Gaussian Voronoi Diagrams

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New Directions in Algebraic Statistics

UT Austin

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Joint work with Joe Kileel

Motivating example

- Patient has a tumor with 14cm perimeter and we want to classify it as benign/malignant

[1] Wolberg, Mangasarian, Street (1993). Breast Cancer Wisconsin Diagnostic Dataset.

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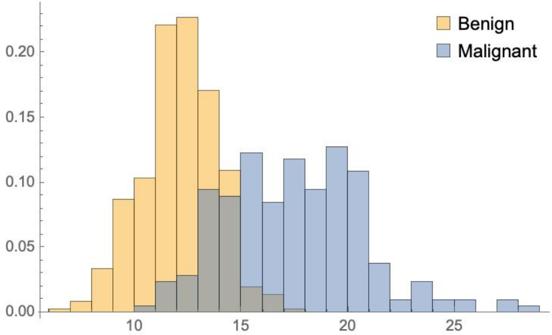
- Patient has a tumor with 14cm perimeter and we want to classify it as benign/malignant
- Have data on perimeters of tumors from the Breast Cancer Wisconsin Diagnostic Dataset[1]



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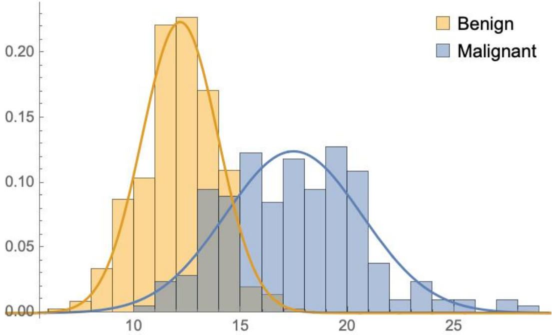
- Perimeter of malignant tumors are roughly $\mathcal{N}(17.5, 3.2)$ and benign are $\mathcal{N}(12.2, 1.8)$



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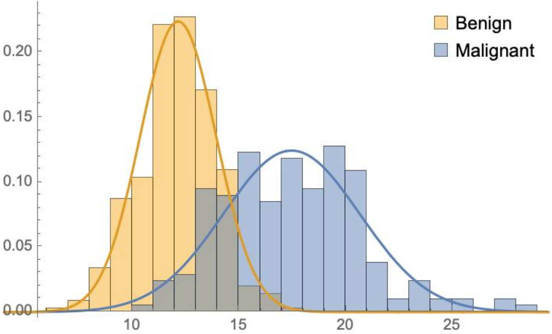

- More likely tumor is benign (probability 0.65)

Gaussian discriminant analysis

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- Assume each class $i \in [d]$ is distributed as $\mathcal{N}(\mu_i, \Sigma_i)$, $\mu_i \in \mathbb{R}^n$, $\Sigma_i \succ 0$ and

$$f(x|\mu_i, \Sigma_i) = \frac{1}{\sqrt{(2\pi)^d \det(\Sigma_i)}} \exp\left(-\frac{1}{2}(x - \mu_i)^T \Sigma_i^{-1}(x - \mu_i)\right)$$

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- GDA: Classify new point $x \in \mathbb{R}^n$ as class i if

$$f(x|\mu_i, \Sigma_i) \geq f(x|\mu_j, \Sigma_j) \quad \forall j \in [d]$$

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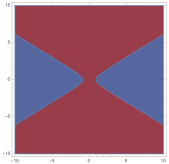

Figure: GVor_X when $X = \left\{ \left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right), \left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 4 & 0 \\ 0 & \frac{1}{3} \end{bmatrix} \right) \right\}.$

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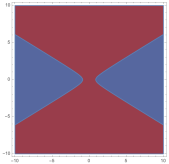

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- $\mathrm{GVor}_X(\mu_i, \Sigma_i)$ is defined by $d-1$ quadratic inequalities (quadratic discriminant analysis)

Example: $\Sigma_i = I_n$

- Consider $X = \{(\mu_1, I_n), \ldots, (\mu_d, I_n)\} \subset \mathbb{R}^n \times \{I_n\}$

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- When $\Sigma_i = I_n$ for all $i \in [d]$, then Gaussian Voronoi cells are just standard *Voronoi cells*

- If $X = \{(\mu_1, \Sigma), \dots, (\mu_d, \Sigma)\}$, then $\mathrm{GVor}_X(\mu_i, \Sigma)$ is a linear transformation of the Voronoi cell of μ_i with respect to the set $\{\mu_1, \dots, \mu_d\}$ $\Rightarrow$ linear discriminant analysis (LDA)

Another example

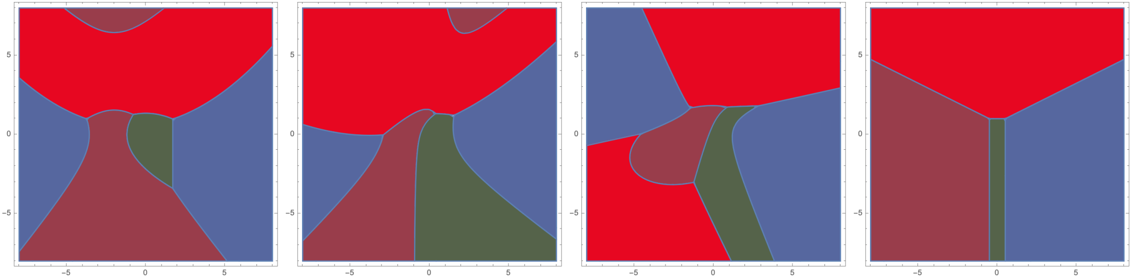
Consider when $n = 2$ and the sets $X_1, X_2, X_3, X_4 \subset \mathbb{R}^2 \times \mathrm{PD}_2$ where each X_i has the same means

$$\mu_1 = \begin{bmatrix} -1 \\ 0 \end{bmatrix}, \quad \mu_2 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \mu_3 = \begin{bmatrix} 0 \\ 2 \end{bmatrix}, \quad \mu_4 = \begin{bmatrix} 0 \\ 0 \end{bmatrix},$$

and the variances are as follows:

$$X_1 = \left\{ \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix}, \begin{bmatrix} 4 & 0 \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right\} \qquad X_2 = \left\{ \begin{bmatrix} 1 & 1 \\ 1 & 2 \end{bmatrix}, \begin{bmatrix} 4 & 1 \\ 1 & 1 \end{bmatrix}, \begin{bmatrix} 2 & 1/2 \\ 1/2 & 1 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right\}$$

$$X_3 = \left\{ \begin{bmatrix} 1 & 1/2 \\ 1/2 & 1 \end{bmatrix}, \begin{bmatrix} 3 & -1 \\ -1 & 1 \end{bmatrix}, \begin{bmatrix} 2 & 2 \\ 2 & 4 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right\} \qquad X_4 = \left\{ \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right\}$$



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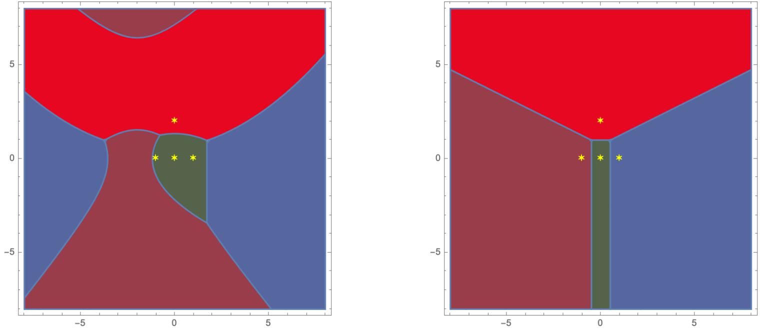

Figure: Gaussian Voronoi cells of X (left) and standard Voronoi cells of Y (right).

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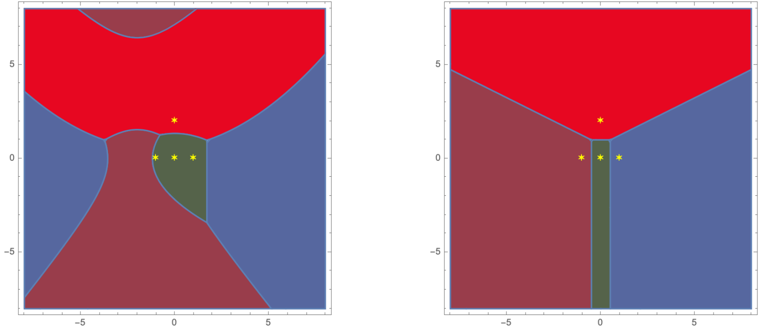

Figure: Gaussian Voronoi cells of X (left) and standard Voronoi cells of Y (right).

- **Goal:** Understand geometry and combinatorics of Gaussian Voronoi cells/diagrams

Motivation for Gaussian Voronoi diagrams

- Gaussian Voronoi diagrams give *all possible* clusterings GMMs are capable of producing
  - Standard Voronoi cells (as in LDA) can only give convex clusterings
  - Kernel methods embed in high dimensional space then use convex clusterings

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- **Question:** Which clusterings are GMMs capable of producing?

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Upper bounds on connected components

- The *decision boundary* of $X = \{(\mu_1, \Sigma_1), \ldots, (\mu_d, \Sigma_d)\} \subset \mathbb{R}^n \times \mathrm{PD}_n$ is

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- Apply Milnor-Thom to $\mathcal{B}_i$ with $\deg(\mathcal{B}_i) = 2(d-1)$ to see:

$$\# \text{ connected components } \mathrm{GVor}_X(\mu_i, \Sigma_i) \leq (2d-2)^{n+1}$$

$$\# \text{ connected components } \mathrm{GVor}_X \leq d(2d-2)^{n+1}$$

Tight upper bound

Theorem (L., Kileel)

For $X = \{(\mu_1, \sigma_1^2), \ldots, (\mu_d, \sigma_d^2)\} \subseteq \mathbb{R} \times \mathbb{R}_{>0}$ *where* $\sigma_i \leq \sigma_{i+1}$ *for* $i \in [d-1]$*. Then:*

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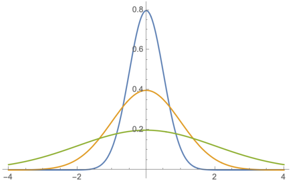
- If $X = \{(0, \sigma_1^2), \ldots, (0, \sigma_d^2)\}$ with $\sigma_i^2 < \sigma_{i+1}^2$ then GVor_X has $2d-1$ connected components



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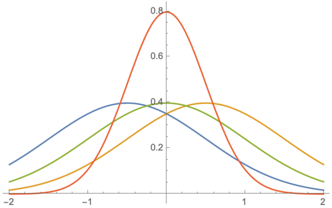

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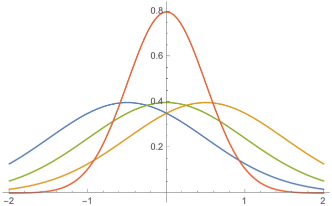

Theorem (L., Kileel)

There exists a collection of Gaussians $X = \{(\mu_1, \Sigma_1), \ldots, (\mu_d, \Sigma_d)\} \subset \mathbb{R}^n \times \mathrm{PD}_n$ *such that* GVor_X *has 3 connected components.*

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- It is possible that GDA will only classify points as 3 classes
- Also shows shortcomings with *Hard EM*

  Input : unlabeled data $\{x_1, \ldots, x_N\} \subset \mathbb{R}^n$
  Initialize : $\{(\mu_1, \Sigma_1), \ldots, (\mu_d, \Sigma_d)\}$
  Until convergence:

  1. Perform GDA to assign each x_j to a class $1, \ldots, d$
  2. Update (μ_i, Σ_i) to be the sample mean and covariance of the points classified as i

Hard EM

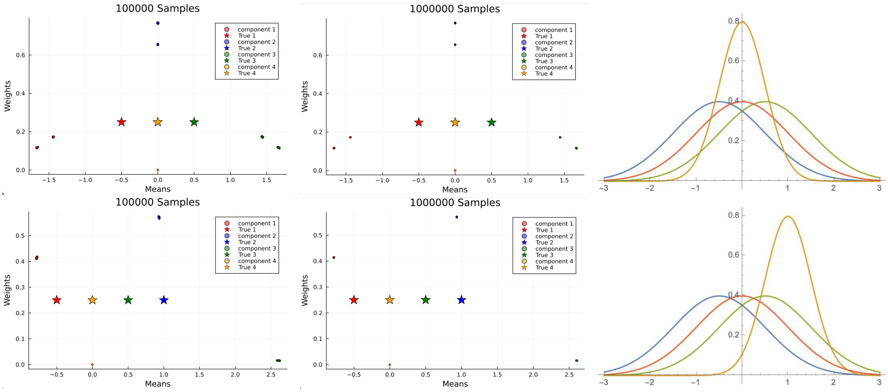

Figure: The results from running 100 trials of Hard EM on Gaussians with ground truth means and weights given and variances in both cases equal to $\sigma_1 = \sigma_3 = \sigma_4 = 1$ and $\sigma_2 = 1/2$. In all cases, we initialized Hard EM at the ground truth.

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One dimensional Gaussian Voronoi cells

- Consider $X = \{(\mu_1, \sigma_1^2), \ldots, (\mu_d, \sigma_d^2)\} \subset \mathbb{R} \times \mathbb{R}_{>0}$

$$\mathrm{GVor}_X(\mu_i, \sigma_i^2) = \{x \in \mathbb{R} \ : \ \frac{1}{\sigma_i^2}(x - \mu_i)^2 + \log(\sigma_i^2) \leq \frac{1}{\sigma_j^2}(x - \mu_j)^2 + \log(\sigma_j^2) \ \ \forall j \in [d]\}$$

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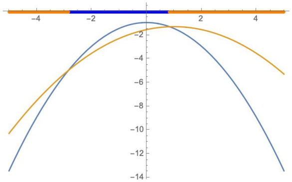
- Ex. $X = \{(0,1),(1,2)\}$



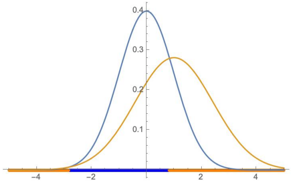


Figure: GVor_X and the log of the densities in X (left) along with the densities (right).

Gaussian sequences

- For $X = \{(\mu_1, \sigma_1^2), \ldots, (\mu_d, \sigma_d^2)\}$, with $\sigma_1^2 \leq \cdots \leq \sigma_d^2$, the *Gaussian d-sequence* corresponding to X is a sequence $S_X = \{i_1, \ldots, i_N\}$ that records the order in which each Gaussian component appears

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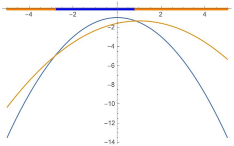
- $X = \{(0,1), (1,2)\}$ has Gaussian 2-sequence $\{2,1,2\}$



Gaussian sequences

- For $X = \{(\mu_1, \sigma_1^2), \dots, (\mu_d, \sigma_d^2)\}$, with $\sigma_1^2 \le \cdots \le \sigma_d^2$, the *Gaussian d-sequence* corresponding to X is a sequence $S_X = \{i_1, \dots, i_N\}$ that records the order in which each Gaussian component appears

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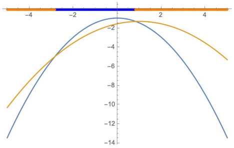

- $X = \{(\mu_1, 1), \dots, (\mu_d, 1)\}$ with $\mu_1 < \dots < \mu_d$ has Gaussian d-sequence $\{1, 2, \dots, d\}$

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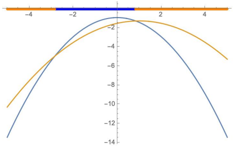

- $X = \{(\mu_1, 1), \ldots, (\mu_d, 1)\}$ with $\mu_1 < \ldots < \mu_d$ has Gaussian d-sequence $\{1, 2, \ldots, d\}$

- **Question :** Which sequences are Gaussian d-sequences?

Gaussian sequences

Theorem (L., Kileel)

Let $S = \{i_1, \ldots, i_N\}$ be a sequence with $i_j \in [d]$ for all $j \in [N]$. Then S is a Gaussian d-sequence if and only if

1. $i_j \neq i_{j+1}$ *for any* $j \in [N]$, *and*
2. *for any indices* $j < \ell$ *where* $i_j = i_\ell$ *then for any* $j < m < \ell$, $i_m \leq i_j$.

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- If an integer $\ell \in [d]$ appears twice in a sequence S, then any integer that appears between the two occurrences of ℓ must be less than or equal to ℓ
- $\{3, 2, 3, 2\}$ can not appear as a part of a larger Gaussian sequence but $\{3, 2, 1, 2\}$ can

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- $\{3, 2, 1, 2, 3\}$, $\{3, 2, 3, 1, 3\}$, $\{3, 1, 3, 2, 3\}$ are all Gaussian 3 sequences of size 5

Stirling permutations

Definition

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Theorem (L., Kileel)

There is a bijection between Gaussian d-sequences of size $2d-1$ and Stirling permutations of order $d-1$. Moreover, the number of Gaussian d-sequences of size $2d-1$ is $(2d-3)!!$.

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Thank you! Questions?