OpSiMore/FIEM

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FIEM: Fast Incremental Expectation Maximization

Here are the codes associated to the paper "Fast Incremental Expectation Maximization for non-convex finite-sum optimization: non asymptotic convergence bounds" available from this web page; author: G. Fort, P. Gach and E. Moulines

In this repository, the subdirectory *ToyExample* contains the MATLAB codes for the toy example (section 4); the subdirectory *MNIST* contains the MATLAB codes for the more challenging example using the MNIST data set.

How to use the matlab files available in the subdirectory ToyExample?

• Statistical model: n observations (Y_1,\ldots,Y_n) . For the value $\theta\in\mathbb{R}^q$ of the parameter: conditionally to (Z_1,\ldots,Z_n) , the random variables Y_i are independent with distribution

$$\mathcal{N}_y(AZ_i,I);$$

the random variables (Z_1,\ldots,Z_n) are independent with the same distribution

$$\mathcal{N}_{p}(X\theta,I)$$
.

The matrices X and A are known.

ullet Statistical analysis: the goal is the estimation of the parameter heta through the minimum of the criterion

$$-rac{1}{n}{\log g(Y_1,\ldots,Y_n; heta)} + rac{arphi}{2}\| heta\|^2$$

where $g(y_1, \cdots, y_n; \theta)$ denotes the distribution of the vector (Y_1, \dots, Y_n) . In this toy example, the solution exists, is unique and is even explicit (see section 4.1).

- Description of the file SampleData.m
 - o The variables :
 - n: the size of the data set
 - lacksquare dim_theta: the size of the vector heta
 - dim_Y: the size of each vector Y_i
 - dim_Z (or p in the paper): the size of each hidden variable Z_i
 - theta_true: the value of the parameter used to generate the observations as described by the above statistical model. The entries of theta_true are sampled uniformly in [-5,5] and then 40% of these entries are set to zero (they are chosen at random).
 - The columns of the dim_Y x dim_Z matrix A are sampled from a stationary AR(1) with variance 1 and coefficient rho = 0.8
 - The columns of the dim_Z x dim_theta matrix X are sampled from a stationary AR(1) with variance 1 and coefficient rho = 0.9
 - o The ouput of the function: the function creates a file DataLong.mat which contains the observations Y_1, \ldots, Y_n , the matrices X and A, and the parameter $theta_true$.
- Description of the file FIEM_Gamma.m
 - o The call
 - >> FIEM_Gamma

will launch the estimation of the parameter θ by the optimized FIEM algorithm described in Section 2.3.4 of the paper. The user is invited to choose different design parameters

- O Choices by the user
 - During the run of FIEM_Gamma graphical controls can be displayed (see the description below). The user is invited to choose if it accepts or not the display.
 - The data are loaded directly in the code. See the line
 - >> load Data.mat

Data.mat contains the matrices A and X which define the statistical model; and the n observations stored in a dim_Y x n matrix called Ymatrix.

- upsilon: the numerical value of the regularization parameter in the penalty term $v \|\theta\|^2/2$. The default value is 0.1
- *NbrMC*: independent runs of FIEM can be launched through a single call to *FIEM_Gamma*; they will be run with the same values of the design parameters and will only differ by the random mecanism for the selection of the examples. The user is invited to indicate this number. The default value is 1e3.
- Kmax: the total length of a FIEM path. The default value is 20 n where n is the number of observations, i.e. 20 epochs.
- The learning rate is constant over the iterations of the path: the two strategies provided in the paper (see Proposition 5 and Proposition 6) are possible, the user can choose between resp. *rate* $n^{\wedge}(2/3)$ and *rate* $n^{\wedge}(1/2)$. Both of these strategies depend on two parameters *mu* and *lambda* and the user is invited to specify these values; the default ones are resp. 0.25 and 0.5. For any other strategies, the user can modify the value of the variable *gamma_gfm* in the definition of *gamma_grid* directly in the code.

- The initial value \hat{S}^0 of the FIEM path can be specified: either it is chosen at random by sampling the entries as standardized independent Gaussian variables; or it is read in a file *InitStat.mat* this file has to contain the variable *Sinit* of size *dim theta x 1*.
- Two sequences of length Kmax containing indices in the range $\{1,\ldots,n\}$ have to be selected: they indicate the examples used in the updating mecanism of the auxiliary variable \tilde{S}^{k+1} and the ones used in the updating mecanism of the statistics \hat{S}^{k+1} . Here again, the user is invited to choose between (i) a random selection; (ii) a choice stored in the file $\mathit{RandomIndex.mat}$ (which contains the NbrMC x Kmax matrix $\mathit{RandomIndexImatrix}$) and $\mathit{RandomIndexFIEM.mat}$ (which contains the NbrMC x Kmax matrix $\mathit{RandomIndexJmatrix}$).
- Finally, by default, the *optimized FIEM* is implemented (see section 2.3.4); the computation of the leverage coefficient λ_{k+1} is done through the call to the function *findlambda.m*. The user can choose other strategies by modifying directly in the code the value of the variable *Coeff*. For example, *Coeff* = 1 corresponds to the original FIEM algorithm (see section 2.3.3), and *Coeff* = 0 corresponds to Online EM (see section 2.3.1)
- The outputs: a file StoreCoeffopt.mat containing
 - lacksquare StoreCoeff: the NbrMC x Kmax values of the leverage coefficient λ_k
 - lacksquare FielH: a NbrMC x Kmax matrix containing the squared norm of $H_{k+1}=(\hat{S}^{k+1}-\hat{S}^k)/\gamma_{k+1}$.
 - lacksquare ExpFieldH: a NbrMC x Kmax matrix containing the squared norm of the mean field $h(\hat{S}^k)$.
 - *ErrorTheta*: a *NbrMC x GG* matrix containing the squared norm of the difference $\theta^{k+1} \theta_{\text{opt}}$ where θ_{opt} is the unique optimum of the objective function, and is explicit in this toy example. This error is evaluated at *GG* time steps in the range $\{1, \dots, Kmax\}$.
- o The displayed graphs:
 - lacktriangle Figure1 and Figure2: the squared norm of $heta^{k+1}- heta_{
 m opt}$ along the path, with a zoom on the first iterations.
 - Figure3: the value of the leverage coefficient λ_k along a FIEM path.
 - lacksquare Figure4: the squared norm of H_{k+1} along a FIEM path.
 - lacksquare Figure5: the evolution of each components of the FIEM statistic \hat{S}^k along the FIEM path.
- \circ The function *findlambda.m* is called by *FIEM_Gamma* and computes the optimal leverage coefficient λ_k see section 2.3.4
- The functions findcstar_1.m and findcstar_2.m are called by FIEM_Gamma and compute the constant learning rate γ_{k+1} resp. provided in Proposition 5 and Proposition 6.

How to use the matlab files available in the subdirectory MNIST ?:

• The data set can be found on https://www.kaggle.com/avnishnish/mnist-original#mnist-original.mat, by downloading the file *mnist-original.mat*. It contains a *label* vector of length 7e4 and a *data* matrix of size 784 x 7e4. The first 6e4 columns are the "learning set" and the last 1e4 columns are the "test set". A parametric statistical model is defined and the parameter of the model is learnt by using examples from the "learning set"; before this estimation phase, the data are pre-processed as described in *readMNIST.m*

First, download the file "mnist-original.mat" in the same directory as the .m following files. Then the call

>> readMNIST

will create the file Data.mat. Then, the call

>> FIEM_MNIST

will run FIEM (which will call "Initialisation.m"). The file RunEstimationFIEM.mat is created (see below for a description od its content).

- Description of the file "readMNIST.m"
 - The first step is to extract the training examples: data_train contains the first n=6e4 columns of data, and label_train contains the first n=6e4 components of labels.
 - Step 2: 67 features among the 784 ones are constant over the n examples: they are removed from the set of features. Therefore, the matrix X of features is of size
 n x d init with d init=717
 - The third step reduces the dimension by ACP: standardize each column of X (expectation zero, standard deviation 1) and compute the singular value decomposition of X'X. Finally, consider the projection of X on the principal components. This yields the n x d_init matrix Xred which is saved in the file Data.mat.
 - o Displayed
 - fig 1. an image from the training set with label equal to 3
 - \blacksquare fig 2. the eignevalues of X'X (the last 5 ones are removed)
 - fig 3. Projection of the *n* examples on the space spanned by the first three principal component.
 - fig 4. Projection of the *n* examples on the space spanned by the first three principal components; the colors indicate the class.
 - fig 5. Projection of the *n* examples on the space spanned by the first two principal components; the colors indicate the class.
 - fig 6. Projection of the *n* examples on the space spanned by the first principal component; the colors indicate the class.
 - Output file: Data.mat contains the n x d_init matrix Xred, with n=6e4 and d_init=717.
- Statistical model:
 - \circ *n* observations (Y_1, ..., Y_n) taking values in $\mathbb{R}^{d_{init}}$ colected in a *d_init x n* matrix. Only $d < d_{init}$ are selected.
 - o The statistical problem at hand consists in fitting a Gaussian Mixture Model in dimension d, with L components, on the features.
 - Therefore, the parameter collects *L* weights (i.e. non negative real numbers with sum equal to one), *L* vectors of length *d* collecting the *L* expectations of the Gaussian distributions, and the covariance matrices. Here, is it assumed that all the components have the same *d x d* covariance matrix. In this example, the objective function to be minimized is the negated normalized log-likelihood

$$-\frac{1}{n}\sum_{i=1}^n \log p(Y_i,\theta)$$

where for any observation $Y \in \mathbb{R}^d$, we have

$$p(Y, heta) = \sum_{k=1}^L lpha_k \, \mathcal{N}_d(\mu_k,\Sigma)(Y) \qquad heta = (lpha_1,\ldots,lpha_L,\mu_1,\ldots,\mu_L,\Sigma).$$

- Description of the file "FIEM_MNIST.m":
 - o General variables to be fixed:
 - RunInit: a binary variable to indicate if the initial parameter is read in a file called * .mat* or has to be constructed. The default value is 1.
 - DisplayPlot: a binary variable to indicate of some graphical controls are displayed during the run or not. The default value is 1.
 - Variables:
 - L is the number of classes in the Gaussian Mixture Model. The default value is L=1.2
 - kswitch defines the number of epochs of Online-EM before switching to epochs of FIEM. The default value is kswitch=6.
 - *NbrEpoch* is related to the number of conditional expectation evaluations: this number of evaluations will be set to *NbrEpoch* x n for an OnlineEM epoch and to *NbrEpoch* x 2n for a FIEM epoch. The default value is *NbrEpoch* = 53.
 - *minibatch* defines the size of the mini-batches. The default value is *minibatch* = 100.
 - NbrRun is the number of independent runs of the algorithm. The default value is NbrRun = 10.
 - vectpas collects the learning rate; it may be modified at each epoch. Its default value is 5e-3.

Displayed

- fig 1. evolution of the estimated parameter sequence of weights (L curves); along the current run, vs the number of iterations
- fig 2. evolution of the estimated parameter sequence of a vector of expectation the one of the first component of the Gaussian mixture (*d* curves); along the current run, vs the number of iterations.
- fig 3. evolution of the eigenvalues of the estimated sequence of the covariance matrix (d curves); along the current run vs the number of iterations.
- fig 4. evolution of the log-likelihood; along the current run vs the number of epochs.
- Output file "RunEstimationFIEM.mat"
 - RunStoreWeight is a L x NbrRun matrix which collects the estimated weights $\alpha_1, \dots, \alpha_L$ at the end of each NbrRun independent runs of FIEM.
 - \blacksquare RunStoreMean is a d x L x NbrRun tensor which collects the estimated L vectors μ_1, \dots, μ_L at the end of each NbrRun independent runs of FIEM.
 - RunStoreInvCov is a d x d x NbrRun tensor which collects the estimated d x d covariance matrix at the end of each NbrRun independent runs of FIEM.
 - RunLogLikelihood is a NbrRun x (1+NbrEpoch) matrix which collects, for each NbrRun independent runs of FIEM, the value of the normalized log-likelihood at the end of each epoch (the first column is the value for the initial parameter).
 - StoreWeight is a $L \times (1+NbrEpoch)$ matrix which collects the estimated weights $\alpha_1, \ldots, \alpha_L$ at the end of each epoch (the first column is the value for the initial parameter).
 - StoreMean1 is a d x (1+NbrEpoch) matrix which collects the estimated first expectation μ1 at the end of each epoch (the first column is the value for the initial parameter).
 - StoreEigen is a d x (1+NbrEpoch) matrix which collects the eigenvalues of the estimated inverse-covariance matrix at the end of each epoch (the first column is the value for the initial parameter).
 - Sweight is a L x NbrIter matrix which collects the estimated weights $\alpha_1, \ldots, \alpha_L$ at the end of each iteration.
 - Smu is a $d \times Nbr/ter$ matrix which collects the estimated expectation μ_1 at the end of each iteration.
 - Seigen is a d x Nbr/Iter matrix which collects the eigenvalues of the estimated inverse-covariance matrix at the end of each iteration.

For example, the specifications kswitch = 6, minibatch = 100, NbrEpoch = 53 will implement 6 n / 100 iterations of Online EM and then 47 n / 100 iterations of FIEM. The total number of conditional expectations evaluations will be 6 n + 2 x 47 n since each FIEM iteration calls 2 minibatch conditional expectations evaluations.

- Description of the file "Initialisation.m": A method for defining an initial value for the set of parameters (the weights, the expectations and the covariance matrix of a
 Gaussian mixture model) is proposed. This function calls "SampleInvCov.m".
 - o Input variables:
 - X: the d x n matrix of features, modeled as n points from a Gaussian Mixture Model in dimension d.
 - L: the number of components in the Gaussian Mixture Model
 - Output variables:
 - a d x L matrix collecting the L expectations of the Gaussian components in dimension d
 - lacksquare a $d \times (dL)$ matrix concatening L inverse covariance matrices of size $d \times d$