, \ldots, x_d) = \Pr_1(x_1)\Pr_2(x_2)\cdots\Pr_d(x_d).$$

   This assumption is typically inaccurate.

2. **Multivariate Gaussian**.
   Model correlations between features: we've seen this in detail.

3. **Graphical models**.
   Arbitrary dependencies between coordinates.