

Opportunities and challenges of using machine learning ML in quantitative wealth and investment management QWIM

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Why machine learning ML for quantitative investment and wealth management QWIM ?

ML : relevant tools and sources of information

ML in QWIM : classification and pattern recognition

ML in QWIM : network analysis and clustering

ML in QWIM : forecasting of financial time series

ML in QWIM : reinforcement learning RL

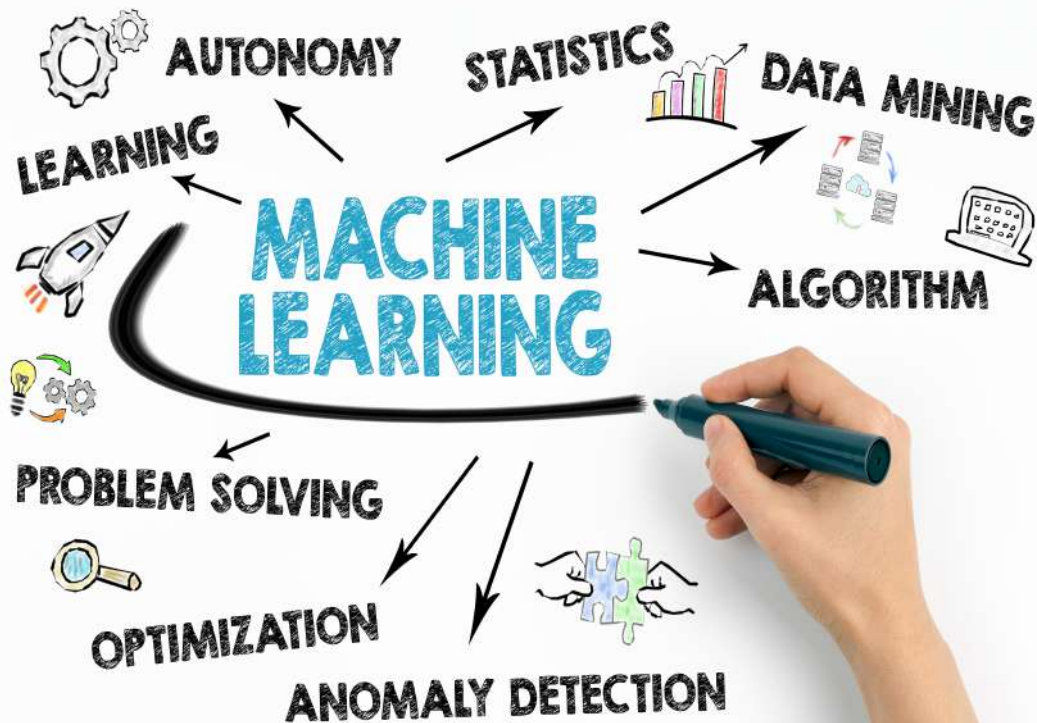
ML in QWIM : importance of market states and regimes

ML in QWIM : other practical applications

ML in QWIM : practical challenges

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The examples are for illustrative purpose only and do not constitute investment advice.



Overview of the presentation

- Increasingly apparent that Financial Machine Learning is a rather specialized area instead of just a combination of standard Machine Learning and Financial Data.
- What is hype and what is reality when applying machine learning **ML** to quantitative investment and wealth management **QWIM**?
- Presentation delves into what appears to work well (or not so well) for **ML** in various areas of **QWIM**, and describes practical challenges
- Area of classification and pattern recognition:
 - classification and partition of the investment universe
 - investing based on alternative data
 - text analysis of company and regulatory documents
 - sentiment analysis of news and social media
 - ESG (Environmental, Social and Governance)
 - investing fund decomposition, inference and replication

Overview of the presentation (cont.)

- Area of network analysis and clustering:
 - clustering-based portfolio optimization
 - network-based portfolio optimization
 - analysis of interconnectedness risk
 - network effects on investment portfolios.
- Area of time series forecasting:
 - forecasting of financial time series
 - empirical asset pricing
- Area of reinforcement learning:
 - pricing and hedging of financial derivatives
 - optimal dynamic trading strategies
 - portfolio allocation
 - goals-based investing

Overview of the presentation (cont.)

- Other practical applications:
 - synthetic financial data generation
 - testing investment strategies and portfolios
 - factor-based investment strategies
 - nowcasting
 - incorporating market states and regimes into investment portfolios.
- Practical challenges include
 - lack of sufficient data
 - need to satisfy privacy, fairness and regulatory requirements
 - model overfitting
 - causality
 - explainability and interpretability
 - hyperparameter tuning

Why machine learning ML for
quantitative investment and
wealth management QWIM?

MIL is everywhere, even to assess wine quality

- Bouri et al. (2018), Le Fur and Outreville (2019): wine as an investment asset class is based on wine quality certification given by human experts, a process both labor intensive and time consuming
- Aich et al. (2019), Gupta (2018): MIL able to assess quality of wines using attributes identified through feature selection
- Accuracy ranging from 92% to 98%



MIL has strong potential in QWIM

- Big data and machine learning have the potential to profoundly change the investment landscape, due to
 - ongoing expansion in amount and type of available data
 - performance and capabilities of MIL packages and platforms
 - computational power and data storage ↑, while costs ↓
 - significant improvements in MIL: methods and software
- Lopez de Prado (2020a), Dixon et al. (2020), Bartram et al. (2020), Jurczenko et al. (2020): considerable advantages of MIL in QWIM: incorporate nonlinearity, pattern recognition, networks and deeper interactions
- Lopez de Prado (2019): *“economic systems exhibit a degree of complexity that is beyond the grasp of classical statistical tools”*
- AI /MIL already used successfully in QWIM: Guida (2019), Lopez de Prado (2018), Kolanovic and Krishnamachari (2017), Sirotiyuk (2019), Lopez de Prado (2020a), Dixon et al. (2020), Jurczenko et al. (2020), Jansen (2020), Bartram et al. (2020)
- AI /MIL can provide powerful new insights using classical investment data, alternative data, or a combination of both

MIL has strong potential in QWIM (cont.)

- Efron and Hastie (2016): *“Our new computation-rich environment has unplugged the mathematical bottleneck, giving us a more realistic, flexible, and far-reaching body of statistical techniques”*
- Lopez de Prado (2020a), Jurczenko et al. (2020): MIL for asset managers
 - MIL can help to discover economic and financial theories; complement rather than replace classical methods
 - Some of MIL strengths include:
 - focus on out-of-sample predictability over variance adjudication;
 - usage of computational methods to avoid relying on (potentially unrealistic) assumptions
 - ability to “learn” complex specifications, including non-linear, hierarchical and non-continuous interaction effects in a high-dimensional space
 - ability to disentangle the variable search from the specification search, robust to multicollinearity and other substitution effects

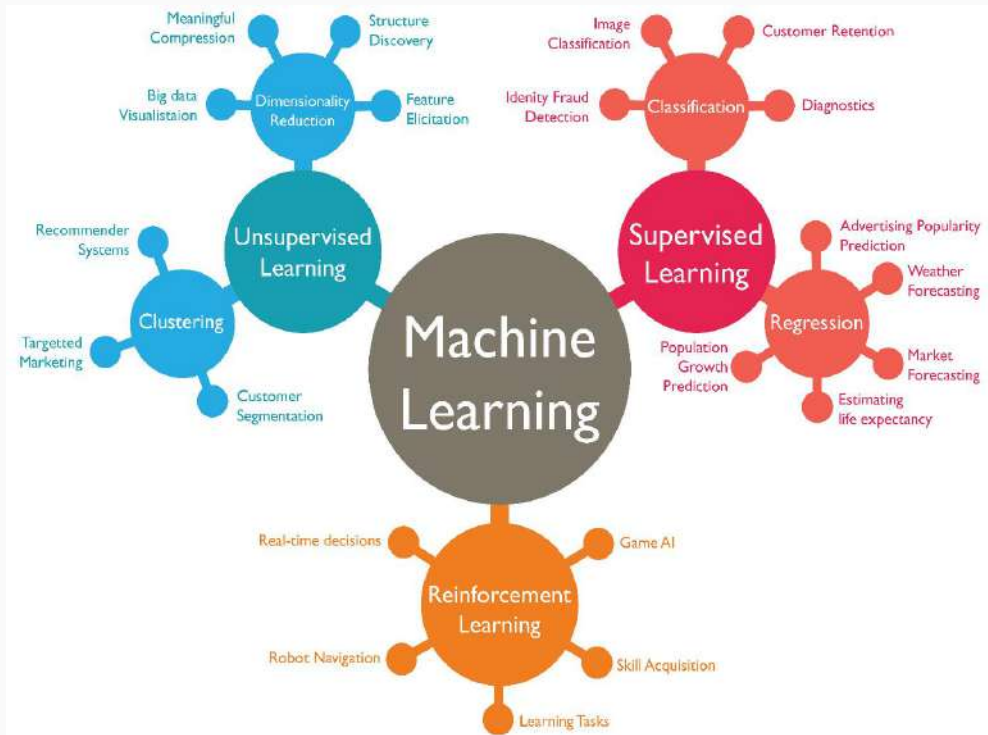
However ...

- To extract significant value from QWIM datasets, standard ML may need to be enhanced (from modeling, numerical and computational perspectives) and augmented with domain expert knowledge
- Lopez de Prado (2018): Financial Machine Learning is rather specialized

Financial ML \neq ML Algorithms + Financial Data

- Heaton (2018): *“financial market data is unlike the data that machine learning works well on in computer vision, speech recognition, and natural language processing.”*
- Thus significant challenges when using AI /ML in QWIM
 - Datasets may not be sufficient (quantity and/or quality) for ML
 - Financial datasets have distinctive stylized characteristics
 - Model overfitting and data mining risks may be higher for ML
 - Forecasting QWIM time series may need more than standard ML
 - Stakeholders and regulators require interpretability and/or explainability for ML

Visual categorization of machine learning algorithms



Source: Jha (2017)

Important ML applications in QWIM

- Classification and pattern recognition can be used for
 - inclusion of alternative data into investment process
 - fund classification, inference and decomposition
 - topic and sentiment analysis
 - risk detection from corporate documents
- Reinforcement learning can be used for
 - goals-based investing
 - construction and risk management of trading and portfolios
 - retirement and financial planning
- Network analysis and clustering can be used for
 - portfolio optimization
 - analysis and improvement of portfolio diversification
 - clustering of financial time series
 - examination of network-related risks

Important ML applications in QWIM (cont.)

- Forecasting and prediction can be used for
 - Short-term, medium-term and long-term forecasting of returns and risks for asset classes and investment vehicles
 - Forecasting of alternative risk premia
 - Prediction of market regimes and structural breaks
 - Forecasting fundamentals and earnings of individual companies
- Other practical applications in QWIM include
 - regime-based investing
 - testing and analysis of trading and investment strategies
 - scenario generation and data augmentation for financial time series
 - ESG-based investing
 - factor-based quantitative investing
 - due diligence and document analysis
 - nowcasting
 - compliance with internal rules and external regulations

ML: relevant tools and sources
of information

- Explosive growth of information related to ML: books, articles, conference presentations, preprints and working papers, Python and R packages, GitHub and GitLab repositories
- One can efficiently find relevant research works through specialized online avenues: ConnectedPapers.com, Dimensions.ai, PapersWithCode, SSRN, arXiv, arXiv Sanity, SemanticScholar, papertalk.org
- Overviews and best practices: Lopez de Prado (2020a), Kolanovic and Krishnamachari (2017), Burkov (2019), Lopez de Prado (2018), Ryll and Seidens (2019), Bloch (2020b), Bloch (2020a), Dixon and Halperin (2019), Sammut and Webb (2017), Hutter et al. (2019), Malik (2020), Goan and Fookes (2020), Raschka et al. (2020), Krohn et al. (2019), Burkov (2019), Boehmke and Greenwell (2019), Chollet (2017), Lapan (2020), Jurczenko et al. (2020), Dixon et al. (2020)
- Machine learning platforms and frameworks
 - TensorFlow, PyTorch, Theano, PlaidML, Keras, Microsoft Cognitive Toolkit, mlr3, MXNet, Caffe, Deeplearning4j, Chainer, SpaCy
 - H2O.ai, DataRobot, OneClick.ai, DarwinAI, Dataiku, Valohai
 - Google TFX, AWS SageMaker, IBM Watson ML, Microsoft Azure ML
- Small data and machine learning: Greco et al. (2019), Li et al. (2018), Qi and Luo (2019), Brigato and Iocchi (2020), Yao et al. (2020a)

Major topics in machine learning

- Deep learning **DL**: Goodfellow et al. (2016), Nakagawa et al. (2019b), Hatcher and Yu (2018), Polson and Sokolov (2018b), Zhang et al. (2018b), Alonso et al. (2019), Polson and Sokolov (2018a), Higham and Higham (2018), Aguilera et al. (2020), Bacciu et al. (2020), Li et al. (2020a), Ozbayoglu et al. (2020), Raghu and Schmidt (2020), Zhang et al. (2020a), Thompson et al. (2020), Samek et al. (2020), Xie et al. (2020), Ren et al. (2020)
- Natural Language Processing: Aggarwal (2018), Kamath et al. (2019), McMahan and Rao (2019), Lane et al. (2019), and Eisenstein (2019), Qiu et al. (2020), Torfi et al. (2020), Ferrario and Naegelin (2020), Chen et al. (2020a)
- Reinforcement learning **RL** (also Deep **RL** and inverse **RL**): Dong et al. (2019), Francois-Lavet et al. (2018), Nachum et al. (2019), Sutton and Barto (2018), Zhang et al. (2018a), Zhao et al. (2019), Xing (2019), Laskin et al. (2020), Lapan (2020)
- Probabilistic graphical models: Benhamou (2018), Denev et al. (2018), Denev and Mutnikas (2016a), Gao et al. (2018), Ma and Zhang (2019)
- Transfer learning: Ada et al. (2019), Fawaz et al. (2018b), He et al. (2019a), Krishna and Menzies (2018), Sun et al. (2019), Nakagawa et al. (2019a)
- Tuning hyperparameters: Cho and Hegde (2019), Yu and Zhu (2020), Feurer and Hutter (2019), Katakami et al. (2019), Kim and Cho (2019), Klein et al. (2019), Sandru and David (2019), Sanders and Giraud-Carrier (2017), Tu and Nair (2018), van Rijn and Hutter (2018), Yang and Shami (2020), Yu and Zhu (2020)

Major topics in machine learning (cont.)

- **Generative Adversarial Networks (GANs):** Saxena and Cao (2020), Jabbar et al. (2020), Koochali et al. (2020), Ni et al. (2020a), Yoon et al. (2019), Vieira (2020)
- **Variational Autoencoders:** Yu (2020), Charte et al. (2018), Imokoyende (2019), Kingma and Welling (2019), Rocca and Rocca (2019), Yacoby et al. (2020)
- **Data augmentation:** Fawaz et al. (2018a), Hoffmann et al. (2018), Kuchnik and Smith (2018), Taylor and Nitschke (2017), Tran et al. (2017), Volpi et al. (2018), He et al. (2019b), Wang et al. (2019a), Xie et al. (2019), Wen et al. (2020), Fang and Lin (2020), Saxena and Cao (2020), Laskin et al. (2020)
- **Feature selection:** Cai et al. (2018), Nogueira et al. (2018), Sreevani and Murthy (2017), Sreevani and Murthy (2017), Stanczyk and Jain (2015), Bolon-Canedo and Alonso-Betanzos (2019), Bugata and Drotar (2019), Draminski and Koronacki (2018), Lu et al. (2018), Piliszek et al. (2019), Yan and Bien (2018), Barandas et al. (2020)
- **Overfitting and how to control it:** Hastie et al. (2011), James et al. (2015), Aparicio and Lopez de Prado (2018), Bailey et al. (2017), Philipp and Carbonell (2018), Suhonen et al. (2017), Zhang et al. (2018a), Koshiyama and Firoozye (2019), Rasekhschaffe and Jones (2019), Lopez de Prado (2020b)
- **Anomaly detection:** Bulusu et al. (2020), Braei and Wagner (2020), Bashchenko and Marchal (2020), Das et al. (2019c), Lee et al. (2020), Wu (2016), Wu and Keogh (2020), Jacob et al. (2020b), Ruff et al. (2020)

Major topics in machine learning (cont.)

- **Network analysis:** Bramson and Vandermarliere (2016), Das et al. (2019a), Fortunato and Hric (2016), Iori and Mantegna (2018), Jeub et al. (2015), Lacasa et al. (2015), Lawyer (2015), Runge (2018), Zanin et al. (2016), Marti et al. (2020)
- **Clustering:** Maharaj et al. (2019), Cai et al. (2016), Cavallo and Demiralp (2018), Durante et al. (2013), Kauffmann et al. (2019), Khaleghi et al. (2016), Murtagh and Contreras (2012), Murtagh and Contreras (2017), Patel and Thakral (2016), Adolfsson et al. (2019), Javed et al. (2020), Sartorio and Fonseca (2020)
- **Interpretability:** Liu et al. (2018), Kim and Doshi-Velez (2017), Poursabzi-Sangdeh et al. (2018), Zhang and Zhu (2018), Avigdor-Elgrabli et al. (2018), Du et al. (2018), Gilpin et al. (2018), Hall et al. (2018), Mohseni et al. (2018), Murdoch et al. (2019), Schmidt and Biessmann (2019), Friedler et al. (2019), Ghorbani et al. (2019), Hazard et al. (2019), Ish-Horowicz et al. (2019), Ahuja et al. (2018), Bachoc et al. (2018), Brown and Petrik (2018), Rudin (2019), Choi et al. (2020), Caruana et al. (2020), Molnar et al. (2020)
- **Explainability:** Arik and Pfister (2019), Adadi and Berrada (2018), Amarasinghe et al. (2018), Choo and Liu (2018), Dosilovic et al. (2018), Horel and Giesecke (2018), Preece (2018), Roscher et al. (2019), Vasic et al. (2019), Ahern et al. (2019), Arras et al. (2019), Gade et al. (2019), Samek and Muller (2019), Singh and Anand (2019), Vaughan et al. (2018), Moore et al. (2019), Ignatiev (2020), Samek et al. (2020), Shi et al. (2020), Xie et al. (2020), Puiutta and Veith (2020), Moreira et al. (2020), Moraffah et al. (2020)

ML in QWIM: classification and pattern recognition

What type of alternative data is available in QWIM?

- Ekster and Kolm (2020): usage of alternative data in QWIM
- Kolanovic and Krishnamachari (2017) and Guida (2019):
 - Alternative data can be generated by:
 - individuals (social media, news and reviews, web searches)
 - business processes (e-commerce, credit card transactions, company data)
 - government agencies (regulations, rules, guidelines, etc.)
 - machines/sensors (satellite imagery, radar, traffic, etc.)
 - Alternative data can incorporate many categories of attributes:
 - asset class: equity, fixed income, FX, commodity
 - investment style: macro, sectors, risk indicators
 - processing type: raw, processed, trading signal, research
 - quality: historical, outliers, missing values, transparency
 - technical: format, latency, frequency, legal

Visual categorization of alternative data



Source: Lipus and Smith (2019)

Classification and partition of investment universe

- Challenges of partition into asset class categories: a) if partition is “too coarse”, portfolio may be missing desired asset/subasset classes versus b) if partition is “too fine”, portfolio may end up with very small allocations, while costs would increase (trading, compliance, etc.)
- [Lamponi \(2015\)](#): data-driven categorization of investable assets
- [Ma et al. \(2019\)](#): unsupervised MIL to identify number of most relevant risk-axes and corresponding asset categories, then supervised MIL to identify most important defining characteristics of an asset category
- [Garvey and Madhavan \(2019\)](#): model output (geographical footprint) identified by MIL may differ significantly from usual groupings
- [Kakushadze and Yu \(2017a\)](#), [Kakushadze and Yu \(2017b\)](#): MIL when industry and sector classification not very clear, or needs to adjust rapidly
- [Yang et al. \(2016\)](#), [Kee \(2019\)](#): automated, text-based industry and sector classification reflecting constant changes in companies’ scope
- [Fang et al. \(2020\)](#): GICS sector categorization can be successfully reconstructed from historical fundamental data using MIL

Classification and partition of investment universe (cont.)

- [Gao et al. \(2020\)](#): text-based industry classification using word embedding schemes and clustering algorithms
- [Mehta et al. \(2020\)](#): industry categorization system using MIL is reproducible and may be as good (or better) than categorization based on human curation
- [Kilburn \(2020b\)](#): many asset managers no longer convinced of asset class labels used for decades; use clustering and network analysis rather than rely on traditional information such as their sector, geography, issuer or credit ratings
- [Kilburn \(2019b\)](#): MIL can group assets better and predict regime shifts
- [Husmann et al. \(2020\)](#): t-distributed stochastic neighbor embedding (t-SNE) and spectral clustering for company classification
- [Massaro et al. \(2020\)](#): MIL delivers very reliable predictions company classification based on sector of economic activity

Text analysis of company and regulatory documents

- Loughran and McDonald (2020): survey of textual analysis in finance
- Feuerriegel and Gordon (2018): text-based and news-based MIL improves forecasts of stock indices and interpretability
- DiPietro (2019), Fleiss et al. (2020): MIL in combination with SEC 13f filing data found to be effective in terms of portfolio cloning
- Das et al. (2019b): NLP to parse corporate email content and news to assess factors that predict escalating risk or potential firm malaise before they manifest in observable data and financial outcomes
- Klevak et al. (2019): scoring of earnings conference call transcripts based on tone (sentiment) and specific events delivers a signal incrementally additive to earnings surprises and short-term returns around earnings announcement
- Ravula (2021a), Ravula (2021b): text analysis in financial disclosures and and bankruptcy prediction using disclosure text features

Text analysis of company and regulatory documents (cont.)

- Agarwal (2020): systematic textual analysis of company annual reports delivers sustainable returns orthogonal to market returns
- Cohen et al. (2019): changes to 10-Ks predict future earnings, profitability, future news announcements, and even future firm-level bankruptcies
- Amel-Zadeh et al. (2020): MIL capable of forecasting sign and magnitude of abnormal stock returns around earnings announcements based on financial statement data alone
- Luo (2020): NLP applied to company management presentations
 - to analyze readability index and language complexity
 - to quantify executive personalities
- NLP delivers alpha factors uncorrelated with traditional factors, offering significant diversification benefits

Sentiment analysis of news and social media

- Naumer and Yurtoglu (2020), Houlihan and Creamer (2017), Liew and Budavari (2017): Social media and news sentiments have significant power in explaining time series variation in stock returns
- Frydman et al. (2021): mechanism describing how market sentiment drives forecasts of stock returns
- Huang et al. (2018): investor sentiment relevant for stocks, bonds, commodities, currencies, housing
- Audrino et al. (2020): sentiment and attention from social media, news articles, information consumption, and search engine data have significant impact on stock market volatility
- Coqueret (2020b): quantifies impact of stock-specific news sentiment on future financial returns
- Tran (2021): bridging model that connects risk-based factor models to sentiment models
- Ravula (2021b): market sentiment analysis using Valence Aware Dictionary and sEntiment Reasoner

Sentiment analysis of news and social media (cont.)

- [Elagamy et al. \(2018\)](#): text mining combined with Random Forest may determine early warning indicators for stock market crisis
- [Kadous et al. \(2017\)](#): investment advice provided on social media is influential even when it has little predictive value.
- [Creamer \(2015\)](#): since Black-Litterman model is meant to incorporate investor views, why not use sentiment from news, social media and corporate social network as source of investors' expectations?
- [Martin-Utrera \(2020\)](#), [Hilliard et al. \(2020\)](#): market sentiment relevant for portfolio optimization
- [Luo \(2020\)](#), [Adammer and Schussler \(2020\)](#): information embedded in news a) has predictive power and b) is not captured by established economic predictors
- [Upreti et al. \(2019\)](#), [Man et al. \(2019\)](#), [Mohammad \(2020\)](#): surveys of ML-based financial news analytics and sentiment analysis

Environmental, Social and Governance ESG Investing

- **BNP Paribas (2019)**: More than 75% of asset owners and 60% of asset managers hold $\geq 25\%$ of their investments in funds incorporating ESG
- **Walker (2019)**: *"There are issues with the fundamental analyst driven nature of ESG factors in investment process. Data can be too infrequent, measuring events are sometimes too extreme, and capturing events can be too late"*.
- **Nauman (2019)**: MIL can go through vast reams of ESG data in a sector where information comes from many sources and is often presented in incompatible ways due to lack of reporting regulations.
- **Laidlaw (2019)**: *"AI is really the catalyst that allows us to find very fine-grain nuggets of information in massive unstructured data"*
- **de Franco (2019b), De Franco et al. (2020)**: MIL can identify patterns between ESG profiles and financial performances for companies in a large investment universe
- **Guo et al. (2020b)**: pipeline of ESG news extraction, news representations, and Bayesian inference of deep learning models

Environmental, Social and Governance ESG Investing (cont.)

- [Antoncic et al. \(2020\)](#): combines **MIL** and a sustainability lens based on United Nations Sustainable Development Goals
- Procedure delivers scores, rankings, ratings and benchmarks
- [Craik \(2019\)](#): How **MIL** can help find ESG opportunities
- However, ESG investing may have significant practical challenges: [Cornell \(2020\)](#), [Billio et al. \(2020\)](#), [Bahra and Thukral \(2020\)](#), [Gidwani \(2020\)](#), [Dimson et al. \(2020\)](#), [Harper \(2020\)](#), [Chen and Mussalli \(2020\)](#), [de Franco \(2019a\)](#), [Cornell and Damodaran \(2020\)](#)
- **MIL** can resolve some of these challenges
- [Lanza et al. \(2020\)](#): overcoming current inconsistencies in ESG scores by using **MIL** to identify indicators that contribute better to portfolios
- [Mannix \(2020\)](#): Investors use **MIL** to incorporate raw data over ratings in ESG alpha hunts
- [Sokolov et al. \(2021\)](#): DL and NLP for automated ESG scoring

Fund decomposition, inference and replication

- Question: *Given only the historic net asset value of a mutual fund, which members of some universe of stocks are held by the fund?*
- Discovering an exact solution is combinatorially intractable
- Byrd et al. (2019): use MIL to produce a computationally efficient inference, and identify ETF constituents with accuracy of 88% to 98%
- Duanmu et al. (2020), Giuzio et al. (2018), Simonian and Wu (2019a): MIL successfully used for replication of less liquid funds (such as hedge funds or private equity funds) using liquid investment vehicles
- Mannix (2019), Wigglesworth (2019): firms using MIL to trade public-market stocks to replicate risk and returns of private equity PE funds.
- Some mimic PE's purported bet on buying small, cheap companies; some bet on sectors; others seek to replicate how PE firms think
- Li and Rossi (2021): MIL to select mutual funds from stocks they hold

ML in QWIM: network analysis and clustering

Beware of correlations which are not consistent with intuition

- In many cases, combination of increasing data, computational power computers and MIL may not deliver better results in QWIM, especially when decision making relies on data-based spurious correlations rather than causality
- **Vigen (2019)**: many examples of such data-based spurious correlations
 - ▶ Divorce rate in Maine has 99% correlation with per capita consumption of margarin
 - ▶ Per capita consumption of mozzarella cheese has 96% correlation with civil engineering doctorates awarded in US
 - ▶ Per capita consumption of chicken has 90% correlation with total US crude oil imports
- Example in QWIM **Laurinaityte et al. (2019)**: population growth of captive Asian elephants explains cross-section of expected returns of usually sorted portfolios with $R^2 = 0.91$ and $tStat = 2.93$ for market price of risk.
- *Does it mean that number of captive elephants is the new outstanding factor in empirical asset pricing?*



Clustering-based portfolio optimization

- Practical problem: correlation matrix lacks the notion of hierarchy.
- Thus all investments are potential substitutes of each other
- Since investment vehicles could be grouped in terms of industry, size, liquidity, region, some investments are “closer” substitutes of one another, while other investments are “complementary” to one another.
- Then it is better if similar investments can be placed together, while dissimilar investments can be placed far apart.
- This can be accomplished by leveraging network analysis and graph theory to better describe the dependencies among investment vehicles.
- Clustering-based hierarchical structure has two desirable features:
 - ▶ portfolio weights primarily are rebalanced among peers at various hierarchical levels
 - ▶ weights are distributed top-down, consistent with how many asset managers construct their portfolios, e.g. from asset class to sectors to individual securities

Clustering-based portfolio optimization (cont.)

- [Durante et al. \(2015\)](#) construction of portfolios diversified in their tail behavior by selecting only a single asset in each cluster
- [Dose and Cincotti \(2005\)](#): enhanced index tracking based on clusters of financial time series
- [Tola et al. \(2008\)](#): clustering improves ratio between predicted and realized portfolio risk.
- [Dees et al. \(2019\)](#): portfolio optimization based on graph cuts/ topology
- [Durante et al. \(2013\)](#): since clusters tend to be comonotone in their extreme low values, diversify over these clusters to avoid contagion during risky scenarios
- [Chang et al. \(2016\)](#): portfolio selection based on Affinity Propagation clustering
- [Lemieux et al. \(2014\)](#): clustering effects on portfolio formation and risk
- Hierarchical clustering (discussed next) refers to formation of a recursive clustering, suggested by the data, not defined a priori

Clustering-based portfolio optimization (cont.)

- Zhang and Maringer (2011) and Zhang and Maringer (2010): clustering asset allocation scheme has better performance
- Lopez de Prado (2016): Hierarchical Risk Parity HRP groups similar investments into clusters, based on a proper dissimilarity metric
- Lohre et al. (2020): use HRP to account for tail dependencies in multi-asset multi-factor allocations
- Raffinot (2017): hierarchical clustering-based asset allocation HCAA is more robust and diversified, and achieve statistically better risk-adjusted performances
- Raffinot (2018): Hierarchical Equal Risk Contribution portfolio merges and enhances HRP and HCAA
- Molyboga (2020): modified HRP to improve diversification within and across clusters
- Leon et al. (2017b) and Leon et al. (2017a): Risk-Adjusted Portfolio Construction based on clustering

Clustering-based portfolio optimization (cont.)

- [Jain and Jain \(2019\)](#): use clustering to account for misspecification of covariance matrix, and to investigate when ML-based portfolios outperform traditional risk-based portfolios
- [Duarte and De Castro \(2020\)](#): framework for asset allocation based on partitional clustering algorithms (intragroup and intergroup)
- [Puerto et al. \(2020\)](#): measuring effect (within portfolio optimization) of clustering on selected assets with respect to non-selected ones
- [Lopez de Prado \(2020a\)](#): practical clustering for portfolio optimization
- [Begusic and Kostanjcar \(2019\)](#): cluster-based shrinkage of correlation matrices for portfolio optimization
- [Kolrep et al. \(2020\)](#): intuition and nature of hierarchical clustering in context of multi-asset multi-factor investing
- [Jaeger et al. \(2021\)](#): Interpretable ML and clustering for diversified portfolio construction

Network-based portfolio optimization

- Networks enable practical usage of high / low centrality concepts
 - significant interconnectedness risk (tail events propagate more quickly) due to assets with high centrality scores
 - "peripheral assets" carry relatively less interconnectedness risk
- Pozzi et al. (2013): investments in “peripheral” stocks (located in poorly connected regions of financial networks) better diversified
- Clemente et al. (2019), Clemente et al. (2021): network-based portfolio consistently outperforms standard portfolios out-of-sample
- Kaya (2015): vol strategy augmented by eccentricity centrality measure
- Zhao et al. (2018), Clemente et al. (2018): optimal portfolios obtained through a network-based approach are composed mainly of peripheral assets
- Li et al. (2019): peripherality in a network used as indicator to identify optimal assets
- Peralta and Zareei (2016): negative relationship between centrality of stocks and their risk-adjusted returns.

Network-based portfolio optimization (cont.)

- [Konstantinov et al. \(2020\)](#): compared factor and asset allocation portfolios using both traditional and network-based approaches
- Demonstrate advantages of graph theory for portfolio management, and dynamic nature of assets and factors with their importance scores
- Centrality scores help to identify crowded exposure and build diversified allocations
- [Vyrost et al. \(2019\)](#): construct financial networks in which nodes are represented by assets and where edges are based on long-run correlations
- Proposed adjustments to portfolio strategies utilize centralization measures from financial networks, and improve OOS risk and left-tail risk-adjusted returns
- [Giudici et al. \(2020\)](#): network models and Random Matrix Theory combined to improve robot advisory portfolio asset allocation
- [Pichler et al. \(2018\)](#): minimize systemic risk through network optimization

Other uses of clustering and networks analysis

- [Vozlyublennaya and Wu \(2018\)](#): measures mutual fund uniqueness using cluster analysis of fund returns
- [Narabin and Boongasame \(2018\)](#): cluster analysis of mutual funds data
- [Lisi and Menardi \(2015\)](#) and [Lisi and Otranto \(2010\)](#): clustering analysis to obtain classes of homogeneous funds with respect to risk levels
- [Sakakibara et al. \(2015\)](#): cluster mutual funds based on investment similarity instead of historical performances
- [Forsberg et al. \(2018\)](#): identifying hedge fund manager skill using cohorts (identified through clustering) that adjusts fund returns for return of cohort of funds applying same, or very similar, strategies.
- [Razafitombo \(2015\)](#): fund analysis and selection using distances and similarities between key performance measures based on clustering
- [Zhang and Gencay \(2019\)](#): mutual fund performance persistence linked to network-based analysis of how fund utilizes market information
- [Eom and Park \(2017\)](#): influence of factors affecting network connectivity is considerable on stocks with many links to other stocks in network

Other uses of clustering and networks analysis (cont.)

- [Konstantinov and Rusev \(2020\)](#): connections between global equity and bond funds from a network perspective; networks can amplify system-wide stress or inefficiencies in the factor bets
- Equity-bond allocations based on centrality scores, factor exposure, and hierarchical clustering of asymmetrically connected assets
- [Konstantinov and Simonian \(2020\)](#): analyze hedge fund market from perspective of a network of interacting individual funds
- Able to identify most important hedge fund styles to affect market and transmit systemwide shocks
- [Baitinger and Papenbrock \(2017b\)](#), [Baitinger and Papenbrock \(2017a\)](#): neglect of interconnectedness risk is not justified, because a) it has limited connection to conventional portfolio optimization input and b) investment strategies based on interconnectedness information outperform
- [Balasubramanian et al. \(2019\)](#): Market regime changes are connected to clustering of co-moving assets and breaking of already existing clusters

ML in QWIM: forecasting of financial time series

Forecasting of time series

- Goal of econometric models is parameter estimation: produce good estimates of parameters β that underlie relationship between y and x
- Goal of (supervised) ML is to produce good predictions out-of-sample
- Mullainathan and Spiess (2017): *“Put succinctly, machine learning belongs in toolbox compartment marked \hat{y} rather than in the more familiar $\hat{\beta}$ compartment”*
- Econometric models adjudicate explanatory power to specific variables; designed to decompose a combined effect as sum of individual effects
- Success of ML largely due to its ability to discover complex structure that was not specified in advance, and to fit complex and very flexible functional forms to data without simply overfitting.
- ML may enable new perspectives, such as recasting time series forecasting as an ordinal regression task Orozco et al. (2018)
- Comparing statistical and ML forecasting methods: Makridakis et al. (2018a), Makridakis et al. (2020), Januschowski et al. (2020), Benidis et al. (2020), Lim and Zohren (2020), Cerqueira et al. (2019), and Hyndman and Athanasopoulos (2020)

Forecasting of financial time series (cont.)

- Traditional methods for time series forecasting include univariate Autoregressive (AR), univariate Moving Average (MA), Autoregressive Integrated Moving Average (ARIMA): Hyndman and Athanasopoulos (2020)
- Siami-Namini and Namin (2018), Qian (2017): ML (in particular Deep Learning) may outperform ARIMA for financial time series forecasting
- Heaton et al. (2017): deep learning can detect and exploit data interactions invisible (at least currently) to any existing financial economic theory
- Siami-Namini and Namin (2018): Long Short-Term Memory (LSTM) delivers 85% reduction in error rates compared to ARIMA
- Bao et al. (2017): combination of wavelet transforms, stacked autoencoders and LSTM outperforms LTSM, WT-LTSM and recurrent neural network RNN
- Fischer and Krauss (2017): LSTM good out-of-sample prediction of directional movements for constituents of *S&P* 500
- Sezer et al. (2020), Alonso et al. (2020): financial time series forecasting with DL

Forecasting of financial time series (cont.)

- Superiority of MIL not apparent when it comes to typical time series forecasting, where data availability is often limited
- M4 competition: Makridakis et al. (2019) and Makridakis et al. (2018b)
 - many (100,000) and diverse time series, mostly medium-frequency data (daily), and some low-frequency data
 - requested both point forecasts and prediction intervals
- Performance for time series forecasting has to be assessed through a combination of metrics Botchkarev (2019) and Gasthaus et al. (2019)
- Januschowski et al. (2020): more practical to compare MIL and statistical forecasting from other perspectives:
 - global versus local methods
 - probabilistic versus point forecasts
 - data driven versus model-driven
 - ensemble versus single models
 - explanatory/interpretable versus predictive

Combinations of forecasting methods

- Combinations of forecasting methods appear to have best results for forecasting of time series of similar granularity as the ones used in QWIM: Qian et al. (2019), Gibbs (2017), and Mancuso and Werner (2013), Atiya (2020), Dantas and Oliveira (2018), Elliott (2017), and Hsiao and Wan (2014), Ma et al. (2018), Thomson et al. (2019) and Post et al. (2019), Shaub (2020)
- First place at M4 Competition Smyl (2020): combination of exponential smoothing ES and LSTM: ES for main components of individual series (seasonality, level), while LSTM for non-linear trends and cross-learning
- Second place at M4 Competition Montero-Manso et al. (2020): combination of 9 statistical and 1 MIL methods, with optimal weights of combination obtained through MIL (gradient boosting)
- Improving on winning entry Smyl (2020) for M4 competition quite challenging task; only a few specialized algorithms have succeeded
- Pure MIL methods (e.g., N-BEATS, GluonTS) discussed in next slides
- More on combinations of MIL and statistical: Joshi (2019), McDonald et al. (2014) and Karathanasopoulos et al. (2017), Gilliland (2020), Allende and Valle (2017), Zhao and Feng (2020)

Combinations of forecasting methods (cont.)

- [Pike and Vazquez-Grande \(2020\)](#): combination weights computed using ML trained on models' past forecast errors
- [Bauer et al. \(2020b\)](#), [Bauer et al. \(2020a\)](#): Telescope is a hybrid multi-step-ahead forecasting approach
 - based on time series decomposition forecasting
 - extracts intrinsic features based on STL decomposition + Fourier
 - XGBoost for composing the forecast component
 - can be used with or without a recommendation system
- Compared to hybrid forecasting methods (including [Smyl \(2020\)](#)), ML methods, established statistical methods, results show that Telescope has best forecast accuracy (based on sMAPE), lowest forecast error variability, much faster than any of the next 3 best (in terms of forecast accuracy) forecasting methods

Exploiting cross-series information

- Athanasopoulos et al. (2019) and Athanasopoulos and Kourentzes (2020): time series are often hierarchical and correlated
- Collection of time series can exhibit dependency relationships between individual time series that can be leveraged in forecasting
 - local co-variate relationships
 - indirect relationships through shared latent causes
 - subtle dependencies through smoothness, temporal dynamics, and noise characteristics
- Instead of one model per each time series, global model is developed exploiting information from many time series simultaneously
- Spiliotis et al. (2020) and Abolghasemi et al. (2019): MIL applied to time series hierarchical forecasting may outperform traditional models
- Sirignano and Cont (2018): model trained on data from all stocks outperforms models trained on time series of any individual stock
- Impressively, results hold for stocks NOT included in training sample

Exploiting cross-series information (cont.)

- Hewamalage et al. (2019): survey of global models in context of deep neural networks.
- Smyl (2020): global model concept with local parameters
- Bandara et al. (2019): clustering groups of related time series, with global model developed per each cluster.
- Salinas et al. (2020): cross-series information applied to Probabilistic Forecasting with Autoregressive Recurrent Networks (DeepAR) model
- Oreshkin et al. (2020): Neural basis expansion analysis (N-BEATS) model
- Wang et al. (2019b): global Deep Neural Networks DNN backbone and local probabilistic graphical models for computational efficiency
- Rangapuram et al. (2018), Wang et al. (2019b): parameterize per-time-series linear state space model with a jointly-learned recurrent neural network

Results on M4 datasets

- [Oreshkin et al. \(2019\)](#): deep neural architecture based on backward and forward residual links and a very deep stack of fully-connected layers.
- N-BEATS: Neural basis expansion analysis.

Table 1: Performance on the M4 test set, sMAPE metric

	Yearly (23K)	Quarterly (24K)	Monthly (48K)	Others (5K)	Average (100K)
Best pure ML	14.397	11.031	13.973	4.566	12.894
Best statistical	13.366	10.155	13.002	4.682	11.986
Best ML/TS combination	13.528	9.733	12.639	4.118	11.720
DL/TS hybrid, M4 winner	13.176	9.679	12.126	4.014	11.374
NBEATS-G	12.855	9.378	12.130	3.979	11.229
NBEATS-I	12.823	9.418	12.048	4.199	11.203
NBEATS-I+G	12.812	9.372	12.064	4.063	11.190

Source: [Oreshkin et al. \(2019\)](#)

Results on M4 datasets (cont.)

Table 2: Performance on the M4 test set, OWA and M4 Rank

	Yearly (23K)	Quarterly (24K)	Monthly (48K)	Others (5K)	Average (100K)	Rank
Best pure ML	0.859	0.939	0.941	0.991	0.915	23
Best statistical	0.788	0.898	0.905	0.989	0.861	8
Best ML/TS combination	0.799	0.847	0.858	0.914	0.838	2
DL/TS hybrid, M4 winner	0.778	0.847	0.836	0.920	0.821	1

NBEATS-G	0.755	0.814	0.823	0.876	0.799	
NBEATS-I	0.753	0.8219	0.820	0.911	0.799	
NBEATS-I+G	0.752	0.814	0.819	0.889	0.797	

Source: [Oreshkin et al. \(2019\)](#)

Table 3: Comparison between DeepAR and Smyl method for M4 dataset

Metric	DeepAR	Smyl
sMAPE	0.1192	0.1137
MASE	1.500	1.54
OWA	0.837	0.821
MSIS	12.07	12.23

Source: [Salinas et al. \(2019\)](#)

Results on M4 datasets (cont.)

- [Loning et al. \(2019\)](#): sktime, a general MML framework for time series, with
 - scikit-learn compatible interfaces
 - tools to build, tune and evaluate composite models
- [Loning and Kiraly \(2020\)](#): framework enhanced to both replicate and extend key results from M4 forecasting study
- Notable results:
 - perfect replication for all naive forecasters
 - small but often statistically significant differences for statistical models
 - large and statistically significant differences for MLP and RNN (likely due to improvements in sk-time and TensorFlow)
 - simple hybrid approaches (such as residual boosting) can boost the performance of statistical models

Empirical asset pricing

- Karolyi and Van Nieuwerburgh (2020), Hou et al. (2021), Nietert and Otto (2020), Barras (2019), Fama and French (2020), Fletcher (2019b), Bektic et al. (2020), Lettau and Pelger (2020), Chen and Zimmermann (2020), Maio (2019), Zaffaroni (2019), Chib et al. (2020): current state-of-the-art on empirical asset premia
- Harvey et al. (2016), Hwang and Rubesam (2019), Feng et al. (2020), Harvey and Liu (2020a), Pukthuanthong et al. (2019): asset pricing literature has produced hundreds of potential risk factors
- Chib and Zeng (2020), Harvey and Liu (2020c), Fletcher (2019a), Messmer and Audrino (2020), Green et al. (2017): Which characteristics really provide independent information?
- Literature mainly builds on linear or linear-like models, due to simplicity, transparency and computational efficiency
- Collot and Hemauer (2021), Giglio and Xiu (2019): Concerns for risk premia estimation: potential omission of factors, measurement error, nonlinearity, clustering or dependency structure

Empirical asset pricing (cont.)

- Suhonen et al. (2017), Shi and Li (2021), Xu (2020), Bryzgalova et al. (2020), Gospodinov and Robotti (2021), Freyberger et al. (2020): current approaches still have challenges
- ML relatively well-equipped to address these concerns, since no prior imposed on functional relation describing expected return process, but “learn” this non-linear dependence structure.
- Gu et al. (2020): ML improved performance compared to traditional methods for both cross section and time series stock return prediction
- Predictive gains traced to inclusion of nonlinear interactions, while ML methods agree on a fairly small set of dominant predictive signals
- Gu et al. (2021): autoencoder asset pricing model delivers OOS errors far smaller compared to other leading factor models
- Bianchi et al. (2021): ML delivers useful bond risk premia forecasts
- Dixon and Polson (2020): DL fundamental factor models capture non-linearity, interaction effects and non-parametric shocks

Empirical asset pricing (cont.)

- [Feng et al. \(2018\)](#): extraction of nonlinear factors information through **DL**, with statistical factor models special cases of shallow learners
- [Coqueret \(2020a\)](#): importance of memory in **MIL**-based models relying on firm characteristics for asset pricing
- [Drobetz and Otto \(2020\)](#): evaluates performance of **MIL**-based forecasting stock returns
- [Rapach and Zhou \(2020\)](#): **MIL** forecasts using time series and cross-sections of stock returns
- [Coqueret and Guida \(2020\)](#): **MIL**-based models for factor investing
- [Andreini et al. \(2020\)](#): **MIL** used to encode information available from hundreds of macroeconomic and financial time-series into a handful of unobserved latent states, which can still be interpreted as in a standard factor models

Empirical asset pricing (cont.)

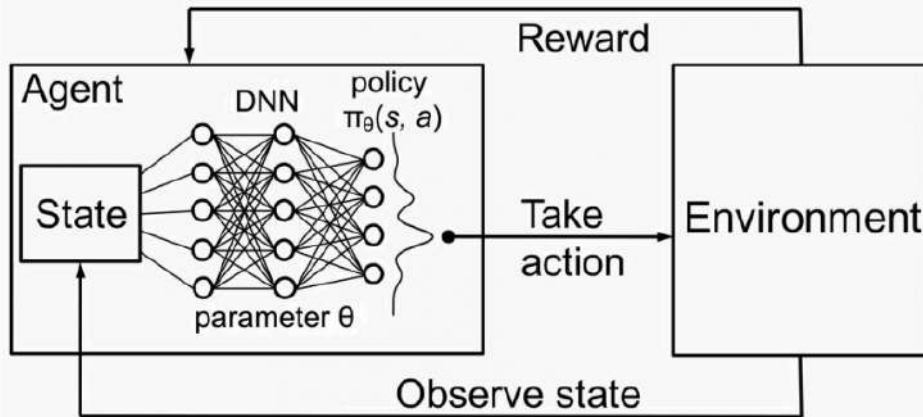
- [Grammig et al. \(2020\)](#): MIL able to predict returns and generate profits in 33 international markets, while using fewer variables as inputs compared to previous studies
- [Jurczenko et al. \(2020\)](#), [Guida \(2019\)](#), [Lopez de Prado \(2020a\)](#): advances and promising results when using MIL for empirical asset pricing
- However, while MIL -based risk premia has many advantages, it also has practical challenges
- [Grammig et al. \(2020\)](#): in a low signal-to-noise environment theory-based risk premia might deliver better results compared to MIL -based risk premia
- [Leung et al. \(2020\)](#): Despite statistical advantage of MIL model predictions, corresponding economic gains somewhat limited, largely dependent on ability to take risk and implement trades efficiently.

ML in QWIM: reinforcement learning RL

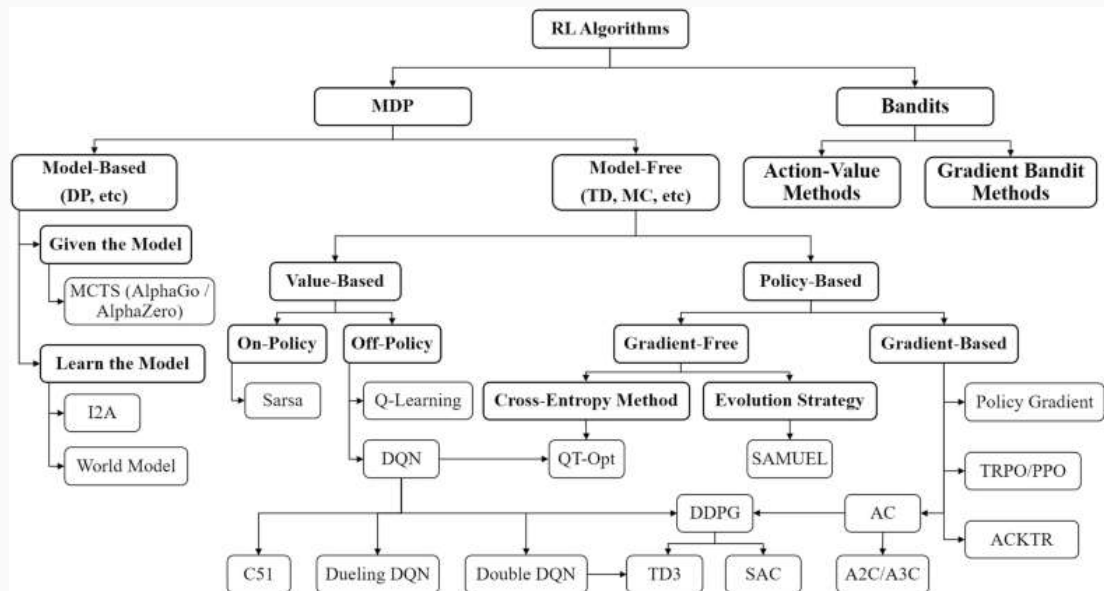
Reinforcement learning \mathbb{RL}

- \mathbb{RL} “learns” how to attain a complex objective (goal), with agent trained in environment by performing actions and adapting to results
- Interactive process, as agent actions actively change its environment
- Deep \mathbb{RL} : agents construct and learn their own knowledge through deep learning of neural networks.

Figure 1: (Deep) Reinforcement learning diagram



Taxonomy of RL algorithms



Source: Zhang and Yu (2020)

Financial applications of RL

- RL can solve financial applications of intertemporal choice, such as:
 - pricing and hedging of financial derivatives
 - investment and portfolio allocation
 - buying and selling securities subject to transaction costs
 - optimal dynamic trading strategy
 - optimization of tax consequences
- There are already good results for RL and DRL in trading and hedging: Kolm and Ritter (2019), Ritter (2019), Kolm and Ritter (2020b), Dixon et al. (2020)
- Buehler et al. (2019): DRL framework for hedging a portfolio of derivatives in presence of transaction costs, liquidity constraints or risk limits
- Du et al. (2020): DRL for option replication subject to discrete trading, round lotting, and nonlinear transaction costs
- Cao et al. (2020): DRL for optimal hedging under transaction costs
- Carboneau (2020), Carboneau and Godin (2020), Cao et al. (2021), Benhamou et al. (2020): DRL for hedging of financial derivatives (including long term)

Using RL in QWIM

- [Fischer \(2018\)](#): RL allows to combine “prediction” and “portfolio construction” tasks into one integrated step, providing better alignment to investor objectives
- [Noguer i Alonso and Srivastava \(2020\)](#): DRL for model-free asset allocation
- [Sato \(2019\)](#): model-free RL for financial portfolios
- [Irlam \(2020\)](#): RL is capable of handling real-world complexity of financial planning; taxes, inflation, longevity, etc.
- [Irlam \(2020\)](#): financial and retirement planning via DRL outperforms
- [Benhamou et al. \(2021\)](#): bridge gap between DRL and MPT; DRL maps directly market conditions to actions by design
- [Benhamou et al. \(2021\)](#): augmented asset management via DRL
- [Hu and Lin \(2019\)](#), [Cong et al. \(2020\)](#): DRL-based portfolio management
- [Alsabab et al. \(2021\)](#): using RL, roboadvisor “learns” over time investor risk preference by observing her portfolio choices under different markets.

Using RL in QWIM: Goals-based investing

- Goal Based Investing GBI: investment approach with performance measured by probabilities of success in achieving investor financial goals (at given time horizons and for specified priority levels)
- Objective is to invest systematically and to manage a portfolio consistent with investor's risk profile and time horizon of goals.
- References for GBI: Kim et al. (2020), Roncalli (2019), Wang et al. (2011), Deguest et al. (2015), Janssen et al. (2013), Dempster et al. (2016), Shalett (2015), Brunel (2011), Parker (2016b), Parker (2016a), Chhabra (2015), Parker (2020)
- Grealish and Kolm (2021), D'Acunto and Rossi (2021): roboadvisors aim to become more holistic; need to incorporate GBI, ML, and more
- Combination of RL and GBI very promising, since investor goals in GBI can be connected to reward function in RL
- GBI portfolio optimization, viewed as optimal control problem performed within data-driven world, can be solved via RL
- Depending on desired purpose, RL-based solutions for GBI may need to incorporate techniques from RL, DRL, IRL

Using RL in QWIM: Goals-based investing (cont.)

- [Das and Varma \(2020\)](#): use RL to solve for GBI, with the solution converging to the solution obtained using dynamic programming
- [Dixon and Halperin \(2020\)](#): GBI using G-Learner, which
 - operates with explicitly defined one-step rewards
 - does not assume a data generation process
 - is suitable for noisy data
- [Dixon and Halperin \(2020\)](#): GIRL extends G-Learner within context of Inverse Reinforcement Learning IRL, where rewards collected by agent are not observed, and should instead be inferred
- Given current state-of-the-art for RL, incorporating multiple goals with their corresponding priority levels within a RL-based solution for GBI appears to be a significant modeling challenge
- It is likely that such a solution will leverage hierarchical RL and curiosity-driven exploration: [Zhao et al. \(2019\)](#), [Rafati and Noelle \(2019\)](#), [Xing \(2019\)](#), [Colas et al. \(2019\)](#), [Roder et al. \(2020\)](#).

ML in QWIM: importance of
market states and regimes

Market states in QWIM

- There are two separate market states Peters (2015), Munnix et al. (2012), Pharasi et al. (2020) Ladekarl et al. (2019), Zakamulin (2020), Zaremba et al. (2020):
 - low uncertainty (relatively stable and resilient) market
 - high uncertainty (relatively chaotic and fragile) market
- Markets in **LOW UNCERTAINTY** state:
 - statistically well behaved
 - can be modeled using standard statistical tools
 - volatility stable and low, correlations relatively stable
 - tail events (≥ 3 std deviations in either direction) quite rare.
- Markets in **HIGH UNCERTAINTY** state:
 - not statistically well behaved
 - vols and correlations change significantly on regular basis
 - Tail events happen with much more regularity
- To account for the two market states, practitioners use a relatively similar concept of **"risk on, risk off"**: Lee (2012), Ma (2015), Dapena et al. (2019)

Structural breaks: market regimes

- The **HIGH UNCERTAINTY** state can incorporate multiple instances and types of significant changes in time series: market regimes, changepoints, bubbles/crashes
- Regime changes, some transitory, some recurring (recessions versus expansions) some permanent (structural breaks), are prevalent across a wide range of financial markets and in behavior of many macro variables [Ang and Timmermann \(2012\)](#), [Hamilton \(2016\)](#), and [Sheikh and Sun \(2012\)](#)
- Examples of regimes considered in academia and/or practitioners:
 - bull vs. bear market regimes
 - inflationary vs. recessionary regimes
 - high vs. low volatility regimes
 - mean reverting vs. trending regimes
- [Kritzman et al. \(2012\)](#) and [Blitz and Van Vliet \(2009\)](#): Regime shifts are challenging for investors because they cause portfolio performance, risk and behavior to depart significantly from ranges implied by long-term averages of means and covariances

Structural breaks: Market regimes (cont.)

- Regime-based asset allocation was shown to deliver improved performance and risk profile Masih (2012), Vo and Maurer (2013), SSgA Research (2015), Nystrup et al. (2018b), Briere and Signori (2012), Nystrup et al. (2015), Kritzman et al. (2012), Kaya (2017), Teiletche et al. (2017), Sheikh and Sun (2012), Jurczenko and Teiletche (2018), Lewin and Campani (2020), Lezmi et al. (2018), Fons et al. (2021), Collin-Dufresne et al. (2020),
- Kinlaw and Turkington (2014): periods characterized by correlation surprise lead to higher risk and lower returns to risk premia than periods characterized by typical correlations.
- Ammann and Verhofen (2006): empirical analysis indicates two clearly separable regimes with different mean returns, volatilities and correlations
- Papenbrock and Schwendner (2015): distinct correlation regimes detected
- Bernhart et al. (2011): correlations between (and within) asset classes are far from being stable, and they vary significantly
- Papenbrock and Schwendner (2015) and Simonian and Wu (2019b): regime-based investing, based on spectral clustering

Forecasting performance depends on market regimes

- Asset allocation is critically dependent on out-of-sample risk premium.
- Question: *Is superior econometric predictability across the business cycle synonymous with predictability at all times?*
- Answer is important since there is asymmetric behavior:
 - **gains during good periods** (when economic benefits may be reduced for high risk-averse and leverage-constrained investors)
 - **losses during bad periods** (when it matters the most for asset allocators to retain assets and their client base intact).
- Li and Piqueira (2019), Dal Pra et al. (2018), Salhi et al. (2016), Nalewaik (2015), Pereiro and Gonzalez-Rozada (2015), Chincoli and Guidolin (2017) Huang et al. (2017), Odendahl et al. (2020), Tsiakas et al. (2020), Hammerschmid and Lohre (2018) : predictability of returns (and of other investment variables) is regime-dependent.
- Baltas and Karyampas (2018): recent advanced forecasting models more accurate in up markets, during expansions, and during low-volatility periods; not necessarily in down markets, during recessions, and during high-volatility periods.

Forecasting performance depends on market regimes (cont.)

- Performance of investment strategies greatly enhanced with introduction of regime switching models \mathbb{RSMs} Costa and Kwon (2020), Nystrup et al. (2015), Nystrup et al. (2018b), Nystrup et al. (2018a), Flint and Mare (2019), Gokhale et al. (2019), Alberico et al. (2018), Collin-Dufresne et al. (2020)
- \mathbb{RSMs} characterize market states using estimates of parameters of some underlying model, and use a transition matrix to quantify probability of moving from one state to another.
- \mathbb{ML} may be effective at detecting change (even in chaotic systems Wolchover (2018)), for example through robust anomaly detection Bulusu et al. (2020), Braei and Wagner (2020)
- It can be enhanced to compute probability of observation in previously observed “market regimes” (defined as clusters in \mathbb{ML})
- Thus clustering algorithms can identify regimes in datasets
- What they have in common with regular regime switching models is ability of producing probabilities of “switching” into another regime
- \mathbb{ML} can also detect preconditions of a break

Identifying market regimes

- Unsupervised learning algorithms can be used for the determination of “natural” clusters and the grouping of market data according to predefined similarity criteria.
- Supervised learning algorithms can be “trained” with known data sets to classify market situations. Then, new data – and especially the current situation – can be assigned to the market phases.
- [Mulvey and Liu \(2016\)](#): identify market regimes via trend filtering
- [Chazal and Michel \(2017\)](#): Topological Data Analysis TDA used to automatically cluster thousands of variables spanning market, macroeconomic, and sentiment data and to create create visual, topological summaries that reveal the key characteristics of the current regime as well as the similarities to past regimes.
- [Gidea and Katz \(2018\)](#): use TDA (persistence homology) to detect and quantify topological patterns that persist across multiple scales; metrics of persistence landscapes exhibit strong growth prior to the primary peak, which ascends during a crash.

Structural breaks: bubbles and crashes

- [Alves et al. \(2018\)](#): Chaotic systems of the real world are comparable to stock market indices evolution.
- [Sornette and Cauwels \(2015\)](#): financial bubble defined as a period of unsustainable growth, when the price of an asset increases ever more quickly, in a series of accelerating phases of corrections and rebounds.
- [Filimonov and Sornette \(2013\)](#) and [Sornette \(2014\)](#): log-periodic power law singularity (LPPLS) model identifies well bubbles and crashes
- [Demos and Sornette \(2017\)](#): LPPLS provides overwhelming evidence that the beginning of bubbles is much better constrained than their end.
- [Demirer et al. \(2019\)](#): LPPLS framework successfully captures, ex-ante, most prominent bubbles across different time scales (Black Monday, Dot-com, and Subprime Crisis).
- Change point detection (CPD) is the problem of finding abrupt changes in data when a property of the time series changes
- Segmentation, edge detection, event detection, and anomaly detection are similar concepts within **MIL** space.

Structural breaks: changepoints

- Ruff et al. (2020), Blazquez-Garcia et al. (2020), Foorthuis (2020), Braei and Wagner (2020), van den Burg and Williams (2020), Aminikhanghahi and Cook (2017): surveys of algorithms for change point detections
- Wu and Keogh (2020), Goswami et al. (2018): existing transition detection methods do not rigorously account for time series uncertainties
- Lee et al. (2018): traditional changepoint detection methods look for statistically-detectable boundaries (defined as abrupt variations in generative parameters of a data sequence)
- However, breakpoints may occur on boundaries non-trivial to detect with these statistical methods, but detectable using DL
- Chalapathy and Chawla (2019), Chalapathy et al. (2020), Wang et al. (2020a), Lee et al. (2018): DL for anomaly detection
- Bashar and Nayak (2020), Geiger et al. (2020): Generative Adversarial Networks for anomaly detection

ML in QWIM: other practical applications

Generating synthetic data for QWIM

- Significant need for additional data in QWIM
 - for adequately training ML models
 - to tackle unbalanced datasets
 - for constructing a very comprehensive set of scenarios incorporating most scenarios which were not observed, yet are plausible and consistent with market and investor behavior and with economic intuition
 - for data anonymization and preserving of data privacy
 - for comprehensive testing of investment strategies and portfolios
 - for constructing much more robust portfolios using scenario-based optimization
 - for better risk management of investment portfolios
- Assefa et al. (2019): synthetic data defined as data obtained from a generative process that learns properties of real data
- Solutions through ML-based data augmentation DAug

Data augmentation and scenario generation

- [Coulombe \(2018\)](#): successful use in NLP of same **DAug** techniques already showing great success in artificial vision
- [Fawaz et al. \(2018a\)](#): **DAug** based on Dynamic Time Warping distance
 - drastically increase of accuracy of deep Convolutional Neural Networks on some time series **TS** datasets
 - significantly improvement of deep model's accuracy when used in an ensemble approach
- [Kuchnik and Smith \(2018\)](#): subsampling policies based on model influence and loss achieve a 90% reduction in augmentation set size while maintaining the accuracy gains of standard data augmentation
- [Zhang et al. \(2018c\)](#): DADA: Deep Adversarial Data Augmentation for Extremely Low Data Regime Classification
- [Hernandez-Garcia and Konig \(2018\)](#) and [Da Silva and Shi \(2019\)](#): generative model for financial **TS** able to create realistic paths that embed underlying structure of markets in a way stochastic processes could not

Generating synthetic financial time series

- Synthetic financial **TS** data is expected to have universal features, commonly referred to as stylized facts ([Kristoufek \(2018\)](#), [Jilla et al. \(2017\)](#), [Cont \(2001\)](#), [Allen and Satchell \(2014\)](#)), together with specialized features of a specific asset class or investment vehicle
- [Buehler et al. \(2020a\)](#): overview of currently used generative modelling approaches and performance evaluation metrics for financial **TS**
- For classical models, these stylized facts are often formulated in terms of distribution of returns
- [Buehler et al. \(2020a\)](#): This returns-based viewpoint (though still interesting) may not convey a sufficiently full picture for distributions of synthetic market paths obtained using generative modeling.
- Most promising **MIL** methods to generate synthetic financial **TS**:
 - generative adversarial networks GANS
 - Variational Autoencoders VAEs
 - Restricted Boltzmann Machine RBM

Generating synthetic financial time series (cont.)

- [Wiese et al. \(2020\)](#): realistic multivariate financial **TS** based on GANs, able to capture longer ranging dependencies
- [Buehler et al. \(2020a\)](#): model based on VAEs works reliably even cases where amount of available training data is notoriously small
- [Kondratyev and Schwarz \(2019\)](#) and [Kondratyev et al. \(2020\)](#): RBM delivers synthetic market data with similar probability distribution of original data, controlling autocorrelation and non-stationarity in generated **TS**
- [Takahashi et al. \(2019\)](#): GANs produce **TS** with desired properties: linear unpredictability, heavy-tailed price return distribution, volatility clustering, leverage effects, coarse-fine vol correlation
- [Koshiyama et al. \(2019\)](#): GANs for financial trading strategies
- [Mariani et al. \(2019\)](#): PAGAN: Portfolio Analysis with GANs
- [Marti \(2020\)](#): GANs to generate realistic financial correlation matrices
- [De Meer Pardo and Lopez \(2020\)](#): training **MIL** on synthetic data generated by Wasserstein GAN with gradient penalty mitigates overfitting

Generating synthetic financial time series (cont.)

- [Franco-Pedroso et al. \(2019a\)](#): virtual multivariate scenarios of financial data of arbitrary length and asset composition, retaining volatility clustering, cross-asset relationships, and their changes over time
- [Franco-Pedroso et al. \(2019b\)](#): While posterior distribution of scenarios has to be consistent with that of real data, it is not sufficient because other properties related to evolution of time series (e.g., autocorrelation of returns) not being evaluated or unknown as being discriminant
- [Franco-Pedroso et al. \(2019b\)](#): evaluation framework to
 - quantify degree of realism of simulated financial time series, whatever simulation method might be
 - discover and improve unknown characteristics not being properly reproduced by analyzed methods
- [Lezmi et al. \(2020\)](#): Boltzmann machines and GANs to generate synthetic data preserving first four statistical moments, stochastic dependence between different dimensions (copula structure) and across time (autocorrelation).

Portfolio construction

- As discussed, network analysis and clustering could be leveraged to construct a more robust and diversified portfolio
- [Snow \(2020\)](#): **MIL** can help with most portfolio construction tasks, such as idea generation, alpha factor design, asset allocation, weight optimization, position sizing, as well as with testing
- [Snow \(2020\)](#): identifies different weight optimization methods within
 - supervised learning framework
 - traditional linear approach using OLS, Ridge, LASSO
 - nonlinear deep learning approach using autoencoders
 - Bayesian sentiment method
 - unsupervised learning framework
 - principal component analysis
 - hierarchical clustering analysis
 - network graphs
 - reinforcement learning framework
 - Deep Determinist Policy Gradient

Testing investment strategies and portfolios

- Harvey et al. (2020b), Giglio et al. (2021), Chordia et al. (2020), Vincent et al. (2020), Perumal and Flint (2018): comparison of various methodologies to test investment strategies
- Backtesting is at high risk of spurious accuracy due to data-mining bias present from considering multiple rules concurrently over same history.
- Harvey and Liu (2018), Barras et al. (2010), Barras et al. (2019), Bailey et al. (2017), Bailey et al. (2014), Bryzgalova et al. (2020), Harvey and Liu (2020b), Hens et al. (2020), Dichtl et al. (2020): majority of investment strategies subject to backtest overfitting (outperforms during backtest, underperforms in practice)
- When strategy selection is done under multiple testing (running many alternative configurations), backtest likely false discovery.
- MIL can be trained to scan billions of data signals in order to design millions of different virtual investment strategies
- Lopez de Prado (2018): Due to backtest overfitting, most quantitative investment firms invest in false discoveries

Testing investment strategies and portfolios (cont.)

- [Lopez de Prado \(2020a\)](#), [Lopez de Prado \(2018\)](#): These false discoveries may have been prevented if academic journals and investors demanded that any reported investment performance incorporates the false positive probability, adjusted for selection bias under multiple testing
- [Fabozzi and Lopez de Prado \(2018\)](#): propose a template to fairly disclose multiple tests involved in testing investment strategies
- [Chordia et al. \(2020\)](#): apply multiple hypothesis testing techniques that account for cross-correlations in signals and returns to produce t-statistic thresholds that control proportion of false discoveries.
- very small number of strategies survive when combining statistical criteria with economic considerations
- [Aparicio and Lopez de Prado \(2018\)](#): model confidence set MCS (see [Hansen et al. \(2011\)](#)) may not be applicable to investment strategies testing since:
 - it is not robust to multiple testing
 - it requires a very high signal-to-noise ratio to be useful.

Testing investment strategies and portfolios (cont.)

- Kellner and Rosch (2020): Bayesian re-interpretation of “significant” empirical financial research indicate rather weak evidence for inferences made under frequentistic framework
- Testing needs to go beyond simple historical data and regular bootstrap
- Harvey and Liu (2015): enhanced bootstrap for multiple comparisons, need to incorporate fictitious yet plausible market scenarios
- Rebonato (2017) describe engineering challenges for testing framework, to incorporate both ‘*scenario analysis*’ and ‘*stress testing*’.
- MIL can generate such additional scenarios (see Data Augmentation)
- Denev and Angelini (2016), Denev et al. (2018): Probabilistic Graphical Models can capture interconnectedness within a stress testing context
- Gao et al. (2018): combination of probabilistic causation and MIL can simulate stress testing scenarios with higher accuracy and lower computational complexity than Monte Carlo simulations.

Testing investment strategies and portfolios (cont.)

- **Arnott et al. (2019):** Backtesting Protocol in the Era of Machine Learning
 - avoid HARKing (Hypothesizing After Results are Known)
 - be aware of multiple testing problem
 - be aware of data integrity
 - outlier exclusions and data transformations set in advance
 - results robust to minor changes in transformations
 - be honest with cross-validation
 - avoid modifying in-sample model to fit OOS data
 - ensure OOS analysis is representative of live trading
 - ensure realistic market frictions such as transactions costs
 - awareness of model dynamics
 - model has to be robust to structural changes
 - minimize model overfitting and tweaking based on live results
 - minimize practical risks such as overcrowding
 - avoid complexity
 - use simplest yet practicable model
 - be able to explain results
 - need to have a scientific research culture
 - reward good processes, not good results
 - are results inconsistent with other research?

Factor-based investment strategies

- Traditional (linear) risk factor models may miss (partially or entirely) key features due to model misspecification
- **MIL** very good at identifying patterns in a high dimensional space
- These patterns associate features (factors) with outcomes
- While nature of relationships can be quite complex, primary focus of analysis can be geared towards finding most important features
- **MIL** will always find patterns, even if none or minimal in reality
- Likelihood of overfitting is high, due to small ratio of size of samples (returns) relative to the number of potential factors.
- To avoid “data mining” (spurious relationships that fail to generalize out of sample) **MIL** has to be paired with economic intuition and financial knowledge

Factor-based investment strategies (cont.)

- Typically two types of methods to identify return predictors:
 - (conditional) portfolio sorts based on one or multiple characteristics, such as size or book-to-market
 - linear regression (panel data or in spirit of Fama-MacBeth)
- **MIL** found to significantly improve selection process, since
 - Portfolio sorts subject to curse of dimensionality
 - linear regressions, as strong functional-form assumptions, are sensitive to outliers
 - **MIL** accommodates many more potential predictor variables
 - **MIL** accommodates richer specifications (e.g. nonlinear)
- Need to identify most relevant features (known as risk factors) and to analyze whether a new factor adds explanatory power
- Feature selection FS is an essential component for **MIL**

Factor-based investment strategies (cont.)

- FS methods aim at ranking and selecting a subset of relevant features according to their degrees of relevance, preference, or importance.
- Feng et al. (2020), Chernozhukov et al. (2015): conventional MIL variable selection techniques need to be augmented to explicitly account for model-selection mistakes (like omitted variables)
- Feng et al. (2020): procedure selects factors that are useful in
 - explaining the cross section of expected returns
 - mitigating the omitted variable bias problem
- Freyberger et al. (2020): use group LASSO to
 - find which characteristics have incremental predictive power for expected returns, given the other characteristics.
 - estimate effect of important characteristics on expected returns without imposing a strong functional form.

Factor-based investment strategies (cont.)

Table 4: Output of selection procedures based on augmented ML

Results	Article
14 out of 99	Feng et al. (2017)
13 out of 62	Freyberger et al. (2018)
14 out of 68	Messmer and Audrino (2017)

- [Feng et al. \(2018\)](#): consider empirical asset pricing problem from perspective of finding alphas in large panel datasets of return with a view to measuring investment performance, as described in [Harvey and Liu \(2019\)](#), [Harvey and Liu \(2018\)](#)
- From this perspective, empirical asset pricing can be recasted into a different solution: searching for a dimension-reduction model from thousands of securities, which is then done through deep learning
- With better measurement through machine learning, risk premia becomes less shrouded in estimation error

Factor-based investment strategies (cont.)

- Factor-based investment strategies particularly suited for MIL , because:
 - measurement of asset's risk premium is in fact prediction
 - large number of candidate conditioning variables for risk premium
 - nonlinearity is likely necessary
 - analysis is required to determine most appropriate functional form of risk factor model
- Gu et al. (2020): comparative analysis of MIL for measuring asset risk premia
- Freyberger et al. (2020): nonlinearities are important; with same set of 11 factors selected by nonlinear model, MIL has out-of-sample Sharpe ratio SR three times larger compared to a linear model
- Feng et al. (2018): predictability of returns explained by nonlinear factors
- Fan et al. (2017): connection between sufficient factor forecasting and deep learning

Additional applications of ML in QWIM

- Kakushadze and Yu (2020): ML to extract factors underlying Treasury yields
- Kakushadze and Yu (2020): LSTM and TCN outperforms analysts in prediction of future earnings per share (EPS)
- Hou et al. (2020): LSTM-DNN hybrid model to integrate company fundamentals information into time-series forecasting
- Gotze et al. (2020): ML improves catastrophe CAT bond pricing models
- Bolhuis and Rayner (2020): nowcast/forecast macroeconomic variables
- Abouseir et al. (2020): ML allows to better integrate macroeconomic data into multi-asset allocation
- Jaeger et al. (2020): use "explainable AI" to compare robustness of diversification strategies in asset allocation, and to extract explanations
- Koshiyama et al. (2020): review of AI and ML, their computational strengths and weaknesses, and their future impact on Capital Markets
- Downey (2020): ensemble ML to predict company fundamentals: earnings, free cash flow, EBITDA, Net Operating Profit After Taxes.

Additional applications of MIL in QWIM (cont.)

- Nunes et al. (2020): bond yield forecasting using LSTM-LagLasso
- Li et al. (2020b): practitioner framework for implementation and interpretation of MIL model predictions applied to investment portfolios.
- Model predictions are decomposed into linear, nonlinear, and interaction components, and evaluated using these components.
- It is shown that MIL models reliably identify known effects and find new nonlinear relationships and interactions.
- Vrontos et al. (2021), Yazdani (2020): MIL prediction of recessions
- Li and Zhang (2020): unified model for detecting, classifying and summarizing financial events
- Wolff and Echterling (2020), Borghi and Rossi (2020): MIL for stock selection and for constructing a multifactor alpha model

Additional applications of MIL in QWIM (cont.)

- Boudt et al. (2020): MIL applied to tactical asset allocation
- Abouseir et al. (2020): integration of macroeconomic data into multi-asset allocation using MIL
- Bolhuis and Rayner (2020): MIL to nowcast (and forecast) (macro)economic variables
- Li and Zhang (2020): unified model for detecting, classifying and summarizing financial events
- Nunes et al. (2020): use learned representations from DNN networks to augment covariance estimation and to create tailored representations best suited to meeting varying financial objectives
- Zhou (2020): use graphical models for portfolio allocation
- Kilburn (2019a), Fornaro and Luomaranta (2020), Monokroussos and Zhao (2020), Babii et al. (2020): MIL for nowcasting

Lessons from COVID-19 pandemic

- For many reasons, 2020 is an exceptional year.
 - COVID-19 virus has shown how vulnerable world is to a pandemic
 - “whatever-it-takes” response from central banks fastest ever seen
 - reminder that the highly unlikely is not the same as impossible, and the highly likely not same as certain
- Pinson and Makridakis (2021), Ioannidis et al. (2020), Taleb et al. (2021): significant challenges remain to deliver “good enough” forecasting methodologies
- Procacci et al. (2020), Cheng (2020): US market structure has dramatically changed during COVID outbreak, while volatility markets underreacted
- Harvey et al. (2020a): strategic risk management useful in market selloff
- Billio and Varotto (2020): economic impact and likely market consequences
- Cepoi (2020): asymmetric dependence between stock market returns and news during COVID-19 financial turmoil
- Lyócsa et al. (2020), Lyócsa and Molnár (2020), Salisu and Akanni (2020), Liu et al. (2020): role of fear and uncertainty in financial markets

Lessons from COVID-19 pandemic (cont.)

- Lipton and Lopez de Prado (2020b), Lipton and Lopez de Prado (2020a): convincing case for more nowcasting, less backtesting (or rather enhanced testing), and strategies that adapt to new regimes
- Nowcasting is becoming much more feasible due to combination of vastly larger amount of available data with MIL advances
- Their list of recommendations includes
 - incorporate short-term ‘nowcasting’
 - backtesting part of validation process, not of research process
 - need for analysis and methods (such as causal MIL, discussed later) towards a stronger link between cause and effect
 - rather than using “all-weather” investment strategies, identify investment strategies that perform well under defined market regimes
- Regime-based investing was already discussed
- Lopez de Prado (2020c): tactical investment algorithms TIAs

Lessons from COVID-19 pandemic (cont.)

- Lopez de Prado (2020c) described a process to construct TIAs
 - define each regime using a particular data-generating process
 - nowcast the probability that current observations are being drawn from each process
 - use those probabilities to build an ensemble portfolio of those optimal strategies
- As these probabilities shift from one data-generating process to another over time, the ensemble portfolio is dynamically adjusted and adapts to prevailing market conditions.
- Lipton and Lopez de Prado (2020b): During coronavirus sell-off, ensemble portfolio could have reduced allocations to models optimised for economic expansions and increased allocations to models optimised for economic recessions and market turmoil.

ML in QWIM: practical challenges

Main challenges

- Challenges due to data [Assefa et al. \(2019\)](#), [Buehler et al. \(2020a\)](#)
 - insufficient data and/or somewhat poor data quality
 - need to satisfy privacy, fairness and regulatory requirements
- Financial datasets have distinctive stylized features [Cont et al. \(1997\)](#), [Cont \(2001\)](#), [Kristoufek \(2018\)](#), [Jilla et al. \(2017\)](#)
- Model overfitting and data mining risks higher for **MIL** (when used inappropriately)
- Standard **MIL** may not be “good enough” for financial time series
- Need to incorporate causality into **MIL**
- Stakeholders and regulators require significant levels of interpretability and/or explainability for **MIL**
- Tuning **MIL** hyperparameters needs to be robust with respect to stylized features of financial time series (such as market regimes)
- Training and testing datasets needs to be representative of realistic investment and trading conditions (including stress periods)

Challenge: insufficient data

- Not having sufficient data (due to medium to low sampling frequency and/or limited historical data) will have an impact on
 - adequately training ML models
 - tackling unbalanced datasets
 - data anonymization and preserving of data privacy
 - comprehensive testing of investment strategies and portfolios
 - robust portfolio construction
 - portfolio risk management
- Synthetic data can be obtained through
 - ML-based data augmentation **DAug**
 - data similarity with data in other time periods
 - combine observations with expert views
 - scenario generation
 - construction of stress scenarios
 - agent based modeling

Methods to generate synthetic data

- Methods to deliver consistent and realistic synthetic data include
 - ▶ **MIL**-based data augmentation **DAug** (discussed in previous section)
 - ▶ time similarity with data in other periods: Marrs (2019), Bai et al. (2019), Echihabi et al. (2018), Kang et al. (2019), Madan and Schoutens (2018), Munnix et al. (2014), Sidi (2020), Yan et al. (2019), Yaros and Imielinski (2015), and Yeh (2020), Paparrizos et al. (2020), Zhu et al. (2020), Suarez et al. (2020), Mishra et al. (2020), Li et al. (2020c), Zhang et al. (2020c), Ontanon (2020), Costa et al. (2020), Edelmann et al. (2019)
 - ▶ combine observations with expert views: Czasonis et al. (2020), Davis and Lleo (2016), Meucci (2009), Yu et al. (2020), Rosen and Saunders (2016), Rosen (2015b), Yu et al. (2014), Kolm and Ritter (2020a)
 - ▶ agent based modeling: Raman et al. (2019), Haldane and Turrell (2018), Beikirch et al. (2018), Bouchaud (2018), Chakrabarti et al. (2019), Mizuta (2019), Lamperti et al. (2018), Lussange et al. (2020), Cramer and Trimborn (2019), Angione et al. (2020), Raman and Leidner (2019), Byrd (2019), Dahlke et al. (2020), Zhang et al. (2020b), Tran et al. (2020), Shiono (2020), Fievet and Sornette (2018)
 - ▶ scenario generation (relevant references on next slide)
 - ▶ construction of stress scenarios (relevant references on next slide)

Methods to generate synthetic data (cont.)

- Methods to deliver consistent and realistic synthetic data also include
 - scenario generation (including factor-based and reduced form modeling): Golub et al. (2018), Dunkler et al. (2014), Engle and Roussellet (2016), Buehler et al. (2020b), Buehler et al. (2020a), Czasonis et al. (2020), Iwana and Uchida (2020), Kondratyev and Schwarz (2020), Yoon (2020), Kaut (2020), Fox and Jha (2019), Hazarika et al. (2020), Waller (2020), Lam and Li (2020), Seib et al. (2020), Kang et al. (2020), Oh et al. (2020), Kondratyev et al. (2020), Ni et al. (2020b), Koochali et al. (2020), Pesenti et al. (2020), Ponomareva et al. (2015), Rosen (2015a), Sironi (2015), Tang et al. (2018), van Beek (2020), Facchinato and Pola (2014), Gosling (2010), Kaut and Lium (2015), Kegel et al. (2017), Liu (2015)
 - construction of stress scenarios: Glasserman et al. (2015), Kopeliovich et al. (2015), Grundke (2012), Rosen and Saunders (2016), Skoglund (2019), Rebonato (2018), Bilgili et al. (2017), Denev and Mutnikas (2016b), Ardia and Meucci (2015), Flood and Korenko (2015), Meucci (2012), Overbeck (2012), Siddique et al. (2019), Traccucci et al. (2019), Ruenzi et al. (2020), Baes and Schaanning (2020), Engle (2020), Cohort et al. (2020), Breuer and Summer (2020), Albanese et al. (2020), Aste (2020), Pesenti et al. (2020), Pesenti et al. (2019)

Challenge: incorporate causality in ML

- When humans rationalize the world, we often think in terms of cause and effect. Causal inference is a statistical tool for ML that enables analysis of ML along the same lines.
- Knight (2019): interview with Yoshua Bengio: *"It's a big thing to integrate [causality] into AI. Current approaches to ML assume that the trained AI system will be applied on the same kind of data as the training data. In real life it is often not the case"*.
- Jacob et al. (2020a), Cui et al. (2020), Guo et al. (2020a): surveys of both traditional and frontier methods in learning causality and connections between causality and ML
- Yao et al. (2020b), Moraffah et al. (2020): reviews of causal inference methods under potential outcome framework, and of causal interpretable models (aiming to answer causal questions)
- Mastakouri et al. (2020): identify direct and indirect causes on time series and provide necessary and sufficient conditions in presence of latent variables

Challenge: incorporate causality in MIL (cont.)

- Gnecco et al. (2020), Pearl and Mackenzie (2018), Pearl (2019): tools of causal inference
- Baldi and Shahbaba (2020): causality within Bayesian statistical framework
- Wang et al. (2020b), Huang et al. (2020a), Wong (2020), Chen et al. (2020b): methods and implementations for causal MIL
- Huang et al. (2020b), da Costa and Dasgupta (2020), Saggioro et al. (2020): detect causal relationships identified from time series
- Little and Badawy (2020): causal bootstrapping to resample observational data such that, if an interventional relationship is identified from that data, new data representing that relationship can be simulated
- Based on such resampled data, MIL-based forecasting is both statistically powerful and causally robust
- Lowe et al. (2020): Amortized Causal Discovery leverages shared dynamics to learn to infer causal relations from time-series data.
- Parafita and Vitria (2020): causal inference using Deep Causal Graphs

Challenge: interpretability and explainability

- Question: *If a machine learning model performs well, why not just trust the model and ignore why it made a certain decision?*
- Kilburn (2020a): based on survey of practitioners, this question becomes especially relevant when using ML in QWIM
- Stakeholders and regulators require significant levels of interpretability and/or explainability for ML in QWIM
- Explainability and interpretability are often used interchangeably, although they are not similar
- Zhou (2019): *interpretability* (describing HOW ML arrived at its conclusions) versus *explainability* (answering WHY)
- Molnar (2020a), Choi (2020), Samek et al. (2020), Stewart (2020), Kim (2019), Biecek and Burzykowski (2021), Doshi-Velez and Kim (2017): surveys and methods for ML interpretability
- Molnar et al. (2020): pitfalls to avoid when interpreting ML

Interpretability

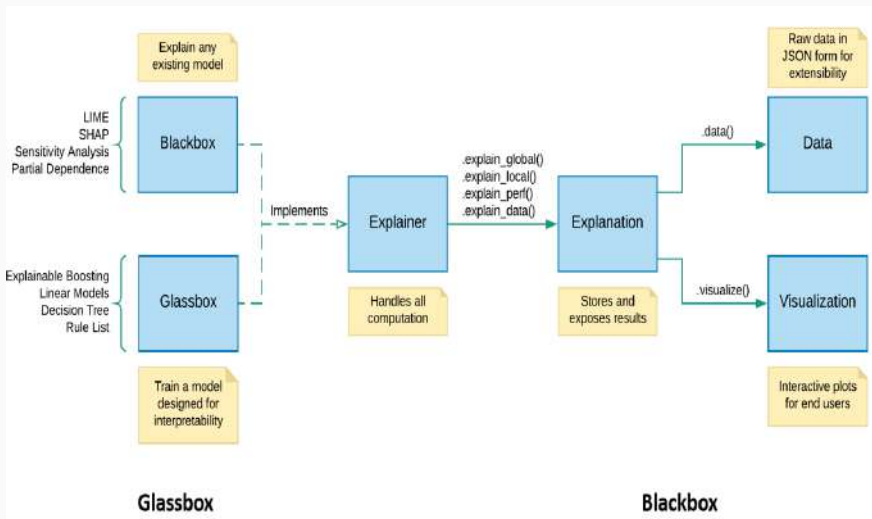
- Molnar (2020b): Methods to quantify interpretability:
 - Model-agnostic methods
 - Global and Local surrogate models
 - Feature importance and interaction
 - Individual Conditional Expectations
 - Shapley Additive exPlanations SHAP
 - Scoped rules (anchors)
 - Partial Dependence Plot PDP
 - Accumulated Local Effects Plot ALEP
 - Merging Path Plot MPP
 - Break Down Plot BDP
 - Permutational Variable Importance Plot PVIP
 - Cateris Paribus Plot CPP
 - Example-based explanations
 - Counterfactual explanations
 - Adversarial examples
 - Prototypes and criticisms
 - Influential instances
- Hall (2020): comprehensive list of resources on interpretability

Interpretability (cont.)

- [Ribeiro et al. \(2016a\)](#), [Ribeiro et al. \(2016b\)](#): LIME (“Local Interpretable Model-Agnostic Explanations”) used to fit local surrogate models:
 - Choose instance of interest for which to have an explanation
 - Perturb dataset and get black box predictions for these new points.
 - Weight new samples by their proximity to instance of interest.
 - Fit weighted, interpretable model on dataset with variations.
 - Explain prediction by interpreting the local model.
- [Ribeiro et al. \(2018\)](#): “Anchors” to address LIME weaknesses
 - Inability to know how widely one can apply a “local” explanation
 - Dependence on assumptions of linearity
 - Dependence on rather vague concepts of closeness/distance
- [Ribeiro et al. \(2018\)](#): further enhancements “bLIMEy” and “LIMEtree”
- [Linden et al. \(2019\)](#): argue that global importance introduced by LIME does not reliably represent the model’s global behavior, and introduce Global Aggregations of Local Explanations (GALE)

Software packages for interpretability

- While there are many such packages, we mention two software suites which have proven quite powerful: InterpretML and DALEX
- **Nori et al. (2019)**: InterpretML uses glassbox and blackbox

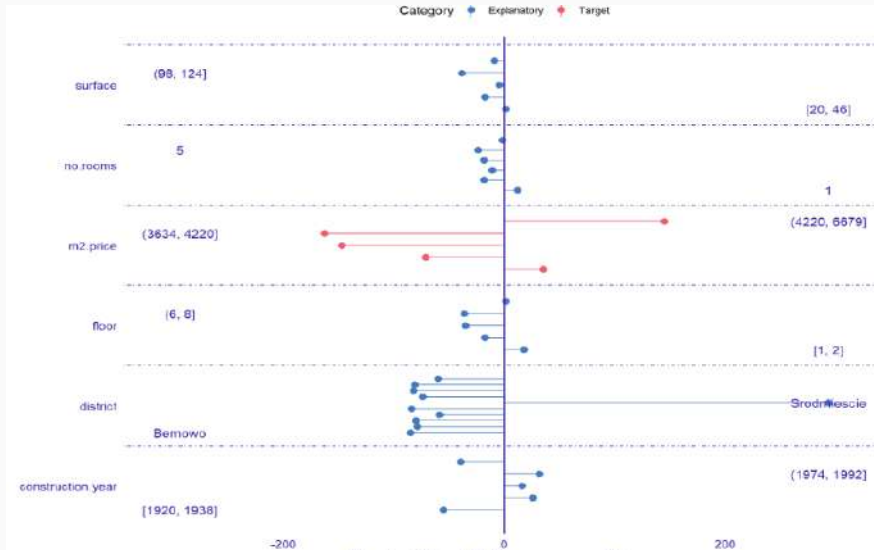


Source: **Nori et al. (2019)**

Software packages for interpretability (cont.)

- Biecek and Burzykowski (2021), Biecek (2018): Descriptive mACHine Learning EXplanations DALEX suite

Figure 2: Champion (left) vs. Challenger (right)



Source: Biecek and Maksymiuk (2019)

Explainability

- According to DARPA, eXplainable artificial intelligence \mathbb{XAI} aims to *“produce more explainable models, while maintaining a high level of learning performance (prediction accuracy); and enable human users to understand, appropriately, trust, and effectively manage the emerging generation of artificially intelligent partners”*
- Biecek and Burzykowski (2021), Choi (2020), Caruana et al. (2020), Ignatiev (2020), Adadi and Berrada (2018), Danilevsky et al. (2020), Camburu (2020), Dosilovic et al. (2018), Samek et al. (2019), Arya et al. (2020), Heuillet et al. (2020), Xie et al. (2020), Puiutta and Veith (2020): surveys on current state-of-the-art, developments, and challenges for \mathbb{XAI} , including \mathbb{XDL} (explainable deep learning) and \mathbb{XRL} (explainable reinforcement learning)
- Arrieta et al. (2019): concept of Responsible Artificial Intelligence for large-scale implementation of \mathbb{AI} organizations with fairness, model explainability and accountability at its core
- Schneider and Handali (2019): concept of personalized explanation in \mathbb{XAI} based on three key explanation properties: complexity, decision information and presentations

Explainability (cont.)

- Spinner et al. (2020), Choo and Liu (2018), Samek et al. (2017), Zhang and Zhu (2018): visual analytics and information visualization within context of XAI
- Horel and Giesecke (2020), Horel and Giesecke (2018), Horel and Giesecke (2019): computationally efficient significance tests for MIL features and feature interactions of any order in a hierarchical manner; generates a model-free notion of feature importance
- Horel et al. (2019): XML applied to wealth management compliance
- Roscher et al. (2020) : survey on XML combined with domain knowledge
- Chen et al. (2020c): significance, relevance and explainability for MIL, from econometrics and financial data science perspectives
- Chen et al. (2020c) and Hoepner et al. (2021): practitioner framework for Adaptive Explainable Neural Networks within context of quantitative finance

Explainability (cont.)

- Virgolin et al. (2019), Udrescu et al. (2020), Udrescu and Tegmark (2020): symbolic regression can improve ML explainability
- Marcinkevics and Vogt (2020): emphasise divide between interpretability and explainability and illustrate these two different research directions with concrete examples of state-of-the-art.
- Spinner et al. (2020): framework for interactive XAI to allow users to
 - understand ML models
 - diagnose model limitations using different XAI methods
 - refine and optimize the models
- Framework combines iterative XAI pipeline with eight global monitoring and steering mechanisms, including quality monitoring, provenance tracking, model comparison, and trust building

Challenge: fairness, bias, and data privacy

- Miresghallah et al. (2020), De Cristofaro (2020): review of data privacy challenges and possible countermeasures
- Rodriguez-Barroso et al. (2020), Triastcyn and Faltings (2020), Shen et al. (2021) Ntoutsis et al. (2020): methodologies and software tools for preserving data privacy
- Term “bias” is used in conjunction with ML in many different contexts, and with many different meanings
- Hellstrom et al. (2020), Ntoutsis et al. (2020): taxonomy and analysis of how different types of biases are connected and depend on each other
- Saleiro et al. (2020): mitigation frameworks for bias and fairness when building and deploying data science systems
- Sharma et al. (2019): CERTIFAI - Counterfactual Explanations for Robustness, Transparency, Interpretability, and Fairness of AI models
- Segal et al. (2020), Dwork et al. (2020), Makhlouf et al. (2020), Oneto and Chiappa (2020), Ruf et al. (2020), del Barrio et al. (2020): concepts, metrics and procedures to assess and ensure fairness in ML

Challenge: tuning hyperparameters

- ML hyperparameters versus parameters
 - ML hyperparameters define model configuration (activation functions, optimization methods, training/testing sets)
 - ML model parameters: learned during model training
- Bakhteev and Strijov (2020), Yu and Zhu (2020), Yang and Shami (2020), Feurer and Hutter (2019): Hyperparameter search can be performed on a predefined grid, via rules-of-thumb, random search, systematic (such as automated ML and multiobjective optimization)
- van Rijn and Hutter (2018): *“Given an algorithm, what are its most important hyperparameters, and what are typically good values for these?”*
- Probst et al. (2019): measuring tunability of hyperparameters
- Nystrup et al. (2020), Feurer and Hutter (2019): systematic hyperparameter tuning delivers better investment portfolios
- Parameters may also be specialized to tasks, such as finding optimal number of clusters: Kawamoto and Kabashima (2017b), Kawamoto and Kabashima (2017a), Riolo et al. (2017)

Challenge: tuning hyperparameters (cont.)

- Bezrukavnikov and Linder (2021), Halvari et al. (2020), Milutinovic et al. (2020), Tuggenier et al. (2019), Hanussek et al. (2020), Zoller and Huber (2020): recent advances in automated hyperparameter search (automated ML)
- Hyperparameter optimization HPO frameworks: HyperOpt, Spearmint, SMAC, Autotune, Vizier, Katib, Tune, Hyperband, GPyOpt
- Various choice of parameter-sampling algorithms: Gaussian processes in Spearmint and GPyOpt, tree-structured Parzen estimator in HyperOpt, random forests in SMAC
- Recent frameworks (Vizier, Katib, Tune) support pruning algorithms, which stop unpromising trials prematurely to speed up the exploration
- Klein et al. (2019): meta-surrogate benchmarking for HPO, to generate inexpensive and realistic scenarios
- Jomaa et al. (2019): HPO as a sequential decision problem (which hyperparameter to test next) solved with reinforcement learning
- Akiba et al. (2019): Optuna: A Next-generation HPO Framework



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