Lecture 18 — **G**aussian **M**ixture **M**odels.

Alex Schwing and Matus Telgarsky

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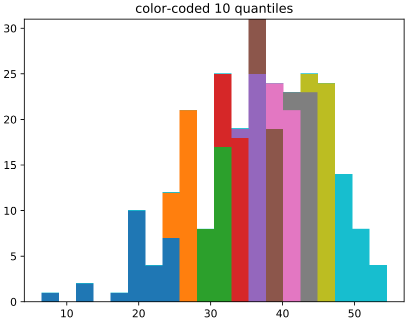
Announcements.

- Midterm has been graded;
  grades are in compass;
  midterms handed back in TA office hours.
  This week there **is** a Friday TA office hour.
- Midterm grade histogram, with 10 quantiles:



Schedule for today.

- k-means review.
- (Almost) Deriving GMMs by extending k-means.
- Probability model behind GMMs.
- GMMs Examples.
- Ancillary topics.

k-means review.

k-means review.

Key points with k-means.

- The objective function.
- The standard algorithm (Lloyd's method).
- Standard application: vector quantization.

k-means review: objective function.

The **exemplar-based**, **hard-assignment** k-means clustering objective.

$$\min_{\mu_1,\ldots,\mu_k} \sum_{i=1}^{n} \min_{j} \|x_i - \mu_j\|_2^2 = \min_{\mu_1,\ldots,\mu_k} \min_{\substack{A\in\{0,1\}^{n\times k} \\ A\mathbf{1}_k=\mathbf{1}_n}} \sum_{i=1}^{n} \sum_{j=1}^{k} A_{ij} \|x_i - \mu_j\|_2^2.$$

Remarks.

- Second form makes assignment of data to centers explicit.
- NP-hard even when $d = 2$; methods do not globally optimize.

k-means review: standard algorithm.

1. Let initial clusters $(C_1, \ldots, C_k)$ be given.
2. Alternate the following two steps:
   - 2.1 **(Recentering.)** Hold $(C_1, \ldots C_k)$ fixed, optimally update centers: for all j, $\mu_j := \text{mean}(C_j)$.
   - 2.2 **(Reassignment.)** Hold $(\mu_1, \ldots, \mu_k)$ fixed, optimally update clusters: put x_i in C_j iff $\|x_i - \mu_j\| = \min_l \|x_i - \mu_l\|$ (breaking ties arbitrarily).

Remarks.

- This is **alternating minimization**.
- Initialization is crucial; standard initialization now is "`kmeans++`" (see k-means lecture).
- With good initialization, in practice method quickly finds good clusters; in theory, not so much.

k-means review: vector quantization.

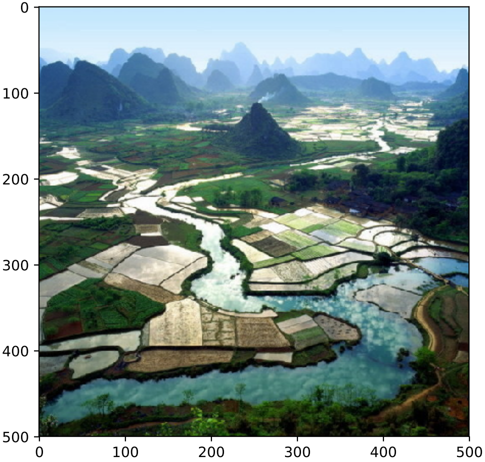
A standard application of k-means is **vector quantization**.

1. Obtain data $(x_i)_{i=1}^n$.
2. Run k-means on $(x_i)_{i=1}^n$, obtain $(\mu_1, \ldots, \mu_k)$.
3. Output new data $(\mu(x_i))_{i=1}^n$ where $\mu(x_i) = \arg\min_{\mu_j} \|x_i - \mu_j\|_2$, the center closest to x_i.

Remarks.

- In words: replace data points with their closest means.
- This gives a quick way to "compress" data.
- This is useful in speech and vision data (amongst others).

k-means review: vector quantization.



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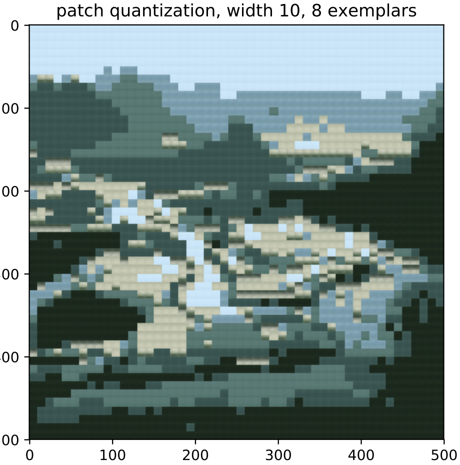

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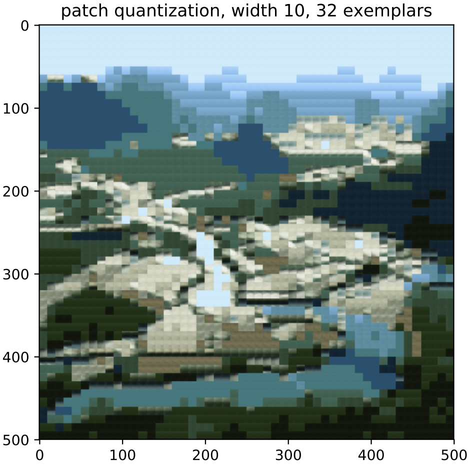

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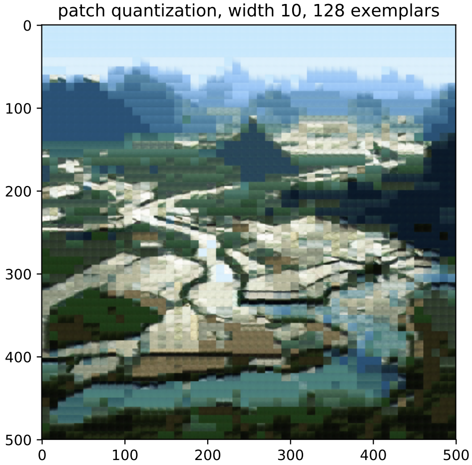

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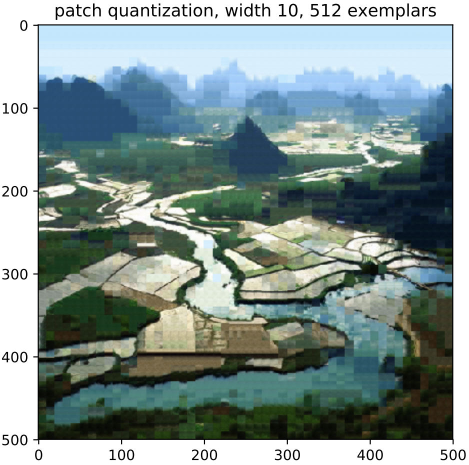

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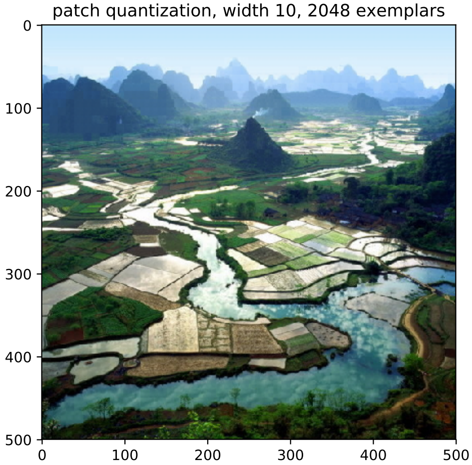

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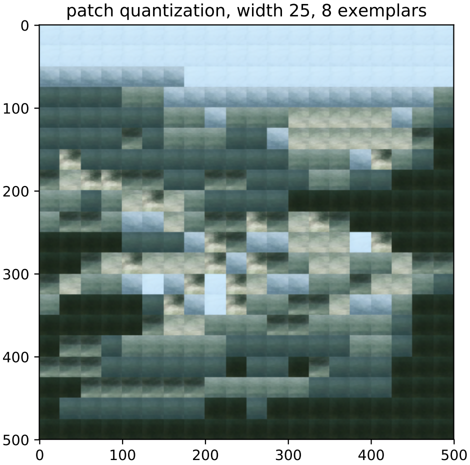

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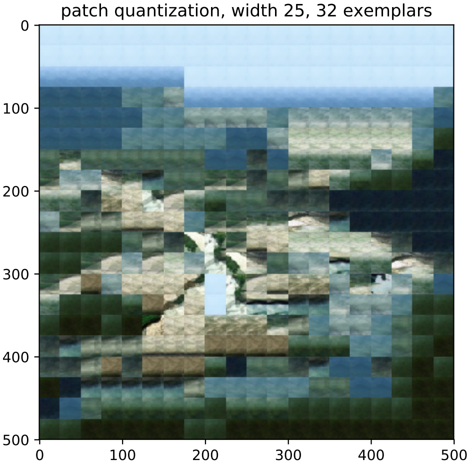

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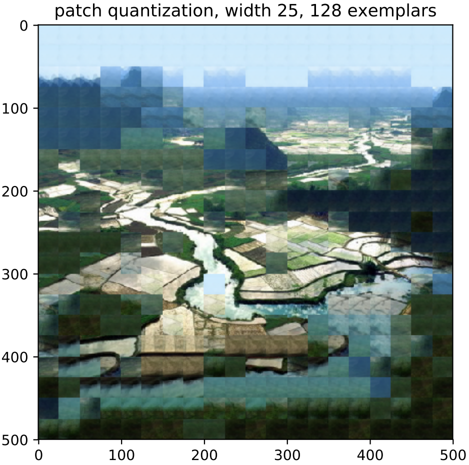

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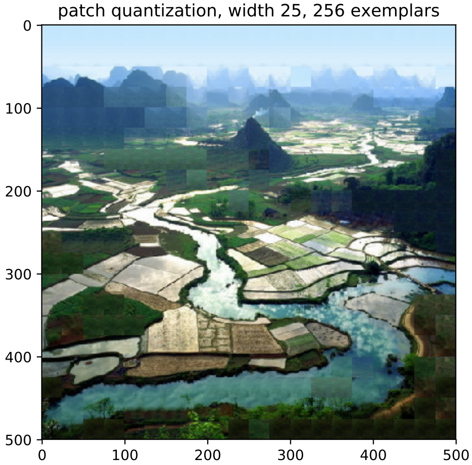

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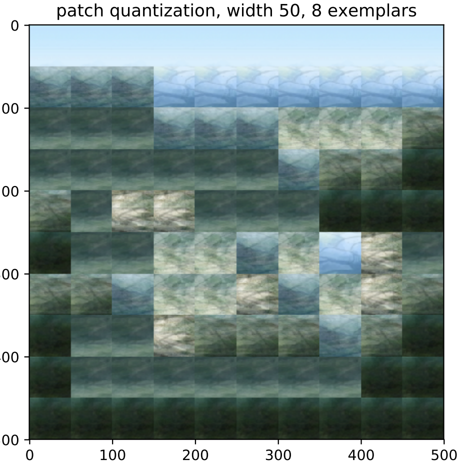

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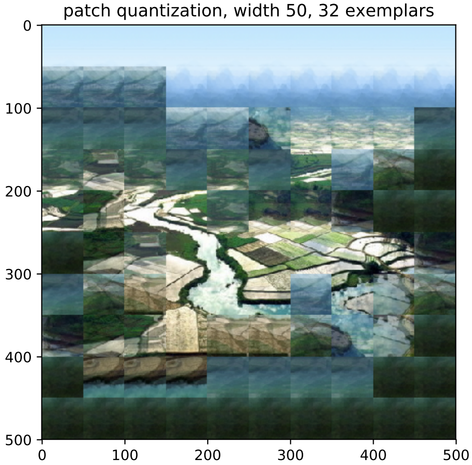

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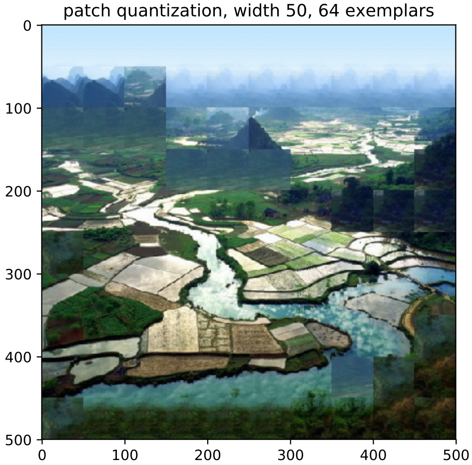

(Almost) Deriving GMMs by extending k-means.

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Let's extend k-means in two ways:

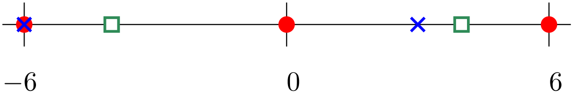
- Soft assignments.
- Non-spherical clusters.

k-means with soft assignments.

Suppose assignment matrix $A \in [0,1]^{n\times k}$ has *probability vectors* for rows:

$$\min_{\mu_1,\ldots,\mu_k} \min_{\substack{A\in[0,1]^{n\times k}\\ A\mathbf{1}_k=\mathbf{1}_n}} \sum_{i=1}^{n}\sum_{j=1}^{k} A_{ij}\|x_i-\mu_j\|_2^2.$$

Example:



Soft assignments give a “more pleasing” fit?

- red = data, blue = hard centers, green = soft centers.
- Soft clustering allows a symmetric solution; hard does not!

k-means with soft assignments.

Directly (min over a larger set),

$$\min_{\mu_1,\ldots,\mu_k} \min_{\substack{A\in[0,1]^{n\times k}\\ A\mathbf{1}_k=\mathbf{1}_n}} \sum_{i=1}^{n}\sum_{j=1}^{k} A_{ij}\|x_i-\mu_j\|_2^2 \leq \min_{\mu_1,\ldots,\mu_k} \min_{\substack{A\in\{0,1\}^{n\times k}\\ A\mathbf{1}_k=\mathbf{1}_n}} \sum_{i=1}^{n}\sum_{j=1}^{k} A_{ij}\|x_i-\mu_j\|_2^2.$$

On the other hand,

k-means with soft assignments.

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On the other hand,

$$\begin{aligned}
&\min_{\mu_1,\ldots,\mu_k} \min_{\substack{A\in[0,1]^{n\times k}\\ A\mathbf{1}_k=\mathbf{1}_n}} \sum_{i=1}^{n}\sum_{j=1}^{k} A_{ij}\|x_i-\mu_j\|_2^2 \\
&\geq \min_{\mu_1,\ldots,\mu_k} \min_{\substack{A\in[0,1]^{n\times k}\\ A\mathbf{1}_k=\mathbf{1}_n}} \sum_{i=1}^{n}\sum_{j=1}^{k} A_{ij}\min_{l}\|x_i-\mu_l\|_2^2 \\
&\geq \min_{\mu_1,\ldots,\mu_k} \min_{\substack{A\in[0,1]^{n\times k}\\ A\mathbf{1}_k=\mathbf{1}_n}} \sum_{i=1}^{n}\left(\sum_{j=1}^{k} A_{ij}\right)\min_{l}\|x_i-\mu_l\|_2^2 \\
&= \min_{\mu_1,\ldots,\mu_k} \min_{\substack{A\in\{0,1\}^{n\times k}\\ A\mathbf{1}_k=\mathbf{1}_n}} \sum_{i=1}^{n}\sum_{j=1}^{k} A_{ij}\|x_i-\mu_j\|_2^2.
\end{aligned}$$

k-means with soft assignments.

Therefore

$$\min_{\mu_1,\ldots,\mu_k} \min_{\substack{A\in[0,1]^{n\times k} \\ A\mathbf{1}_k=\mathbf{1}_n}} \sum_{i=1}^{n}\sum_{j=1}^{k} A_{ij}\|x_i-\mu_j\|_2^2 = \min_{\mu_1,\ldots,\mu_k} \min_{\substack{A\in\{0,1\}^{n\times k} \\ A\mathbf{1}_k=\mathbf{1}_n}} \sum_{i=1}^{n}\sum_{j=1}^{k} A_{ij}\|x_i-\mu_j\|_2^2,$$

and even soft assignment has a globally optimal **hard assignment**!

- Therefore: minimization alone won't give soft A_{ij} choice.
- In earlier example, symmetric local optimum was not global!

k-means with spherical clusters.

Consider a single cluster C_j; the cost is

$$\sum_{x_i \in C_j} \|x_i - \mu_j\|_2^2 = (x_i - \mu_j)^\top (x_i - \mu_j).$$

How can this be made this non-spherical?

k-means with spherical clusters.

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How can this be made this non-spherical?
Introduce a positive definite matrix $M = Q\Lambda Q^\top$:

$$\sum_{x_i \in C_j} (x_i - \mu_j)^\top M (x_i - \mu_j) = \sum_{x_i \in C_j} \left(Q^\top (x_i - \mu_j)\right)^\top \Lambda \left(Q^\top (x_i - \mu_j)\right).$$

"Non-spherical" because $\{x \in \mathbb{R}^d : x^\top M x = 1\}$ is an ellipse.

k-means with spherical clusters.

Great. Let's optimize

$$\min_{\substack{\mu_1,\ldots,\mu_k \\ M_1,\ldots,M_k \\ M_j \succ 0}} \min_{\substack{A \in [0,1]^{n \times k} \\ A\mathbf{1}_k = \mathbf{1}_n}} \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij}(x_i - \mu_j)^\top M_j (x_i - \mu_j)$$

...

k-means with spherical clusters.

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Fix: *regularize M.*

k-means with spherical clusters.

To determine regularization, consider a single cluster:

$$\sum_{x_i \in C_j} (x_i - \mu_j)^\top M_j (x_i - \mu_j) + \mathrm{Reg}(M).$$

Apply ∇_M and set to zero:

$$\sum_{x_i \in C} (x_i - \mu_j)(x_i - \mu_j)^\top = -\nabla_M \mathrm{Reg}(M).$$

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Natural choice: $\mathrm{Reg}(M) := -\ln\det M$, so $\nabla_M \mathrm{Reg}(M) = -M^{-1}$, and

$$\sum_{x_i \in C} (x_i - \mu_j)(x_i - \mu_j)^\top = -\nabla_M \mathrm{Reg}(M) = M^{-1},$$

the *inverse sample covariance*!

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the *inverse sample covariance*!

Remark. If $\ln\det$ seems weird, try diagonal covariances.

Extensions to k-means.

Soft assignment: objective function

$$\min_{\mu_1,\ldots,\mu_k} \min_{\substack{A\in[0,1]^{n\times k}\\ A\mathbf{1}_k=\mathbf{1}_n}} \sum_{i=1}^{n}\sum_{j=1}^{k} A_{ij}\|x_i-\mu_j\|_2^2.$$

- Gives some symmetric solutions, but doesn't decrease cost; Unclear how to optimize.

Elliptical clusters: replace cluster cost $\sum_{x_i\in C_j}\|x_i-\mu_j\|^2$ with

$$\sum_{x_i\in C_j}(x_i-\mu_j)^\top M_j(x_i-\mu_j) - \ln\det M.$$

- Setting gradient to zero, get $M^{-1}=\sum_{x_i\in C_j}(x_i-\mu_j)(x_i-\mu_j)^\top$.

Probability model behind GMMs.

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First recall *maximum likelihood*: choose parameters according to

$$\arg\max_{\theta\in\Theta} \prod_{x\in S} p_\theta(x) = \arg\min_{\theta\in\Theta} -\ln\left(\prod_{x\in S} p_\theta(x)\right) = \arg\min_{\theta\in\Theta} \sum_{x\in S} \ln\frac{1}{p_\theta(x)}.$$

Probability model behind GMMs.

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If $\theta = (\mu, \Sigma)$ and $\Theta = \{(\mu, \Sigma) \in \mathbb{R}^d \times \mathbb{R}^{d^2} : \Sigma \succ 0\}$ and

$$p_\theta(x) = \left((2\pi)^d \det \Sigma\right)^{-1/2} \exp\left(-\frac{1}{2}(x-\mu)^\top \Sigma^{-1}(x-\mu)\right)$$

(Gaussian), so

$$\arg\max_{\theta\in\Theta} \prod_{x\in S} p_\theta(x) = \arg\min_{\theta\in\Theta} \sum_{x\in S} (x-\mu)^\top \Sigma^{-1}(x-\mu) + \ln\det\Sigma.$$

Familiar?

Probability model behind GMMs.

What we have so far: letting p_θ denote Gaussian density,

$$\underset{(\theta_1,\ldots,\theta_k)\in\Theta^k}{\arg\max} \min_{\substack{A\in[0,1]^{n\times k}\\ A\mathbf{1}_k=\mathbf{1}_n}} \sum_{i=1}^{n}\sum_{j=1}^{k} A_{ij} \ln p_\theta(x_i).$$

- This is just a reinterpretation of the previous section.
- We still don't have a way to choose soft $A \in [0,1]^{n\times k}$! For this, need a *complete* likelihood model.

Complete likelihood model for GMMS.

Data points are created in two steps:

$$\begin{aligned} Y &\sim \text{Discrete}(\pi_1, \ldots, \pi_k) && \text{(choose cluster component)}, \\ (X|Y = j) &\sim \mathcal{N}(\mu_j, \Sigma_j) && \text{(sample Gaussian } j\text{)}. \end{aligned}$$

- Random variable Y corresponds to a row of $A \in [0,1]^{n \times k}$.
- Given full parameters

  $$\theta = ((\pi_1, \theta_1), \ldots, (\pi_k, \theta_k)) = ((\pi_1, \mu_1, \Sigma_1), \ldots, (\pi_k, \mu_k, \Sigma_k)),$$

  then

  $$p_\theta(x) = \sum_{j=1}^{k} \pi_j p_{\theta_j}(x).$$

Complete likelihood model for GMMS.

Suppose we knew the true assignments $A \in [0,1]^{n \times k}$.
Then fitting the parameters to data means

$$\arg\max_{\theta \in \Theta} \sum_{i=1}^{n} \sum_{j=1}^{k} A_{ij} \ln p_{\theta_j}(x_i)$$

$$= \arg\max_{\theta \in \Theta} \sum_{i=1}^{n} \sum_{j=1}^{k} A_{ij} \left(2 \ln \pi_j - (x_i - \mu_j)^\top \Sigma_j^{-1} (x - \mu_j) - \ln \det(\Sigma_j) \right).$$

(For each i, A_{ij} isolates the single true mixture component.)

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(For each i, A_{ij} isolates the single true mixture component.)
As before, *sequentially* setting derivatives to zero gives update

$$\pi_j' := \frac{\sum_i A_{ij}}{\sum_{i,j} A_{ij}} = \frac{\sum_i A_{ij}}{n} \propto \sum_i A_{ij},$$

$$\mu_j' := \frac{\sum_i A_{ij} x_i}{\sum_i A_{ij}} = \frac{\sum_i A_{ij} x_i}{n\pi_j'},$$

$$\Sigma_j' := \frac{\sum_i A_{ij}(x_i - \mu_j')(x_i - \mu_j')^\top}{\sum_i A_{ij}} = \frac{\sum_i A_{ij}(x_i - \mu_j')(x_i - \mu_j')^\top}{n\pi_j'}.$$

("*Sequentially*" is why μ_j' not μ_j for Σ_j'.)

Complete likelihood model for GMMS.

- If we fixed the data and model parameters, we can update A_{ij} by expectations:

$$A'_{ij} := \Pr[Y_i = j | X_i = x_i] \quad = \frac{\Pr[Y_i = j]\Pr[X_i = x_i | Y_i = j]}{\Pr[X_i = x_i]}$$

$$= \frac{\pi_j p_{\theta_j}(x_i)}{\sum_l \pi_l p_{\theta_l}(x_i)}.$$

- For now this merely seems reasonable; we will justify it next lecture.

Full update rule for GMMs.

Initialize in some way; then alternate the following two steps.

1. Fix model parameters, update assignments:

$$A_{ij} := \frac{\pi_j p_{\theta_j}(x_i)}{\sum_l \pi_l p_{\theta_l}(x_i)},$$

   where p_{θ_j} is Gaussian density with parameters $\theta_j = (\mu_j, \Sigma_j)$.

2. Fix assignments, update parameters:

$$\pi'_j := \frac{\sum_i A_{ij}}{n},$$

$$\mu'_j := \frac{\sum_i A_{ij} x_i}{n\pi'_j},$$

$$\Sigma'_j := \frac{\sum_i A_{ij}(x_i - \mu'_j)(x_i - \mu'_j)^\top}{n\pi'_j}.$$

Expectation-maximization.

- This method is called Expectation-Maximization (E-M).
- Matrix $A \in [0,1]^{n\times k}$ is often called "responsibilities".
- Next lecture we will justify the method,
  in particular the choice of A_{ij},
  and establish it increases likelihood.

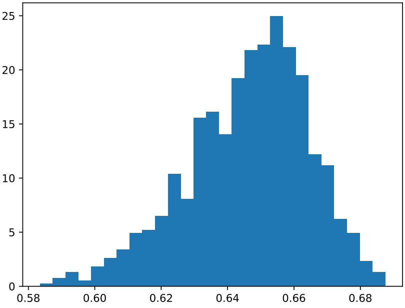
Examples.

Examples.

- Univariate example: Pearson's crabs!
- Bivariate example: synthetic data.

Pearson's crabs.

Statistician Karl Pearson wanted to understand the distribution of "forehead breadth to body length" for 1000 crabs



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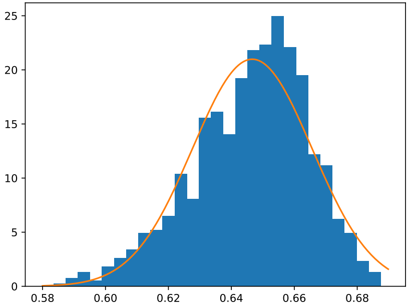

Doesn't look Gaussian!

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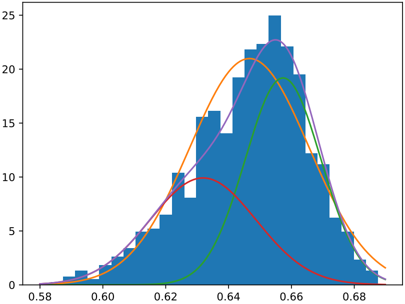

Pearson fit a **mixture of two Gaussians**.

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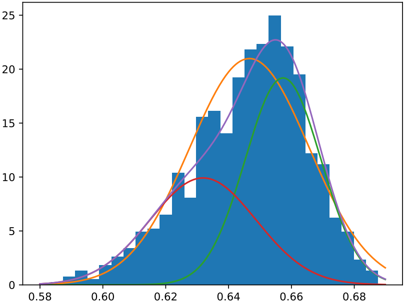


Pearson fit a **mixture of two Gaussians**.

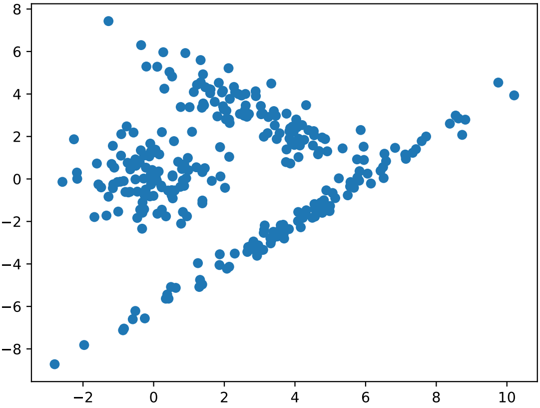
Remark. Pearson did *not* use E-M. For this he invented the "method of moments" and obtained a solution by hand.

Aside: why Gaussians at all?

- You can argue Gaussian is a good model for *single* populations thanks to the CLT (Central Limit Theorem).
- Pearson, seeing the skewed distribution, felt there are two populations.
- Treating these populations as independent, one gets a mixture of Gaussians.

Example: synthetic bivariate data.

Plot of contours of $p_\theta(x) = \sum_{i=1}^{k} \pi_j p_{\theta_j}(x)$.



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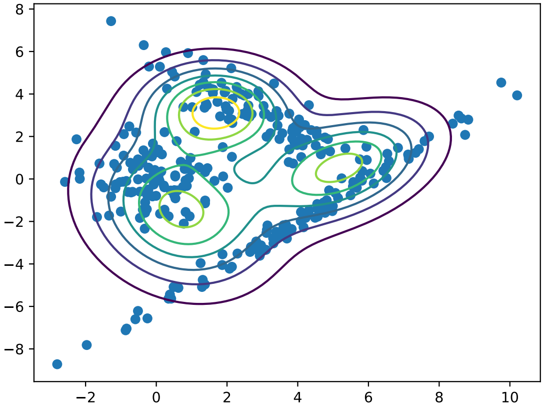

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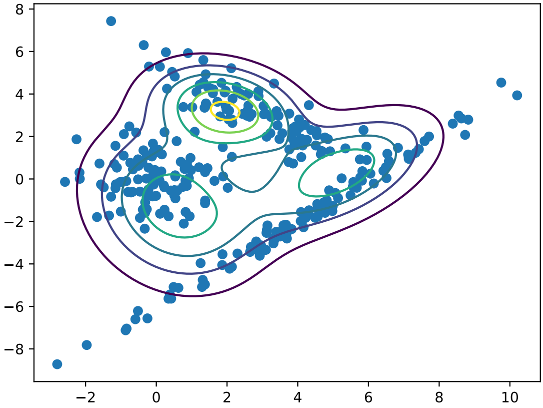

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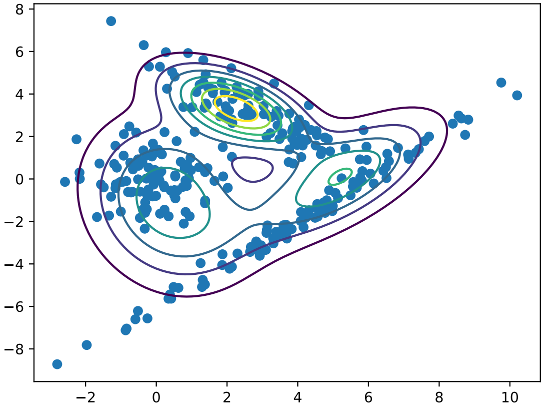

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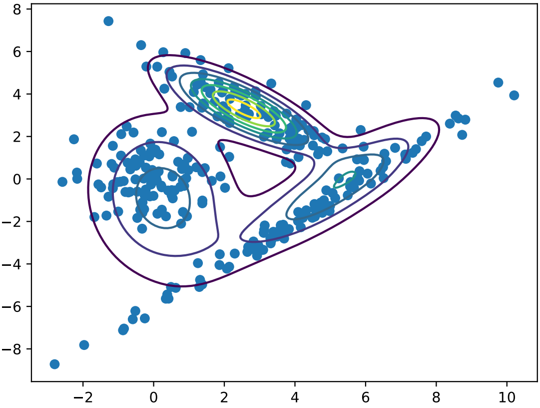

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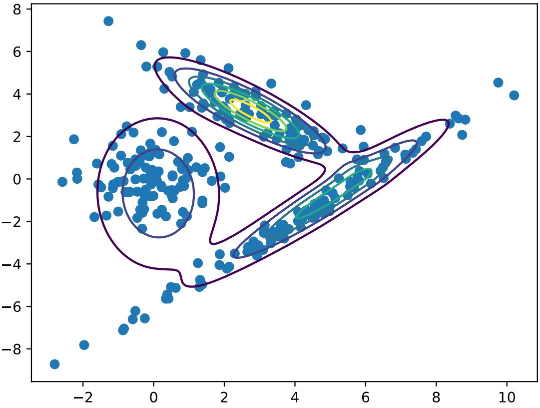

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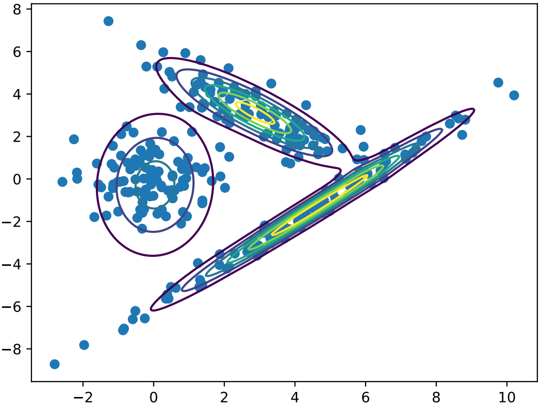

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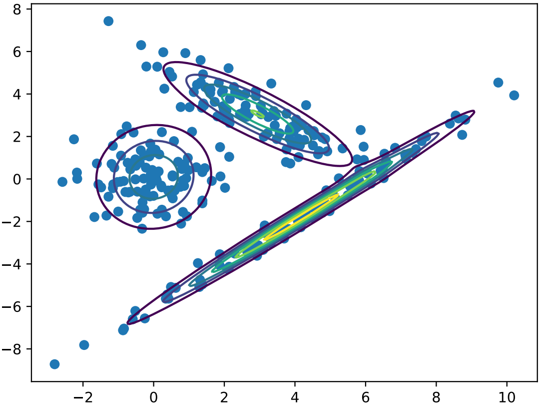

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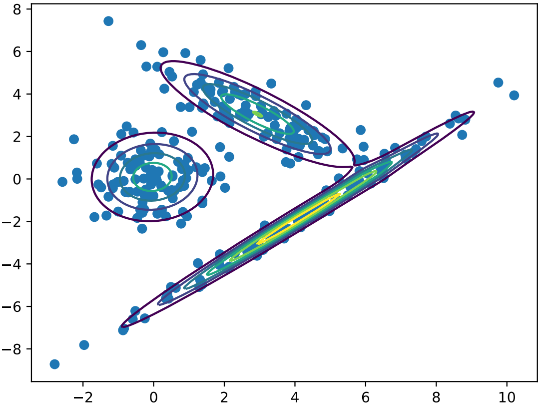

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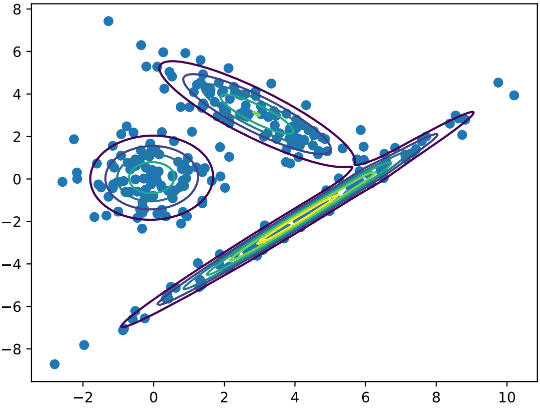

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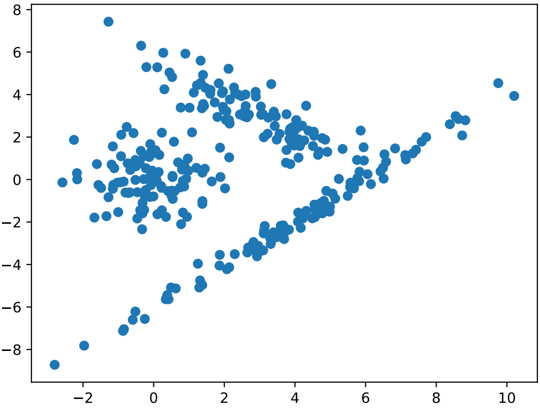
Common simplification: *diagonal* covariance matrices.
(Now $\mathcal{O}(kd)$ parameters, not $\mathcal{O}(kd^2)$.)



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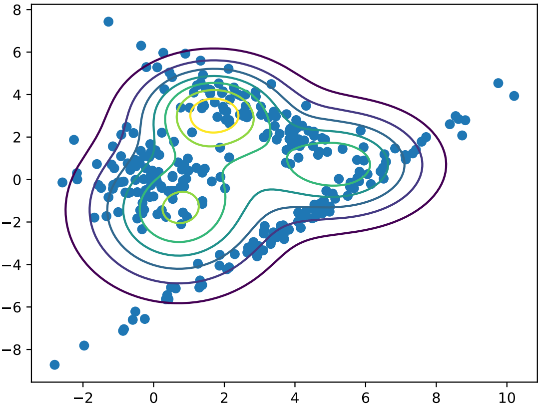

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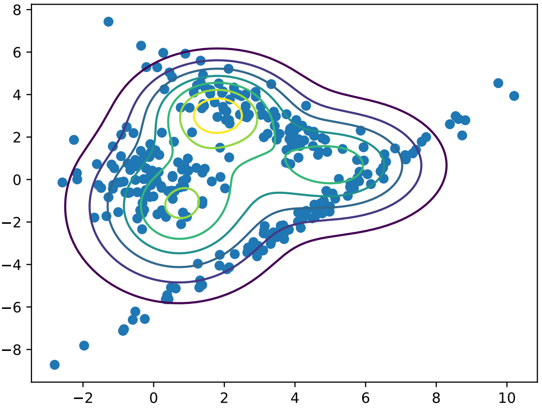

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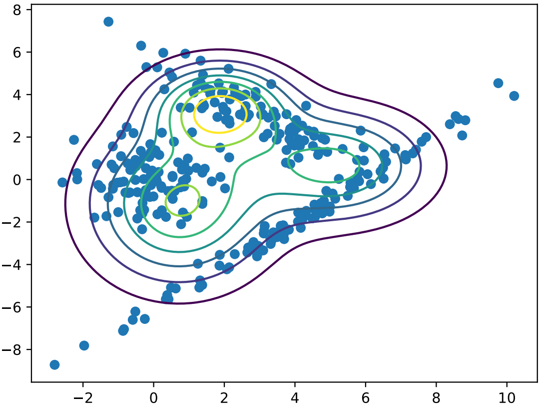

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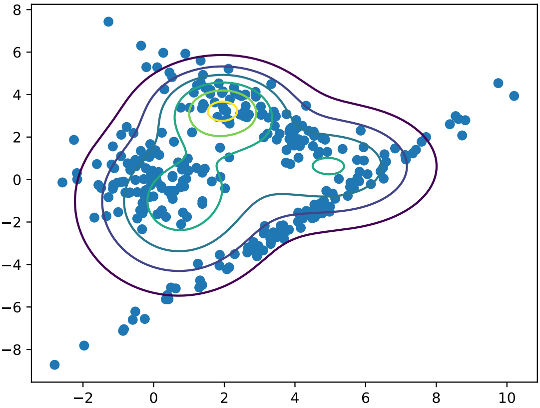

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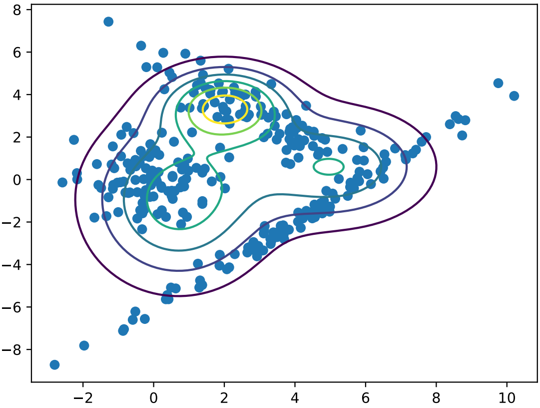

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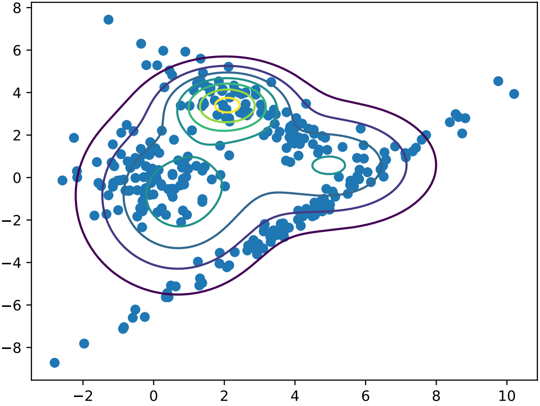

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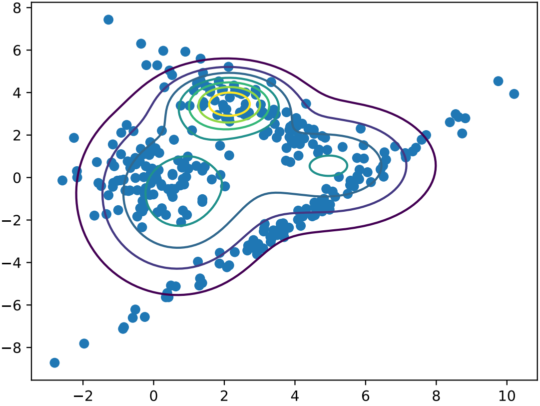

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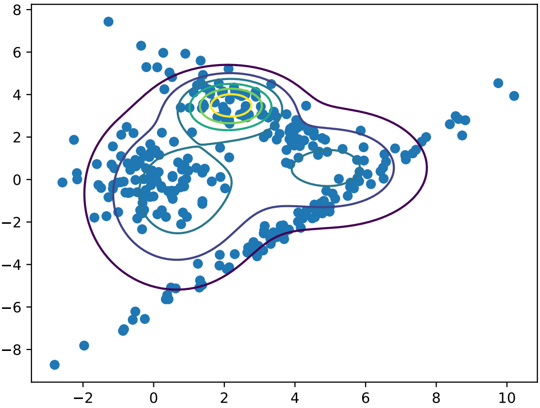

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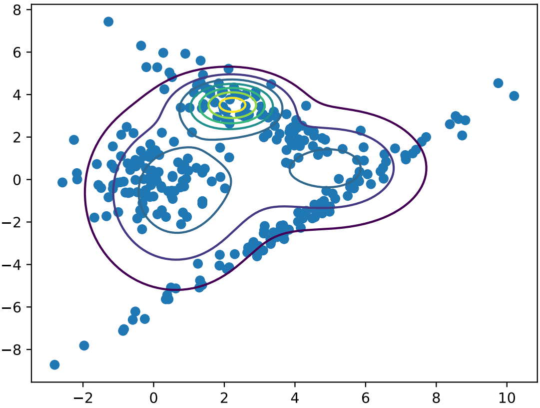

Ancillary topics.

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- Choosing k: use *elbow* as before.
  (Or some “Bayesian Information Criterion”.)
- Initialization: random, or k-means.
- “Singularaties” / collapsing components.
- Deriving k-means from GMMs.

“Singularities”.

Consider two data points in $\mathbb{R}$, two centers.
E-M can shrink a cluster onto one point and delete it!

(More details in lecture.)

In practice, implementations impose lower bounds on covariance eigenvalues, and sometimes randomly re-initialize small clusters.

Deriving k-means from GMMs.

Consider $\Sigma_j := \sigma^2 I$ with $\sigma \to 0$,
make mixture proportions $(\pi_1, \ldots, \pi_k) = (1/k, \ldots, 1/k)$ uniform,
otherwise leave algorithm as before.

1. **(Re-assignment.)** Since $A_{ij} \propto p_{\theta_j}(x_i)$, soft assignments become hard assignments as $\sigma \to 0$.
2. **(Parameter maximization.)** as in k-means, mean update is just sample mean!

Key points from this lecture.

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1. The GMM likelihood model: $p_\theta(x) = \sum_j \pi_j p_{\theta_j}(x)$ where p_{θ_j} is a multivariate Gaussian density.
2. The E-M algorithm for GMMs.