HOMEWORK 5

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Instructions: Use this latex file as a template to develop your homework. We are changing our reproducibility policy on code submissions going forward. **Instead of uploading it on GitHub, please submit a separate zip file that contains your code. You will submit two files to Canvas, one is your pdf, and the other one is a zip file.** Late submissions may not be accepted. You can choose any programming language (i.e. python, R, or MATLAB). Please check Piazza for updates about the homework.

This homework is more difficult than previous homework. The total amount of points for this homework is **150**. The extra credit reflects the level of difficulty.

1 Clustering

1.1 K-means Clustering (14 points)

1. **(6 Points)** Given n observations $X_1^n = \{X_1, \ldots, X_n\}$, $X_i \in \mathcal{X}$, the K-means objective is to find k ($< n$) centres $\mu_1^k = \{\mu_1, \ldots, \mu_k\}$, and a rule $f : \mathcal{X} \to \{1, \ldots, K\}$ so as to minimize the objective

$$J(\mu_1^K, f; X_1^n) = \sum_{i=1}^{n} \sum_{k=1}^{K} \mathbb{1}(f(X_i) = k)\|X_i - \mu_k\|^2 \tag{1}$$

Let $\mathcal{J}_K(X_1^n) = \min_{\mu_1^k, f} J(\mu_1^K, f; X_1^n)$. Prove that $\mathcal{J}_K(X_1^n)$ is a non-increasing function of K.

Lets begin by finding what f, μ_K are. Although we cannot find the best μ and f at the same time, we can:

- fix μ, we find the best f exactly. Also called the Assignment Step.

$$\begin{aligned}
\mathcal{J}_K(X_1^n) &= \min_f J(\mu_1^K, f; X_1^n) \\
&= \min_f \sum_{i=1}^{n} \sum_{k=1}^{K} \mathbb{1}(f(X_i) = k)\|X_i - \mu_k\|^2 \\
&= \min_f \sum_{k=1}^{K} \mathbb{1}(f(X_1) = k)\|X_1 - \mu_k\|^2 + \ldots + \sum_{k=1}^{K} \mathbb{1}(f(X_n) = k)\|X_n - \mu_k\|^2
\end{aligned}$$

Thus we can minimize each of the above term individually by setting

$$f(X_i) = \arg\min_k \|X_i - \mu_k\|^2$$

Which means to assign the point to the cluster whose centroid is closest.

- fix f, we find the best μ exactly. Also called the Update Step.

$$\begin{aligned}
\mathcal{J}_K(X_1^n) &= \min_{\mu_1^K} J(\mu_1^K, f; X_1^n) \\
&= \min_{\mu_1^K} \sum_{i=1}^{n} \sum_{k=1}^{K} \mathbb{1}(f(X_i) = k)\|X_i - \mu_k\|^2 \\
&= \min_{\mu_1^K} \sum_{i=1}^{n} \mathbb{1}(f(X_i) = 1)\|X_i - \mu_1\|^2 + \ldots + \sum_{i=1}^{n} \mathbb{1}(f(X_i) = K)\|X_i - \mu_K\|^2
\end{aligned}$$

The individual terms can be minimized by setting:

$$\mu_k = \arg\min_{\mu} \sum_{i=1}^{n} \mathbb{1}(f(X_i) = k)\|X_i - \mu\|^2 = \frac{\sum_{i=1}^{n} \mathbb{1}(f(X_i) = k)X_i}{\sum_{i=1}^{n} \mathbb{1}(f(X_i) = k)}$$

Thus pick a centroid of a cluster as the mean of all points in that cluster.

Now lets pick a setting where we increase the number of clusters by 1 i.e. total clusters are $\mathbf{K+1}$.
Let $f^K(X_i)$ assign the cluster to a point in a setting with K cliusters.

- Assignment Step proof:
  A point will be assigned to this new cluster if and only if its closer to the center of this new cluster

  $$\|X_i - \mu_{K+1}\|^2 < \|X_i - \mu_k\|^2 \; \forall \; k = 1, 2, ..., K$$

  Thus decreasing the total objective value than before. The worst case scenario is when no point is assigned to this new cluster in which case the objective value remains the same.

  Hence proved the objective value can never increase during assignment step when increasing K.
- Update Step proof: If a point is assigned from cluster k to $K+1$.
  - Let the cluster k with less points be called k'.
    The new $\mu_{k'}$ will change from before if and only if it decreases the total objective value of leftover points in its cluster. If the new $\mu_{k'}$ increases the total objective value then it was better off staying at μ_k.

    $$\sum_{i=1}^{n} \mathbb{1}(f^{K+1}(X_i) = k')\|X_i - \mu_{k'}\|^2 \leq \sum_{i=1}^{n} \mathbb{1}(f^{K+1}(X_i) = k')\|X_i - \mu_k\|^2$$

  - As for the point assigned to $K+1$.
    Now if the sum of objective value in the original setting is less than in the current one i.e.:

    $$\sum_{i=1}^{n} \mathbb{1}(f^{K+1}(X_i) = K+1)\|X_i - \mu_{f^K(X_i)}\|^2 \leq \sum_{i=1}^{n} \mathbb{1}(f^{K+1}(X_i) = K+1)\|X_i - \mu_{K+1}\|^2$$

    Where $\mu_{f^K(X_i)}$ is the centroid of their cluster in the original setting with only K cluster
    Then:

    $$\mu = \frac{\sum_{i=1}^{n} \mathbb{1}(f^{K+1}(X_i) = K+1)\mu_{f^K(X_i)}}{\sum_{i=1}^{n} \mathbb{1}(f^{K+1}(X_i) = K+1)}$$

    gives equal objective value as the original setting and is a better choice of μ_{K+1}. Thus the sum of objective values for newly assigned points can also never increase.

  Thus increasing K will increase the total objective value for neither the set of points that don't change cluster nor those which do during the Update Step.

2. **(8 Points)** Consider the K-means (Lloyd's) clustering algorithm we studied in class. We terminate the algorithm when there are no changes to the objective. Show that the algorithm terminates in a finite number of steps.

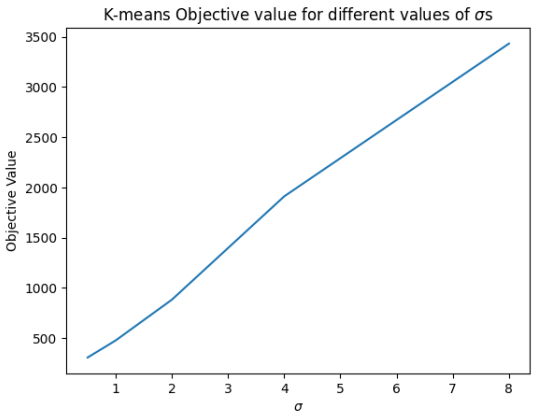
   We can see above that the K-mean algorithm moves in a fashion to reduce the objective $\mathcal{J}_K(X_1^n) = \min_{\mu_1^k, f} J(\mu_1^K, f; X_1^n)$. Now for **fixed set of points** $X_1^n = \{X_1, \ldots, X_n\}$, $X_i \in \mathcal{X}$ and a **fixed** K there can only be a finite set of assignments of points to the clusters i.e. only a **finite number of objective values** and even if the algorithm iterates over all of them it will eventually choose the one with minimum objective value $\mathcal{J}_K(X_1^n)$ and terminate after those finite set of iterations and converge to a solution.

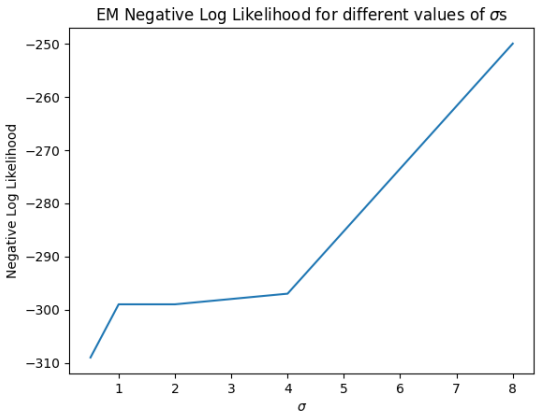
1.2 Experiment (20 Points)

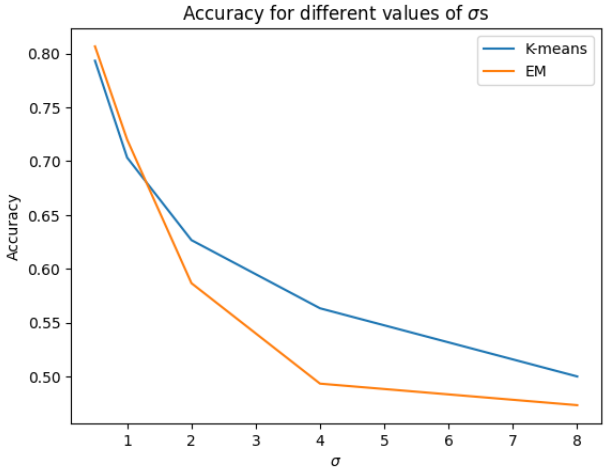
In this question, we will evaluate K-means clustering and GMM on a simple 2 dimensional problem. First, create a two-dimensional synthetic dataset of 300 points by sampling 100 points each from the three Gaussian distributions shown below:

$$P_a = \mathcal{N}\left(\begin{bmatrix}-1\\-1\end{bmatrix}, \sigma\begin{bmatrix}2, & 0.5\\0.5, & 1\end{bmatrix}\right), \quad P_b = \mathcal{N}\left(\begin{bmatrix}1\\-1\end{bmatrix}, \sigma\begin{bmatrix}1, & -0.5\\-0.5, & 2\end{bmatrix}\right), \quad P_c = \mathcal{N}\left(\begin{bmatrix}0\\1\end{bmatrix}, \sigma\begin{bmatrix}1 & 0\\0, & 2\end{bmatrix}\right)$$

Here, σ is a parameter we will change to produce different datasets.







- First implement K-means clustering and the expectation maximization algorithm for GMMs. Execute both methods on five synthetic datasets, generated as shown above with $\sigma \in \{0.5, 1, 2, 4, 8\}$. Finally, evaluate both methods on *(i)* the clustering objective (1) and *(ii)* the clustering accuracy. For each of the two criteria, plot the value achieved by each method against σ.
- Both algorithms are only guaranteed to find only a local optimum so we recommend trying multiple restarts and picking the one with the lowest objective value (This is (1) for K-means and the negative log likelihood for GMMs). You may also experiment with a smart initialization strategy (such as kmeans++).
- To plot the clustering accuracy, you may treat the 'label' of points generated from distribution P_u as u, where $u \in \{a, b, c\}$. Assume that the cluster id i returned by a method is $i \in \{1, 2, 3\}$. Since clustering is an unsupervised learning problem, you should obtain the best possible mapping from $\{1, 2, 3\}$ to $\{a, b, c\}$ to compute the clustering objective. One way to do this is to compare the clustering centers returned by the method (centroids for K-means, means for GMMs) and map them to the distribution with the closest mean.

Points break down: 7 points each for implementation of each method, 6 points for reporting of evaluation metrics.

2 Linear Dimensionality Reduction

2.1 Principal Components Analysis (10 points)

Principal Components Analysis (PCA) is a popular method for linear dimensionality reduction. PCA attempts to find a lower dimensional subspace such that when you project the data onto the subspace as much of the

information is preserved. Say we have data $X = [x_1^\top; \ldots; x_n^\top] \in \mathbb{R}^{n \times D}$ where $x_i \in \mathbb{R}^D$. We wish to find a d ($< D$) dimensional subspace $A = [a_1, \ldots, a_d] \in \mathbb{R}^{D \times d}$, such that $a_i \in \mathbb{R}^D$ and $A^\top A = I_d$, so as to maximize $\frac{1}{n} \sum_{i=1}^n \|A^\top x_i\|^2$.

1. **(4 Points)** Suppose we wish to find the first direction a_1 (such that $a_1^\top a_1 = 1$) to maximize $\frac{1}{n} \sum_i (a_1^\top x_i)^2$. Show that a_1 is the first right singular vector of X.

   We have $a_1^\top x_i = x_i^\top a_1$

   $$\max_{||a||_2^2=1} \frac{1}{n} \sum_i (a_1^\top x_i)^2 = \max_{||a||_2^2=1} \frac{1}{n} \sum_i (a_1^\top x_i)(x_i^\top a_1) = \max \frac{1}{n} \sum_i (a_1^\top x_i x_i^\top a_1)$$

   Now for the above expression

   $$\frac{1}{n} \sum_i x_i x_i^\top = \frac{1}{n} X^\top X$$

   From the Singular Value Decomposition of X

   $$\begin{aligned} X &= U \Sigma V^\top \\ X^\top X &= V \Sigma^\top U^\top U \Sigma V^\top \\ &= V \Sigma^\top \Sigma V^T \end{aligned}$$

   Follows from the fact that $U^T U = I$
   Substituting above:

   $$\max \frac{1}{n} a_1^T X^T X a_1 = \max \frac{1}{n} a_1^T V \Sigma^2 V^T a_1$$

   Let $z = V^T a_1$:

   $$\max \frac{1}{n} z^T \Sigma^2 z = \max \frac{1}{n} \text{tr}(z^T \Sigma^2 z) = \max \frac{1}{n} \text{tr}(z z^T \Sigma^2) = max \frac{1}{n} \sum_{i=1}^D \sigma_i^2 z_i^2$$

   Now if $V = [v_1, \ldots, v_D] \in \mathbb{R}^{D \times D}$, such that $v_i \in \mathbb{R}^D$. Each element of Z is $z_i = v_i^\top a_1$ is the projection of a_1 on the orthogonal set of vectors of V. Now we know $\sigma_1^2 > \sigma_2^2 > \cdots > \sigma_D^2$.

   Thus to maximize the objective function the factor of σ_1 needs to be the largest i.e. $\mathbf{v_1^\top a_1 > v_i^\top a_1}$ $\forall i \neq 1$. Knowing that v_i are a set of orthogonal vectors the mentioned criteria can only be achieved if $\mathbf{v_1 = a_1}$. Hence Proved

2. **(6 Points)** Given $a_1, \ldots, a_k$, let $A_k = [a_1, \ldots, a_k]$ and $\tilde{x}_i = x_i - AA^\top x_i$. We wish to find a_{k+1}, to maximize $\frac{1}{n} \sum_i (a_{k+1}^\top \tilde{x}_i)^2$. Show that a_{k+1} is the $(k+1)^{th}$ right singular vector of X.

   $$\begin{aligned} \tilde{x}_i &= x_i - AA^\top x_i \\ (x_i^\top AA^\top) \cdot \tilde{x}_i &= (x_i^\top AA^\top) \cdot (x_i - AA^\top x_i) = (x_i^\top AA^\top x_i) - (x_i^\top AA^\top x_i) = 0 \end{aligned}$$

   Therefore $x_i^\top AA^\top \perp x_i - AA^\top x_i$
   Now,

   $$AA^\top x_i = \sum_{j=1}^k a_j a_j^\top x_i = \sum_{j=1}^k a_j x_i^\top a_j = \sum_{j=1}^k (x_i^\top a_j) a_j = x_i^\top AA^\top \Rightarrow AA^\top x_i \perp x_i - AA^\top x_i$$

   Consequently $\|x_i\|^2 = \|AA^\top x_i\|^2 + \|x_i - AA^\top x_i\|^2$
   Thus $\tilde{x}_i$ is the component of x_i orthogonal to $AA^\top x_i$ and is a way to split x_i into two orthogonal components.
   Stacking $x_i^\top$ we get $\tilde{X}^\top = X^\top - AA^\top X^\top$

   $$AA^\top X^\top = XAA^\top = U \Sigma V^\top AA^\top$$

From the previous proof we can see every row of $V^\top A$ is $v_i A$ which is a $(1 \times k)$ row vector with 1 at i^{th} place and 0 at all other places up-to the k_{th} vector and a zero for all vectors from $k+1$ to D. This gives us,

$$U\Sigma V^\top AA^\top = \sum_i^D \sigma_i u_i v_i^T AA^T = \sum_i^k \sigma_i u_i v_i$$

Thus $\tilde{X}$ is essentially equal to removing the approximation of X along the first k components of right singular vector from X or removing the best-k-rank approximation of X from itself. Hence our problem boils down to

$$\max \frac{1}{n} \sum_i (a_{k+1}^\top \tilde{x}_i)^2 = \max \frac{1}{n} \sum_{k+1}^D \sigma_i^2 z_i^2$$

Where $z_i = v_i^\top a_{k+1}$ and following from the proof in 2.1.1 this is maximized when $\mathbf{a_{k+1}} = \mathbf{v_{k+1}}$

2.2 Dimensionality reduction via optimization (22 points)

We will now motivate the dimensionality reduction problem from a slightly different perspective. The resulting algorithm has many similarities to PCA. We will refer to method as DRO.
As before, you are given data $\{x_i\}_{i=1}^n$, where $x_i \in \mathbb{R}^D$. Let $X = [x_1^\top; \ldots x_n^\top] \in \mathbb{R}^{n \times D}$. We suspect that the data actually lies approximately in a d dimensional affine subspace. Here $d < D$ and $d < n$. Our goal, as in PCA, is to use this dataset to find a d dimensional representation z for each $x \in \mathbb{R}^D$. (We will assume that the span of the data has dimension larger than d, but our method should work whether $n > D$ or $n < D$.)
Let $z_i \in \mathbb{R}^d$ be the lower dimensional representation for x_i and let $Z = [z_1^\top; \ldots; z_n^\top] \in \mathbb{R}^{n \times d}$. We wish to find parameters $A \in \mathbb{R}^{D \times d}$, $b \in \mathbb{R}^D$ and the lower dimensional representation $Z \in \mathbb{R}^{n \times d}$ so as to minimize

$$J(A, b, Z) = \frac{1}{n} \sum_{i=1}^n \|x_i - Az_i - b\|^2 = \|X - ZA^\top - \mathbf{1}b^\top\|_F^2. \tag{2}$$

Here, $\|A\|_F^2 = \sum_{i,j} A_{ij}^2$ is the Frobenius norm of a matrix.

1. **(3 Points)** Let $M \in \mathbb{R}^{d \times d}$ be an arbitrary invertible matrix and $p \in \mathbb{R}^d$ be an arbitrary vector. Denote, $A_2 = A_1 M^{-1}$, $b_2 = b_1 - A_1 M^{-1} p$ and $Z_2 = Z_1 M^\top + \mathbf{1}p^\top$. Show that both (A_1, b_1, Z_1) and (A_2, b_2, Z_2) achieve the same objective value J (2).

$$J(A_1, b_1, Z_1) = \|X - Z_1 A_1^\top - \mathbf{1}b_1^\top\|_F^2.$$

$$J(A_2, b_2, Z_2) = \|X - Z_2 A_2^\top - \mathbf{1}b_2^\top\|_F^2.$$

Substituting the given values
$A_2 = A_1 M^{-1}$, $b_2 = b_1 - A_1 M^{-1} p$ and $Z_2 = Z_1 M^\top + \mathbf{1}p^\top$.

$$J(A_2, b_2, Z_2) = \|X - (Z_1 M^\top + \mathbf{1}p^\top)(A_1 M^{-1})^\top - \mathbf{1}(b_1 - A_1 M^{-1} p)^\top\|_F^2$$
$$J(A_2, b_2, Z_2) = \|X - Z_1 M^\top (M^{-1})^\top A_1^\top - p^\top (M^{-1})^\top A_1^\top - b_1^\top + p^\top (M^{-1})^\top A_1^\top\|_F^2$$
$$J(A_2, b_2, Z_2) = \|X - Z_1 (M^{-1} M)^\top A_1^\top - \mathbf{1}b_1^\top\|_F^2$$
$$J(A_2, b_2, Z_2) = \|X - Z_1 A_1^\top - \mathbf{1}b_1^\top\|_F^2 = J(A_1, b_1, Z_1)$$

Hence, we can observe above that both objectives are equal.
Therefore, in order to make the problem determined, we need to impose some constraint on Z. We will assume that the z_i's have zero mean and identity covariance. That is,

$$\bar{Z} = \frac{1}{n} \sum_{i=1}^n z_i = \frac{1}{n} Z^\top \mathbf{1}_n = 0, \qquad S = \frac{1}{n} \sum_{i=1}^n z_i z_i^\top = \frac{1}{n} Z^\top Z = I_d$$

Here, $\mathbf{1}_d = [1, 1 \ldots, 1]^\top \in \mathbb{R}^d$ and I_d is the $d \times d$ identity matrix.

2. **(16 Points)** Outline a procedure to solve the above problem. Specify how you would obtain A, Z, b which minimize the objective and satisfy the constraints.

   Hint: The rank k approximation of a matrix in Frobenius norm is obtained by taking its SVD and then zeroing out all but the first k singular values.

We need to minimize:

$$g(x_i, z_i|A, b) = \frac{1}{n}\sum_{i=1}^{n} \|x_i - Az_i - b\|^2 = \|X - ZA^\top - \mathbf{1}b^\top\|_F^2$$

What we are trying to achieve here is express X in a lower dimensional basis of Z and then reduce the reconstruction error when reverting from z-space back to x-space.

Lets assume our new basis space as $A = [a_1; a_2; \ldots; a_d]$ such that $a_i \in \mathbb{R}^D$ and $a_i \perp a_j \ \forall\ i \neq j$ and b is added to account for any shift in centre of X.

Coordinate in lower dimension d:

$$z_j^i = (x_i - b)^\top a_j \ \forall\ i \in [1, n]; j \in [1, d]$$

First lets solve for b:

$$\nabla_b g(x_i, z_i|A, b) = \frac{2}{n}\sum_{i=1}^{n}(x_i - Az_i - b) = 0$$

$$\Rightarrow \sum_{i=1}^{n} x_i - A\sum_{i=1}^{n} z_i - nb = 0$$

$$\Rightarrow \sum_{i=1}^{n} x_i - 0 - nb = 0$$

$$\Rightarrow \mathbf{b} = \frac{\mathbf{1}}{\mathbf{n}}\sum_{\mathbf{i=1}}^{\mathbf{n}} \mathbf{x_i}$$

Now we need to find $A = [a_1; a_2; \ldots; a_d]$ by minimizing:

$$\frac{1}{n}\sum_{i=1}^{n} \|x_i - b - \sum_{j=1}^{d} z_j^i a_j\|^2$$

Now we should also note that x_i can be represented by a n-dimensional projection as $x_i = b + \sum_{j=1}^{n} a_j z_j^i$:
Substituting :

$$\frac{1}{n}\sum_{i=1}^{n} \|(b + \sum_{j=1}^{n} a_j z_j^i) - (b + \sum_{j=1}^{d} a_j z_j^i)\|^2 = \frac{1}{n}\sum_{i=1}^{n} \|(\sum_{j=d+1}^{n} a_j z_j^i)\|^2$$

$$\Rightarrow\Longrightarrow \frac{1}{n}\sum_{i=1}^{n}(\left(\sum_{j=d+1}^{n} z_j^i a_j^T\right)\left(\sum_{j=d+1}^{n} a_j z_j^i\right))$$

$$\Rightarrow \frac{1}{n}\sum_{i=1}^{n}(\sum_{j=d+1}^{n}(z_j^i)^2)$$

This follows from the fact that $a_i \perp a_j \ \forall\ i \neq j$
Substituting value of z_i

$$\frac{1}{n}\sum_{i=1}^{n}\sum_{j=d+1}^{n}(a_j^T(x_i - b)(x_i - b)^T a_j)$$

$$\Longrightarrow \frac{1}{n}\sum_{j=d+1}^{n}(a_j^T[\sum_{i=1}^{n}(x_i - \bar{x})(x_i - \bar{x})^T]a_j)$$

This is nothing but the covariance matrix. So our optimization becomes

$$\min \sum_{j=d+1}^{n} (a_j^T \Sigma a_j)$$

Where $\Sigma = \frac{1}{n}\sum_{i=1}^{n}(x_i - \frac{1}{n}\sum_{i=1}^{n} x_i)(x_i - \frac{1}{n}\sum_{i=1}^{n} x_i)^T$

To minimize the above i.e, $j = d+1 \to n$ is equivalent to maximizing $j = 1 \to d$. *This follows from the fact that a_{d+1} to a_n, need to explain the least variance in demeaned X, thus in turn a_1 to a_d need to explain the maximum variance in X.* Arriving again at the condition where we have to :

$$\max \sum_{j=1}^{d} (a_j^T \Sigma a_j)$$

This can be maximized by setting $\mathbf{a_j}$'s in the direction of **right singular values of demeaned X** and picking the **first d right singular vectors** as proven already in 2.1.1.

3. **(3 Points)** You are given a point x_* in the original D dimensional space. State the rule to obtain the d dimensional representation z_* for this new point. (If x_* is some original point x_i from the D–dimensional space, it shoud be the d–dimensional representation z_i.)

$$z_* = (x_* - b)^\top A$$

2.3 Dimensionality reduction via a generative model (42 points)

We will now study dimensionality reduction via a generative model. We will refer to method as DRLV. We will assume a $d(< n)$ dimensional latent space and the following generative process for the data.

$$z \sim \mathcal{N}(\mathbf{0}, I), \quad z \in \mathbb{R}^d$$
$$x|z \sim \mathcal{N}(Az + b, \eta^2 I), \quad x \in \mathbb{R}^D$$

The model says that we first sample a d dimensional Gaussian with zero mean and identity variance. Then we map it to D dimensions by computing $Az + b$. Finally, we add some spherical Gaussian noise with variance η^2 on each dimension.
We will use an expectation maximization (EM) procedure to learn the parameters A, b, η. So far we have only studied EM with discrete latent variables. In this problem, we will look at EM with a continuous latent variable which has a parametric distribution. The following results will be useful.

Fact 1 (Conditional of a Gaussian)**.** *Say $(Y_1, Y_2), Y_i \in \mathbb{R}^{d_i}$ is Gaussian distribued.*

$$\begin{pmatrix} Y_1 \\ Y_2 \end{pmatrix} = \mathcal{N}\left(\begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{12}^\top & \Sigma_{22} \end{bmatrix}\right)$$

Then, conditioned on $Y_1 = y_1$ the distribution for Y_2 is

$$Y_2|Y_1 = y_1 \sim \mathcal{N}(\mu_2 + \Sigma_{12}^\top \Sigma_{11}^{-1}(y_1 - \mu_1),\ \Sigma_{22} - \Sigma_{12}^\top \Sigma_{11}^{-1} \Sigma_{12})$$

Fact 2 (Some Matrix Derivatives)**.** *Let $X \in \mathbb{R}^{r \times c}$, and $u \in \mathbb{R}^r$, $v, w \in \mathbb{R}^c$.*

$$\nabla_X v^\top X^\top u = uv^\top$$
$$\nabla_X v^\top X^\top X w = X(vw^\top + wv^\top)$$

1. **(10 Points)** Assuming some given values for A, b, and η^2, write down the joint distribution of (z, x). Use this to derive the marginal distribution of x and the conditional distribution $z|x$.

$$p(z) = \frac{1}{(2\pi)^{d/2}} \exp\left(-\frac{1}{2} z^\top z\right)$$

$$p(x|z) = \frac{1}{\eta(2\pi)^{D/2}} \exp\left(-\frac{1}{2\eta}(x - Az - b)^\top (x - Az - b)\right)$$

Now for estimating $p(z, x)$ we use the formula for conditional of a Gaussian. But first lets state the form of $p(z, x)$

$$p(z, x) = \mathcal{N}\left(\begin{pmatrix} \mathbf{0} \\ \mu_2 \end{pmatrix}, \begin{bmatrix} I & \Sigma_{12} \\ \Sigma_{12}^\top & \Sigma_{22} \end{bmatrix}\right)$$

Thus using the above equation for $p(x|z)$ gives:

$$p(x|z) = \mathcal{N}(\mu_2 + \Sigma_{12}^\top z,\ \Sigma_{22} - \Sigma_{12}^\top \Sigma_{12})$$

Comparing with our equation it gives:

$$\mu_2 = b$$

$$\Sigma_{12} = A^\top$$

$$\Sigma_{22} - \Sigma_{12}^\top \Sigma_{12} = \eta^2 I \Rightarrow \Sigma_{22} = \eta^2 I + AA^\top$$

Therefore,

$$\mathbf{p(z, x)} \sim \mathcal{N}\left(\begin{bmatrix} \mathbf{0} \\ \mathbf{b} \end{bmatrix}, \begin{bmatrix} \mathbf{I} & \mathbf{A}^\top \\ \mathbf{A} & \boldsymbol{\eta^2 I + AA^\top} \end{bmatrix}\right)$$

$$\mathbf{p(x)} \sim \mathcal{N}(\mathbf{b},\ \boldsymbol{\eta^2 I + AA^\top})$$

$$\mathbf{p(z|x)} \sim \mathcal{N}(\mathbf{A}^\top(\boldsymbol{\eta^2 I + AA^\top})^{-1}(\mathbf{x - b}),\ \mathbf{I - A}^\top(\boldsymbol{\eta^2 I + AA^\top})^{-1}\mathbf{A})$$

Now we need

$$(\eta^2 I + AA^\top)^{-1} = C^{-1} = \eta^{-2} I - \eta^{-2} A M^{-1} A^\top$$

$$M = A^\top A + \eta^2 I$$

$$\mathbf{p(z|x)} \sim \mathcal{N}(\mathbf{M^{-1}A}^\top(\mathbf{x - b}),\ \boldsymbol{\eta^{-2}M})$$

2. **(4 points)** Write the log likelihood in terms of parameters A, b, and η^2.

$$p(x|A, b, \eta) \sim \mathcal{N}(b,\ \eta^2 I + AA^\top)$$

$$p(x|A, b, \eta) = \frac{1}{(2\pi)^{D/2}\sqrt{|\eta^2 I + AA^\top|}} \exp\left(-\frac{1}{2}(x - b)^\top (\eta^2 I + AA^\top)^{-1}(x - b)\right)$$

Taking log on both sides,

$$\log p(x|A, b, \eta) = -\frac{D}{2}\log 2\pi - \frac{1}{2}\log|\eta^2 I + AA^\top| - \left(\frac{1}{2}(x - b)^\top (\eta^2 I + AA^\top)^{-1}(x - b)\right)$$

3. **(4 Points)** First obtain the Maximum Likelihood Estimate for b. This does not require EM.

$$\nabla_b \sum_{i=1}^{n} \log p(x_i|A, b, \eta) = 0 + 0 - \sum_{i=1}^{n} 2 * \frac{1}{2}(x_i - b)^\top (\eta^2 I + AA^\top)^{-1} = 0$$

$$\Rightarrow \sum_{i=1}^{n} (x_i - b) = 0$$

$$\Rightarrow \mathbf{b} = \frac{\mathbf{1}}{\mathbf{n}} \sum_{\mathbf{i=1}}^{\mathbf{n}} \mathbf{x_i}$$

4. **(10 Points)** To apply the EM algorithm, let $Q(z_i)$ denote some distribution over z_i for each z_i. Obtain a lower bound on the log likelihood via Jensen's inequality.

$$\begin{aligned}\sum_{i=1}^{n} \log p(x_i|A,b,\eta) &= \sum_{i=1}^{n} \log\left(\int_{-\infty}^{\infty} p(x_i,z_i|A,b,\eta)dz_i\right)\\ &= \sum_{i=1}^{n} \log\left(\int_{-\infty}^{\infty} Q(z_i)\frac{p(x_i,z_i|A,b,\eta)}{Q(z_i)}dz_i\right)\\ &\geq \sum_{i=1}^{n}\int_{-\infty}^{\infty} Q(z_i)\log\left(\frac{p(x_i,z_i|A,b,\eta)}{Q(z_i)}\right)dz_i\end{aligned}$$

This follows from Jensen's inequality using two facts:

- $\int_{-\infty}^{\infty} Q(z_i)\frac{p(x_i,z_i|A,b,\eta)}{Q(z_i)}dz_i = \mathbb{E}_{z_i\sim Q(z_i)}\left[\frac{p(x_i,z_i|A,b,\eta)}{Q(z_i)}\right]$
- $\log(\mathbb{E}(x)) \geq \mathbb{E}(\log(x))$ because log is a strictly concave function

$$\begin{aligned}\log\left(\frac{p(x_i,z_i|A,b,\eta)}{Q(z_i)}\right) &= \log p(x_i,z_i|A,b,\eta) - \log Q(z_i)\\ &= -\frac{D+d}{2}\log 2\pi - \frac{1}{2}\log|\Sigma_{x,z}| - \left(\frac{1}{2}\begin{bmatrix} z_i \\ x_i-b\end{bmatrix}^{\top}(\Sigma_{x,z})^{-1}\begin{bmatrix} z_i \\ x_i-b\end{bmatrix} + \log Q(z_i)\right)\end{aligned}$$

Now we know $\int_{-\infty}^{\infty} Q(z_i)d_{z_i} = 1$, Therefore the final lower bound on log likelihood is:

$$-\frac{n}{2}\left((D+d)\log 2\pi + \log|\Sigma_{x,z}|\right) - \sum_{i=1}^{n}\int_{-\infty}^{\infty} Q(z_i)\left(\frac{1}{2}\begin{bmatrix} z_i \\ x_i-b\end{bmatrix}^{\top}(\Sigma_{x,z})^{-1}\begin{bmatrix} z_i \\ x_i-b\end{bmatrix} + \log Q(z_i)\right)dz_i$$

where $\Sigma_{x,z} = \begin{bmatrix} I & A^{\top} \\ A & \eta^2 I + AA^{\top}\end{bmatrix}$

5. **(4 Points)** Recall, from the lectures, that we chose $Q(z_i) = \mathbb{P}(z_i|x_i)$ in the E-step to obtain the tightest possible lower bound for the log likelihood. Here, $\mathbb{P}(z_i|x_i)$ is the conditional distribution of z_i given x_i under the current estimates for A, b, and η. Write down the E-step update for the next iteration.
N.B: Unlike in GMMs, where the latent variable was discrete, here the latent variable is continuous. Fortunately, it has a parametric form we can represent $Q(z_i)$ using a finite number of parameters.
(Hint: See part 1)

E-step: $Q(z_i) = \mathbb{P}(z_i|x_i;A,b,\eta) \sim \mathcal{N}(A^{\top}(\eta^2 I + AA^{\top})^{-1}(x_i-b),\ I - A^{\top}(\eta^2 I + AA^{\top})^{-1}A)$

$$Q(z_i) = -\frac{1}{(2\pi)^{d/2}\sqrt{|I-\beta A|}}\exp\left(-\frac{1}{2}(z_i-\beta(x_i-b))^{\top}(I-\beta A)^{-1}(z_i-\beta(x_i-b))\right)$$

where $\beta = A^{\top}(\eta^2 I + AA^{\top})^{-1}$

Using M and simplifying it becomes:

$$Q(z_i) = -\frac{\eta}{(2\pi)^{d/2}\sqrt{|M|}}\exp\left(\frac{1}{2\eta^2}(z_i - M^{-1}A^{\top}(x_i-b))^{\top}(M^{-1})(z_i - M^{-1}A^{\top}(x_i-b))\right)$$

6. **(10 Points)** Now write down the M-step update for parameters A and η, obtained by maximizing the lower bound obtained from parts 3 and 4.

The M-step needs the maximization of the lower bound of log likelihood calculated in part 4. Lets call that $g(x_i|A,b,\eta)$

For update of parameter A and η We solve the following:

$$\nabla_A g(x_i|A,b,\eta) = \nabla_{\Sigma_{x,z}} g(x_i|A,b,\eta) \cdot \nabla_A \Sigma_{x,z} = 0$$
$$\nabla_\eta g(x_i|A,b,\eta) = \nabla_{\Sigma_{x,z}} g(x_i|A,b,\eta) \cdot \nabla_\eta \Sigma_{x,z} = 0$$

First lets calculate $\nabla_A \Sigma_{x,z}, \nabla_\eta \Sigma_{x,z}$:

$$\nabla_A \Sigma_{x,z} = \begin{bmatrix} 0 & I \\ I & 2A \end{bmatrix} \qquad \nabla_\eta \Sigma_{x,z} = \begin{bmatrix} 0 & 0 \\ 0 & 2\eta I \end{bmatrix}$$

Now for $\nabla_{\Sigma_{x,z}} g(x_i|A,b,\eta)$:

$$\nabla_{\Sigma_{x,z}} g(x_i|A,b,\eta) = \frac{n}{2}\Sigma_{x,z} - \sum_{i=1}^{n} \int_{-\infty}^{\infty} Q(z_i) \frac{1}{2} \begin{bmatrix} z_i \\ x_i - b \end{bmatrix} \begin{bmatrix} z_i \\ x_i - b \end{bmatrix}^\top dz_i$$
$$n \begin{bmatrix} I & A^\top \\ A & \eta^2 I + AA^\top \end{bmatrix} - \sum_{i=1}^{n} \int_{-\infty}^{\infty} Q(z_i) \begin{bmatrix} z_i z_i^\top & z_i (x_i - b)^\top \\ (x_i - b) z_i^\top & (x_i - b)(x_i - b)^\top \end{bmatrix} dz_i$$

Now from Part 4 we know:

$$\mathbb{E}_{z_i \sim Q(z_i)}[z_i] = \int_{-\infty}^{\infty} Q(z_i) z_i dz_i = M^{-1} A^\top (x_i - b)$$
$$\mathbb{E}_{z_i \sim Q(z_i)}[z_i z_i^\top] = \int_{-\infty}^{\infty} Q(z_i) z_i z_i^\top dz_i = \eta^2 M^{-1} - \mathbb{E}_{z_i \sim Q(z_i)}[z_i] \mathbb{E}_{z_i \sim Q(z_i)}[z_i]^\top$$

Substituting above and solving we get:

$$\mathbf{A_{new}} = \left(\sum_{\mathbf{i=1}}^{\mathbf{n}} (\mathbf{x_i} - \mathbf{b}) \mathbb{E}_{\mathbf{z_i} \sim \mathbf{Q(z_i)}}[\mathbf{z_i}]^\top \right) \left(\sum_{\mathbf{j=1}}^{\mathbf{n}} \mathbb{E}_{\mathbf{z_i} \sim \mathbf{Q(z_i)}}[\mathbf{z_i z_i^\top}] \right)^{-1}$$

$$\eta_{\mathbf{new}} = \frac{\mathbf{1}}{\mathbf{nD}} \sum_{\mathbf{i=1}}^{\mathbf{n}} \left((\mathbf{x_i} - \mathbf{b})^\top (\mathbf{x_i} - \mathbf{b}) - \mathbf{2} \mathbb{E}_{\mathbf{z_i} \sim \mathbf{Q(z_i)}}[\mathbf{z_i}]^\top \mathbf{A_{new}^\top} (\mathbf{x_i} - \mathbf{b}) + \mathrm{tr} \left(\sum_{\mathbf{j=1}}^{\mathbf{n}} \mathbb{E}_{\mathbf{z_i} \sim \mathbf{Q(z_i)}}[\mathbf{z_i z_i^\top}] \mathbf{A_{new}^\top A_{new}} \right) \right)$$

2.4 Experiment (42 points)

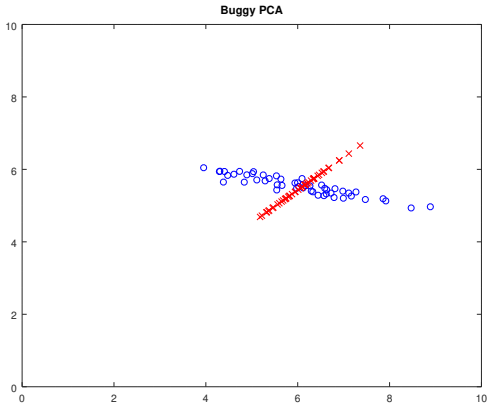
Here we will compare the above three methods on two data sets.

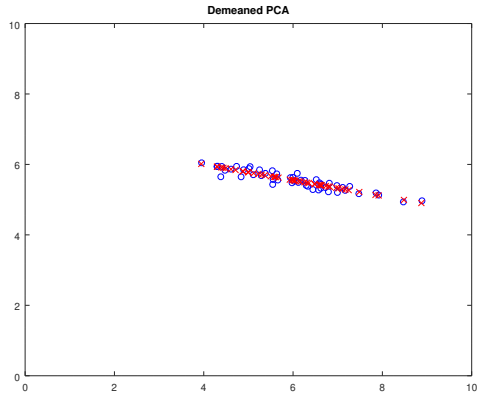
- We will implement three variants of PCA:
  1. "buggy PCA": PCA applied directly on the matrix X.
  2. "demeaned PCA": We subtract the mean along each dimension before applying PCA.
  3. "normalized PCA": Before applying PCA, we subtract the mean and scale each dimension so that the sample mean and standard deviation along each dimension is 0 and 1 respectively.
- One way to study how well the low dimensional representation Z captures the linear structure in our data is to project Z back to D dimensions and look at the reconstruction error. For PCA, if we mapped it to d dimensions via $z = Vx$ then the reconstruction is $V^\top z$. For the preprocessed versions, we first do this and then reverse the preprocessing steps as well. For DRO we just compute $Az + b$. For DRLV, we will use the posterior mean $\mathbb{E}[z|x]$ as the lower dimensional representation and $Az + b$ as the reconstruction.
  We will compare all four methods by the reconstruction error on the datasets.
- Please implement code for the five methods: Buggy PCA (just take the SVD of X) , Demeaned PCA, Normalized PCA, DRO, DRLV. In all cases your function should take in an $n \times d$ data matrix and d as an argument. It should return the the d dimensional representations, the estimated parameters, and the reconstructions of these representations in D dimensions. For DRLV, use the values obtained from DRO as initializations for A. Set η based on the reconstruction errors of DRO. Use 10 iterations of EM.

- You are given two datasets: A two Dimensional dataset with 50 points `data2D.csv` and a thousand dimensional dataset with 500 points `data1000D.csv`.
- For the $2D$ dataset use $d = 1$. For the $1000D$ dataset, you need to choose d. For this, observe the singular values in DRO and see if there is a clear "knee point" in the spectrum. Attach any figures/ Statistics you computed to justify your choice.
- For the $2D$ dataset you need to attach the a plot comparing the orignal points with the reconstructed points for all five methods. For both datasets you should also report the reconstruction errors, that is the squared sum of differences $\sum_{i=1}^{n} \|x_i - r(z_i)\|^2$, where x_i's are the original points and $r(z_i)$ are the D dimensional points reconstructed from the d dimensional representation z_i.
- **Questions:** After you have completed the experiments, please answer the following questions.
  1. Look at the results for Buggy PCA. The reconstruction error is bad and the reconstructed points don't seem to well represent the original points. Why is this?
     Hint: Which subspace is Buggy PCA trying to project the points onto?
  2. The error criterion we are using is the average squared error between the original points and the reconstructed points. In both examples DRO and demeaned PCA achieves the lowest error among all methods. Is this surprising? Why?
- Point allocation:
  - Implementation of the three PCA methods: **(10 Points)**
  - Implementation of DRO and DRLV: **(20 points)**
  - Implementing reconstructions and reporting results: **(5 points)**
  - Choice of d for $1000D$ dataset and appropriate justification: **(3 Points)**
  - Questions **(4 Points)**

Partial answers: These were our errors on all methods for the $2D$ dataset and the reconstructions obtained for Buggy PCA and Demeaned PCA. We have provided them to cross-check with your solution. Our implementation may have bugs so if your answer does not tally, first double check with your peers and then speak to the TA/Instrutor.

```
Reconstruction Errors:
Buggy PCA: 0.886903
Demeaned PCA: 0.010006
Normalized PCA: 0.049472
DRO: 0.010006
DRLV: 0.010081
```



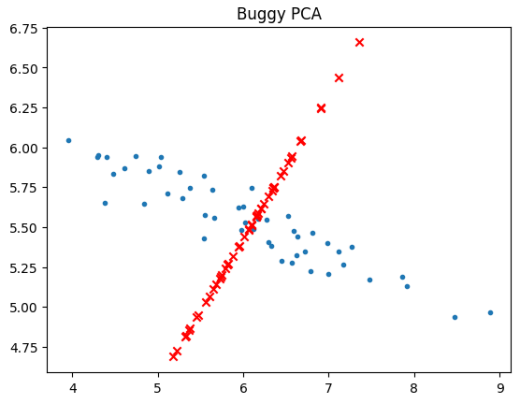


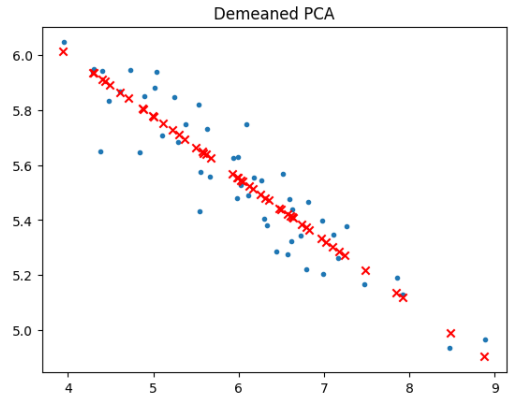
The blue circles are from the original dataset and the red crosses are the reconstructed points.

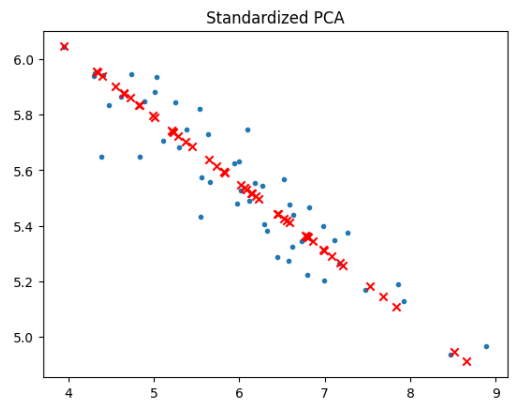
For 2D dataset the Reconstruction Errors are:

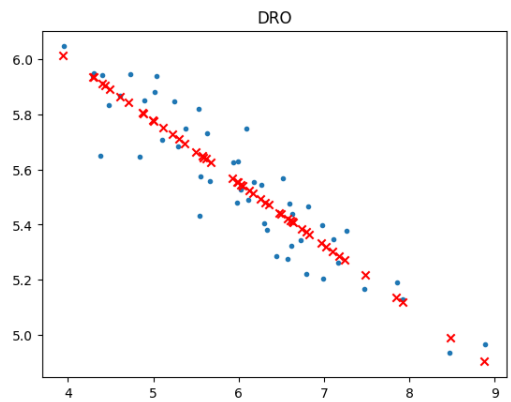
- Buggy PCA : 0.886903

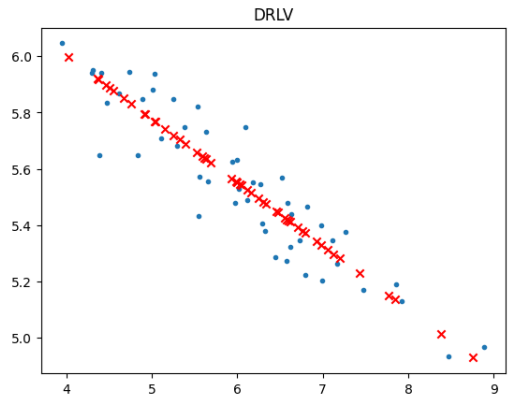
- Demeaned PCA : 0.010006
- Normalized PCA : 0.04947
- DRO : 0.010006
- DRLV : 0.01212



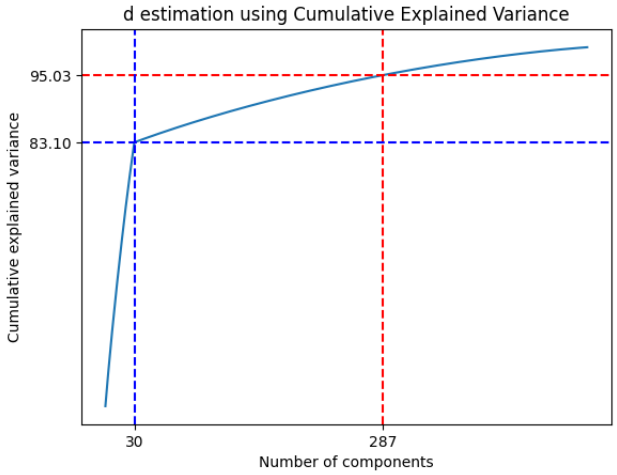








For 1000D dataset we first estimate the lower dimension using **cumulative explained variance**.



Error using d=30 dimensions:

- Buggy PCA Loss : 802.731
- Demeaned PCA Loss : 273.046
- Standardized PCA Loss : 273.629
- DRO : 273.046
- DRLV : 273.130

Error using d=300 dimensions:

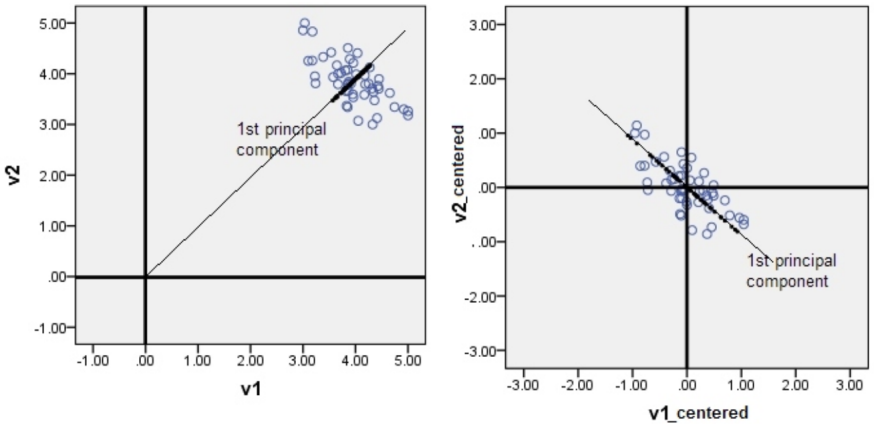
- Buggy PCA Loss : 43.384
- Demeaned PCA Loss : 43.06
- Standardized PCA Loss : 44.567
- DRO : 43.06
- DRLV : Too long to run

Choice of d for 100D
The number of dimensions after which we can explain atleast 95% of the variance in the dataset is considered a good number of components for PCA. In our case that number turns out of 287. Rounding it upto an even 300 is a good number of components and much less than the original 1000 we had.
We also observe a knee point at around **30 components** which is able to explain 83.10% variance in the data and while its a good estimate with much less number of components its not always be a satisfactory estimate and may result in errors which we see above.

Questions

1. Look at the results for Buggy PCA. The reconstruction error is bad and the reconstructed points don't seem to well represent the original points. Why is this?
   Hint: Which subspace is Buggy PCA trying to project the points onto?

   When we perform PCA, the principal components are a subspace of origin-centered vectors. All the principal components pass through the origin as they are just a linear combination of the original components, which also pass through the origin. Hence, we don't center the data before applying PCA; the new components do not consider the shift in data and try to fit the components along the data in the best way possible, resulting in error. (https://stats.stackexchange.com/users/2403/alec)



2. The error criterion we are using is the average squared error between the original points and the reconstructed points. In both examples DRO and demeaned PCA achieves the lowest error among all methods. Is this surprising? Why?

   We can clearly see that DRO and Demeaned PCA use the same final closed-form solution to arrive at the error. When we see DRO, it tries reducing the Mean squared error(MSE) as its objective function, which is also our error evaluation function and hence has the least error. DRLV tries reducing the log-likelihood, which is not directly related to MSE; Buggy PCA has the issue of demeaning; and Standardized PCA, while being more accurate for general representation, fails here as it also captures inter-dimensional variance and not just the variance in the actual data.

References

(https://stats.stackexchange.com/users/2403/alec), A. (2012). How does centering the data get rid of the intercept in regression and pca? Cross Validated. URL:https://stats.stackexchange.com/q/22329 (version: 2017-04-13).