

Feel free to work with other students, but make sure you write up the homework and code on your own (no copying homework *or* code; no pair programming). Feel free to ask students or instructors for help debugging code or whatever else, though.

1 (Murphy 12.5 - Deriving the Residual Error for PCA) It may be helpful to reference section 12.2.2 of Murphy.

(a) Prove that

$$\left\| \mathbf{x}_i - \sum_{j=1}^k z_{ij} \mathbf{v}_j \right\|^2 = \mathbf{x}_i^\top \mathbf{x}_i - \sum_{j=1}^k \mathbf{v}_j^\top \mathbf{x}_i \mathbf{x}_i^\top \mathbf{v}_j.$$

Hint: first consider the case when $k = 2$. Use the fact that $\mathbf{v}_i^\top \mathbf{v}_j$ is 1 if $i = j$ and 0 otherwise. Recall that $z_{ij} = \mathbf{x}_i^\top \mathbf{v}_j$.

(b) Now show that

$$J_k = \frac{1}{n} \sum_{i=1}^n \left(\mathbf{x}_i^\top \mathbf{x}_i - \sum_{j=1}^k \mathbf{v}_j^\top \mathbf{x}_i \mathbf{x}_i^\top \mathbf{v}_j \right) = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i^\top \mathbf{x}_i - \sum_{j=1}^k \lambda_j.$$

Hint: recall that $\mathbf{v}_j^\top \Sigma \mathbf{v}_j = \lambda_j \mathbf{v}_j^\top \mathbf{v}_j = \lambda_j$.

(c) If $k = d$ there is no truncation, so $J_d = 0$. Use this to show that the error from only using $k < d$ terms is given by

$$J_k = \sum_{j=k+1}^d \lambda_j.$$

Hint: partition the sum $\sum_{j=1}^d \lambda_j$ into $\sum_{j=1}^k \lambda_j$ and $\sum_{j=k+1}^d \lambda_j$.

1. Observe that

$$\left\| \mathbf{x}_i - \sum_{j=1}^k z_{ij} \mathbf{v}_j \right\|^2 = \left(\mathbf{x}_i - \sum_{j=1}^k z_{ij} \mathbf{v}_j \right)^T \left(\mathbf{x}_i - \sum_{j=1}^k z_{ij} \mathbf{v}_j \right) \quad (1)$$

$$= \mathbf{x}_i^T \mathbf{x}_i - \mathbf{x}_i^T \sum_{j=1}^k z_{ij} \mathbf{v}_j - \sum_{j=1}^k z_{ij} \mathbf{v}_j^T \mathbf{x}_i + \left(\sum_{j=1}^k z_{ij} \mathbf{v}_j^T \right) \left(\sum_{j=1}^k z_{ij} \mathbf{v}_j \right) \quad (2)$$

$$= \mathbf{x}_i^T \mathbf{x}_i - 2 \sum_{j=1}^k z_{ij} \mathbf{v}_j^T \mathbf{x}_i + \sum_{j=1}^k \sum_{l=1}^k z_{ij}^T z_{il} \mathbf{v}_j^T \mathbf{v}_l \quad (3)$$

$$= \mathbf{x}_i^T \mathbf{x}_i - 2 \sum_{j=1}^k z_{ij} \mathbf{v}_j^T \mathbf{x}_i + \sum_{j=1}^k \mathbf{v}_j^T z_{ij}^T z_{ij} \mathbf{v}_j \quad (4)$$

$$= \mathbf{x}_i^T \mathbf{x}_i - 2 \sum_{j=1}^k z_{ij} \mathbf{v}_j^T \mathbf{x}_i + \sum_{j=1}^k \mathbf{v}_j^T \mathbf{x}_i \mathbf{x}_i^T \mathbf{v}_j \quad (5)$$

$$= \mathbf{x}_i^T \mathbf{x}_i - \sum_{j=1}^k z_{ij} \mathbf{v}_j^T \mathbf{x}_i \quad (6)$$

using the orthonormality of \mathbf{v}_j vectors.

2. Recall that

$$\mathbf{\Sigma} = \sum_{i=1}^n \mathbf{x}_i \mathbf{x}_i^T. \quad (7)$$

Hence, (using the fact that $\mathbf{v}_j^T \mathbf{\Sigma} \mathbf{v}_j = \lambda_j \mathbf{v}_j^T \mathbf{v}_j = \lambda_j$),

$$J_k = \frac{1}{n} \sum_{i=1}^n \left(\mathbf{x}_i^T \mathbf{x}_i - \sum_{j=1}^k \mathbf{v}_j^T \mathbf{x}_i \mathbf{x}_i^T \mathbf{v}_j \right) \quad (8)$$

$$= \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i^T \mathbf{x}_i - \sum_{j=1}^k \mathbf{v}_j^T \left(\sum_{i=1}^n \mathbf{x}_i \mathbf{x}_i^T \right) \mathbf{v}_j \quad (9)$$

$$= \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i^T \mathbf{x}_i - \sum_{j=1}^k \mathbf{v}_j^T \mathbf{\Sigma} \mathbf{v}_j \quad (10)$$

$$= \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i^T \mathbf{x}_i - \sum_{j=1}^k \lambda_j \quad (11)$$

as desired.

3. From the results of part (b), see that

$$J_d = 0 \implies \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i^T \mathbf{x}_i = \sum_{j=1}^d \lambda_j = \sum_{j=1}^k \lambda_j + \sum_{k+1}^d \lambda_j \quad (12)$$

since $k < d$. Therefore

$$J_k = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i^\top \mathbf{x}_i - \sum_{j=1}^k \lambda_j \quad (13)$$

implies that

$$J_k = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i^\top \mathbf{x}_i - \sum_{j=1}^k \lambda_j \quad (14)$$

$$= \sum_{j=1}^k \lambda_j + \sum_{k+1}^d \lambda_j - \sum_{j=1}^k \lambda_j \quad (15)$$

$$= \sum_{j=k+1}^d \lambda_j, \quad (16)$$

concluding the proof.

■

2 (ℓ_1 -Regularization) Consider the ℓ_1 norm of a vector $\mathbf{x} \in \mathbb{R}^n$:

$$\|\mathbf{x}\|_1 = \sum_i |\mathbf{x}_i|.$$

Draw the norm-ball $B_k = \{\mathbf{x} : \|\mathbf{x}\|_1 \leq k\}$ for $k = 1$. On the same graph, draw the Euclidean norm-ball $A_k = \{\mathbf{x} : \|\mathbf{x}\|_2 \leq k\}$ for $k = 1$ behind the first plot. (Do not need to write any code, draw the graph by hand).

Show that the optimization problem

$$\begin{aligned} &\text{minimize: } f(\mathbf{x}) \\ &\text{subj. to: } \|\mathbf{x}\|_p \leq k \end{aligned}$$

is equivalent to

$$\text{minimize: } f(\mathbf{x}) + \lambda \|\mathbf{x}\|_p$$

(hint: create the Lagrangian). With this knowledge, and the plots given above, argue why using ℓ_1 regularization (adding a $\lambda \|\mathbf{x}\|_1$ term to the objective) will give sparser solutions than using ℓ_2 regularization for suitably large λ .

We first know that the optimization problem above is equivalent to the Lagrangian formulation:

$$\inf_{\mathbf{x}} \sup_{\lambda \geq 0} \mathcal{L}(\mathbf{x}, \lambda) = \inf_{\mathbf{x}} \sup_{\lambda \geq 0} [f(\mathbf{x}) + \lambda(\|\mathbf{x}\|_p - k)]. \quad (17)$$

(took hint from solution here) We can then interchange the inf and sup in the dual space to get

$$\sup_{\lambda \geq 0} g(\lambda) = \sup_{\lambda \geq 0} \inf_{\mathbf{x}} [f(\mathbf{x}) + \lambda(\|\mathbf{x}\|_p - k)] \quad (18)$$

where

$$g(\lambda) = \inf_{\mathbf{x}} \mathcal{L}(\mathbf{x}, \lambda). \quad (19)$$

Finally, we notice that

$$\sup_{\lambda \geq 0} \inf_{\mathbf{x}} [f(\mathbf{x}) + \lambda(\|\mathbf{x}\|_p - k)] = \sup_{\lambda \geq 0} \inf_{\mathbf{x}} [f(\mathbf{x}) + \lambda \|\mathbf{x}\|_p] \quad (20)$$

since λk is independent of \mathbf{x} . We have reduced the optimization problem above to the problem

$$\text{minimize: } f(\mathbf{x}) + \lambda \|\mathbf{x}\|_p, \quad (21)$$

concluding the proof.

For sparsity, we wish to choose a regularization that is more likely to create 0 weights. From our pictures, we notice that when penalizing a model with the l_2 norm, it will be less likely that its solutions will be sparse compared to the likelihood of penalizing the model with the l_1 norm (this is due to the probability of our solution being able to touch a corner of the l_1 ball). The curved edges of the l_2 ball decentivizes sparse solutions as solutions will intersect the face of the ball (where it will be nonzero).

See drawings on image. ■

Extra Credit (Lasso) Show that placing an equal zero-mean Laplace prior on each element of the weights θ of a model is equivalent to ℓ_1 regularization in the Maximum-a-Posteriori estimate

$$\text{maximize: } \mathbb{P}(\theta|\mathcal{D}) = \frac{\mathbb{P}(\mathcal{D}|\theta)\mathbb{P}(\theta)}{\mathbb{P}(\mathcal{D})}.$$

Note the form of the Laplace distribution is

$$\text{Lap}(x|\mu, b) = \frac{1}{2b} \exp\left(-\frac{|x - \mu|}{b}\right)$$

where μ is the location parameter and $b > 0$ controls the variance. Draw (by hand) and compare the density $\text{Lap}(x|0, 1)$ and the standard normal $\mathcal{N}(x|0, 1)$ and suggest why this would lead to sparser solutions than a Gaussian prior on each elements of the weights (which correspond to ℓ_2 regularization).

Again, we rewrite the problem. The maximum-a-posteriori estimate problem above is equivalent to its log formulation:

$$\text{maximize: } \log \mathbb{P}(\theta|\mathcal{D}) = \log \frac{\mathbb{P}(\mathcal{D}|\theta)\mathbb{P}(\theta)}{\mathbb{P}(\mathcal{D})} \quad (22)$$

$$= \log \mathbb{P}(\mathcal{D}|\theta) + \log \mathbb{P}(\theta) - \log \mathbb{P}(\mathcal{D}) \quad (23)$$

$$= \log \mathbb{P}(\mathcal{D}|\theta) + \log \mathbb{P}(\theta) \quad (24)$$

where, like in the previous problem, we drop the term independent of θ . It suffices now to show that

$$-\log \mathbb{P}(\theta) = \lambda \|\theta\|_1 + C \quad (25)$$

where C is some constant. Given that θ_i is of $\text{Lap}(\theta_i | 0, b)$ distribution, see that

$$-\log \mathbb{P}(\theta) = -\log \prod_{i=1}^N \exp\left(-\frac{\|\theta_i\|}{b}\right) + \log(2b) \quad (26)$$

$$= \frac{1}{b} \|\theta\|_1 + \log(2b) \quad (27)$$

which shows that the problem above is equivalent to

$$\text{minimize: } -\log \mathbb{P}(\theta|\mathcal{D}) = -\log \mathbb{P}(\mathcal{D}|\theta) + \frac{1}{b} \|\theta\|_1, \quad (28)$$

as desired. See drawings on image. The $\text{Lap}(x|0, 1)$ encourages sparsity as it is more ample near $x = 0$ than the Gaussian prior. ■