commit c1e8645105068c5abcf0ebac7cb0a1981ddf0b94

Author: Lxrd\_AJ <ibraheemaj@icloud.com> Date: Thu May 11 07:32:31 2017 +0100

Uncommented code in viz code

commit c58a1ef05de14344c9294aa61fbb5a371e86e0ff

Author: Lxrd\_AJ <ibraheemaj@icloud.com> Date: Thu May 11 07:24:34 2017 +0100

Dockerfile updated

commit ca0682094dba72b7ae05b0832d28fa89bde951ad
Author: AJ Ibraheem <ibraheemaj@icloud.com>
Date: Wed May 10 21:31:56 2017 +0100

Ethics form added

commit b5e972c8c450fbd71e178c0665d600e57195cc68
Author: AJ Ibraheem <ibraheemaj@icloud.com>
Date: Wed May 10 16:00:46 2017 +0100

Examiner's report complete

commit 456052a60b0ab863b1bd0e213b366488a5b441af
Author: AJ Ibraheem <ibraheemaj@icloud.com>
Date: Tue May 9 14:14:03 2017 +0100

Edits to the report

commit ffb15f6f7279e403787829e650485d63d851f9b5
Author: Lxrd\_AJ <ibraheemaj@icloud.com>
Date: Tue May 9 02:06:07 2017 +0100

docker integration added

commit 8d1bbc9293bb969a6e178c4a558237cfaf238ec5
Author: Lxrd\_AJ <ibraheemaj@icloud.com>
Date: Mon May 8 19:10:52 2017 +0100

Model evaluation and persistence chapter updated

commit 285fa26b994693f76c373c09f3fb369480ee755f
Author: Lxrd\_AJ <ibraheemaj@icloud.com>
Date: Mon May 8 14:02:13 2017 +0100

Model evaluation chapter updated

commit 6086a611892e4fed7b644e68e7c3e0c3203d4ac6
Author: AJ Ibraheem <ibraheemaj@icloud.com>
Date: Mon May 8 08:32:16 2017 +0100

minor changes

 $\verb|commit|| 5a2951843769ad5c4ed3cdb5bf05730b2eb8d081| \\$ 

Author: AJ Ibraheem <ibraheemaj@icloud.com>

Date: Sun May 7 20:34:38 2017 +0100

Machine learning classifier chapter updated

commit 75d253d24b2450373757571c4a0fdadbed336863

Author: Lxrd\_AJ <ibraheemaj@icloud.com>
Date: Sat May 6 04:29:25 2017 +0100

Decision trees chapter complete and neural network chapter updated

commit e03e7b76e3504891423457ca73095ef3bd84a4fe

Author: Lxrd\_AJ <ibraheemaj@icloud.com> Date: Wed May 3 14:57:59 2017 +0100

Support vector machine chapter updated

commit f1ebaed34f23189b2d14227d478d383ebe197098

Author: Lxrd\_AJ <ibraheemaj@icloud.com> Date: Tue May 2 19:21:32 2017 +0100

k-NN Chapter updated

commit cdd846b03d4aa50ff38ec31405a2e7444c7c871b

Author: Lxrd\_AJ <ibraheemaj@icloud.com>
Date: Sun Apr 30 15:26:22 2017 +0100

Clustering section updated

commit d8e1a4d6ff3b74188fec73aa9be2c2bf882ba245

Author: Lxrd\_AJ <ibraheemaj@icloud.com>
Date: Wed Apr 26 14:30:13 2017 +0100

Manifold learning with t-SNE section updated

commit 26659a3f336eb8935e9af792ad660bf43a739b90

Author: Lxrd\_AJ <ibraheemaj@icloud.com>
Date: Tue Apr 25 03:23:58 2017 +0100

Principal component analysis section updated and folder restructuring

commit 4c5ba296629bfcdf391b69aa945b8e5a13b601a5

Author: Lxrd\_AJ <ibraheemaj@icloud.com>
Date: Wed Apr 5 21:55:11 2017 +0100

Data Representation and Preprocessing section added

commit 27aa08e4e8c1a4152d0807ed7c012cfc947b619e

Author: Lxrd\_AJ <ibraheemaj@icloud.com>
Date: Wed Apr 5 19:21:31 2017 +0100

Machine learning chapter restructured and introductory text added

commit 0c1762ce8db382fea1e5909e6a40116eb0eb431f

Author: Lxrd\_AJ <ibraheemaj@icloud.com>
Date: Wed Apr 5 12:55:29 2017 +0100

Morgan Fingerprint chapter written

commit 08ad9afd3ccd20959cb906a25b29faf0508af0e5

Author: Lxrd\_AJ <ibraheemaj@icloud.com>
Date: Thu Mar 30 09:04:04 2017 +0100

Notes added

commit 643b53815001178df46b32141547b96438f63e73

Merge: c528c11 0060ddd

Author: Lxrd\_AJ <ibraheemaj@icloud.com>
Date: Sun Mar 26 12:51:42 2017 +0100

Merge

commit c528c114bc9f6bd0083a289cf8e5ca2832a57b3d

Author: Lxrd\_AJ <ibraheemaj@icloud.com>
Date: Sun Mar 26 12:43:31 2017 +0100

Updated the molecular representation and similarity subsection

commit 0060ddd64e736cc35b15dccb7915748f21b0b5d2

Author: AJ Ibraheem <ibraheemaj@icloud.com>

Date: Thu Mar 23 01:01:04 2017 +0000

Notes added - Molecular Representation

commit baa6bb4ec256eeb2b2b7620d7980d776dc7c36c3

Merge: a508717 60ceb42

Author: AJ Ibraheem <ibraheemaj@icloud.com>

Date: Thu Mar 23 00:06:59 2017 +0000

Merge branch 'master' of https://github.com/Lxrd-AJ/
ml\_blood\_brain\_barrier\_prediction

commit a508717b6c470c6c3059624134c14579a3ebbc8c

Author: AJ Ibraheem <ibraheemaj@icloud.com>

Date: Thu Mar 23 00:06:54 2017 +0000

Brain model added

commit 60ceb4231e445d6a59d3f3ca3e13e89409ff79eb

Author: Lxrd\_AJ <ibraheemaj@icloud.com>
Date: Wed Mar 22 18:22:43 2017 +0000

Background-Cheminformatics-Representing Molecules-SMILES chapter update

commit c15906e92b445eb37842f60a1e1de0a05f64c4a4

Merge: a6ee7f1 3d2b0e3

Author: AJ Ibraheem <ibraheemaj@icloud.com>

Date: Wed Mar 15 23:48:27 2017 +0000

Fix merge

commit a6ee7f1ea1cbf453b122950ece5de2bddade6431
Author: AJ Ibraheem <ibraheemaj@icloud.com>

Date: Wed Mar 15 23:47:11 2017 +0000

Prepping for merge

commit 3d2b0e345feaaf9234517147f78d9db24daa152d
Author: Ibraheem AJ <ibraheemaj@icloud.com>
Date: Wed Mar 15 20:24:14 2017 +0000

Application wrapped in a web server using the Flask framework and option to start the application using a pre-trained scikit-learn model added

commit 4e86ff9b6373cf8bb96cc0fa87e1de5b6e8d58f7
Author: Ibraheem AJ <ibraheemaj@icloud.com>
Date: Sun Mar 12 20:51:34 2017 +0000

TODO notes

commit 7badbe42c498f8c1578792a8bc24a7c4ee6c7f50
Author: Ibraheem AJ <ibraheemaj@icloud.com>
Date: Sun Mar 12 15:09:50 2017 +0000

Bug fix to the decision tree pipeline

commit ebf851047c23de8f689ef292dc57b0dfc72fe521
Author: Ibraheem AJ <ibraheemaj@icloud.com>
Date: Sun Mar 12 01:46:49 2017 +0000

ensemble voting classifier implemented

commit 0c60864304d49ebdb5d6a6a07d0b5598e6880f4c
Author: Ibraheem AJ <ibraheemaj@icloud.com>
Date: Sat Mar 11 22:17:55 2017 +0000

Staging for commit

commit df6bf5fad379462965de7ebac7d37c0d783de0b3
Author: Ibraheem AJ <ibraheemaj@icloud.com>
Date: Wed Mar 1 15:30:48 2017 +0000

Model pipelines + Voting classifier

commit 80e23f82299f9df5f32f387221762f790c3ffb82
Author: Ibraheem AJ <ibraheemaj@icloud.com>

Date: Tue Feb 28 11:04:29 2017 +0000

Custom estimator in progress

commit 0123738dc70b98840360d616dcec72414a444c5f

Author: Ibraheem AJ <ibraheemaj@icloud.com>

Date: Tue Feb 14 18:43:55 2017 +0000

Reinitialised git repo