Big Data for Public Policy

3. Machine Learning Essentials

Elliott Ash & Malka Guillot

Where we are

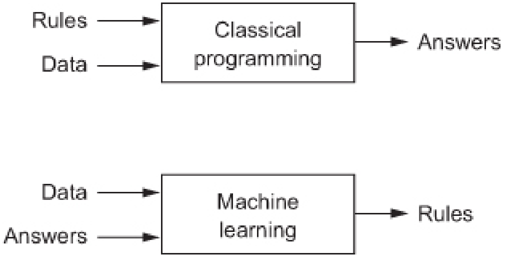
- Past weeks:
  - w1: Overview and motivation
  - w2: Finding datastests using webcrawling and API
- This week (w3): Intro to supervised Machine Learning (ML) - regressions
- Next:
  - w4: Text analysis fundamentals
  - w5: Supervised Machine Learning (ML) - classification
  - w6: Unsupervised Machine Learning (ML)

Today: supervised ML - regressions

- First hour:
  - What is machine learning?
  - Basic steps and concepts
- Second hour:

Application Predicting the prices of houses using given features

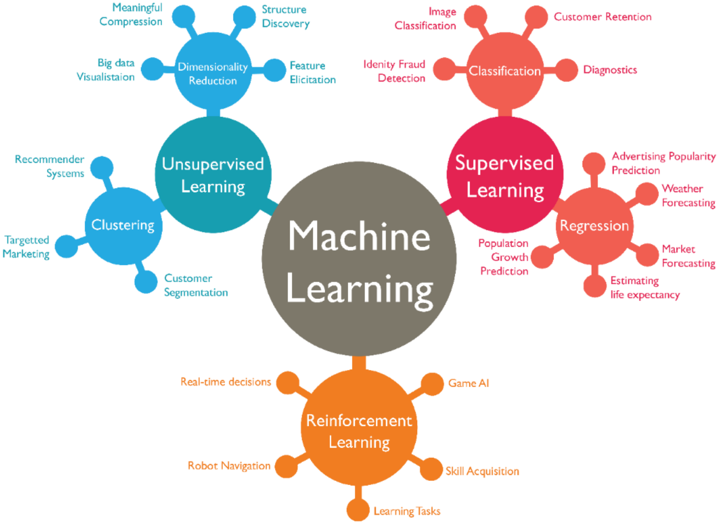
What is machine learning?



- In classical computer programming, humans input the rules and the data, and the computer provides answers.
- In machine learning, humans input the data and the answers, and the computer learns the rules.

$\Longrightarrow$**Machine learning is the science (and art) of programming computers so they can *learn from data*.**

The Machine Learning Landscape



Machine Learning

Usually, ML is diveded in 2 categories:

- the predictive or supervised learning approach
- the descriptive or unsupervised learning approach

Econometrics vs. Machine Learning

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  - goal of estimation: unbiadsedness
  - predicts how outcome y would change if treatment variable x were **exogenously shifted**.
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  - if we collected more data on X, we could predict the associated $\hat{Y}$.
  - but $h(\cdot)$ does not provide a *counterfactual prediction* – that is, how the outcome would change if X's were exogenously shifted.

Example of Applications

- Detect fraud: taxes, social benefits
- Forecasts next year's revenue
- Diagnosis of diseases

Outline

Machine Learning Overview

Overfitting and Regularization

Pipelines and Cross-Validation

Basic Setup

- Suppose we have m observations within a dataset of the form $(y_{i,}, x_i)$ for $i = 1, ..., m$:
  - y_i: dependent /response / label variable
  - x_i: P-dimensional vector of independent variables, covariates or features. Potentially, $P >> N$
- Supervised Learning: Learn a mapping from $x_i$to y_i
  - Classification problem: $y_i$is categorical
  - Regression problem: $y_i$is continuous
- Unsupervised Learning: Learn some structure within the $x_i$observations

What do ML Algorithms do? Minimize a cost function

- A typical cost function for regression problems is Mean Squared Error (MSE):

$$\mathrm{MSE}(X, h) = \frac{1}{m}\sum_{i=1}^{m}(h(x_i) - y_i)^2$$

  - m, the number of rows/observations
  - X, the feature set, with row x_i
  - Y, the outcome, with item y_i
  - $h(x_i)$ the model prediction (hypothesis)

Linear Regression is Machine Learning

- OLS assumes the functional form

$$y_i = x_i'\theta + \epsilon_i$$

and minimizes the MSE

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- This has a closed form solution

$$\hat{\theta} = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{Y}$$

- But
  - this solution does not work well with large *m* and *n*
  - most machine learning models do **not** have a closed form solution.

How do ML Algorithms Work? Gradient Descent

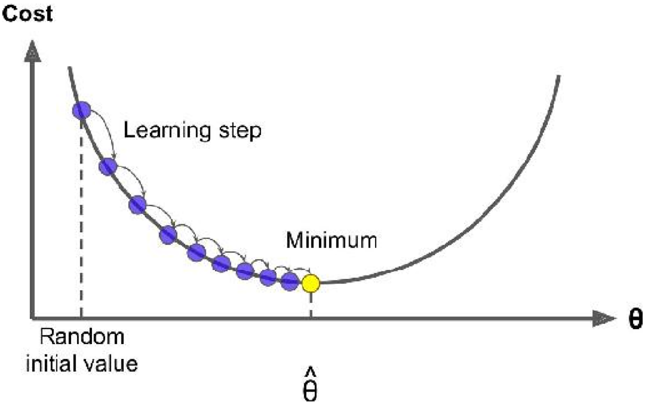

Figure 4-3. Gradient Descent

- Gradient descent measures the local gradient of the error function, and then steps in that direction.
  - Once the gradient equals zero, you have reached a minimum.

Evaluating Algorithms: Cross Validation

Training and Testing

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  - form predictions in 20% test dataset to evaluate performance.

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The Problem of Overfitting

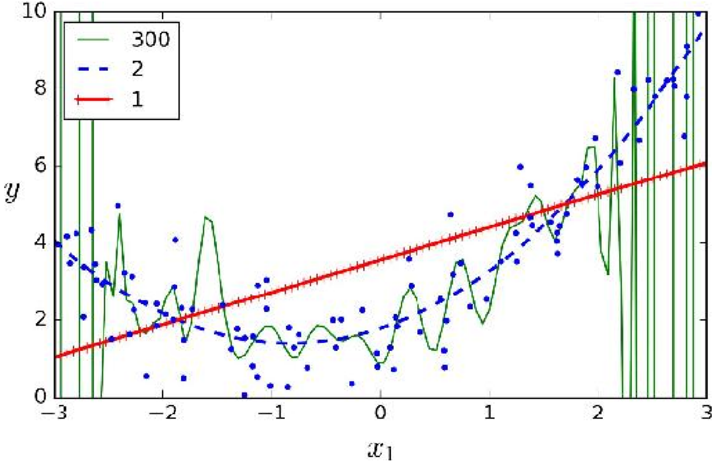

Figure 4-14. High-degree Polynomial Regression

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- *Irreducible error*
  - Error due to noise in the data.

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- If the model is underfitting:
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  - use a more complex model
- If the model is overfitting:
  - adding more training data may help
  - or use regularization
  - cross-validation

Univariate OLS for Ranking Predictive Features

- Consider the univariate regression

$$Y_i = \theta_w x_i^w + \epsilon_i$$

  for each text feature w (e.g., relative word or n-gram frequency).
- Can be estimated with OLS.

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  - Even better, can residualize Y and X on fixed effects before running any regressions.
    - That is, regress $Y_i = \alpha_i + \epsilon_i$ and $x_i^w = \alpha_i + \epsilon_i, \forall w$, take residuals $\tilde{Y}_i = Y_i - \hat{\alpha}_i$ and $\tilde{x}_i^w = x_i^w - \hat{\alpha}_i$

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    - then regress
    $$\tilde{Y}_i = \theta_w \tilde{x}_i^w + \epsilon_i$$
- This can be used for descriptives, and also for feature selection
  - For quick feature selection, can use sklearn's f_regression

Ridge, Lasso, and Elastic Net

- Ridge and lasso regression are tools for dealing with large feature sets where:
  - models have multicollinearity that causes bias
  - models tend to overfit
  - models are computationally costly to fit
- These algorithms work by constraining estimated parameter sizes.

Ridge Regression

- The Ridge cost function is

$$J(\theta) = \mathrm{MSE}(\theta) + \underbrace{\alpha_2 \frac{1}{2} \sum_{i=1}^{n} \theta_i^2}_{\text{Regularization term}}$$

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- Ridge penalizes large coefficients, which reduces over-fitting to the training set.
  - The estimated coefficients, when taken to other data, will generalize better.
- It turns out that the Ridge estimator, like OLS, has a closed-form solution:

$$\hat{\theta}_{\text{Ridge}} = (X'X + \alpha_2 \boldsymbol{I}_n)^{-1} X' \boldsymbol{y}$$

  where $\boldsymbol{I}_n$ is the identity matrix.
  - But it can also be solved by (stochastic) gradient descent.

Lasso Regresison

- *Least Absolute Shrinkage and Selection Operator Regression*
- The Lasso cost function is

$$J(\theta) = \mathrm{MSE}(\theta) + \alpha_1 \sum_{i=1}^{n} |\theta_i|$$

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  - α_1 is a hyperparameter setting the strength of the L1 penalty

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- Lasso automatically performs feature selection and outputs a sparse model.
- It does not have a closed-form solution but can be solved by gradient descent.

Elastic Net

- Elastic Net uses both L1 and L2 penalties:

$$J(\theta) = \mathrm{MSE}(\theta) + \alpha_1 \sum_{i=1}^{n} |\theta_i| + \alpha_2 \frac{1}{2} \sum_{i=1}^{n} \theta_i^2$$

- in general, elastic net is preferred to lasso, which can behave erratically when the number of features is greater than the number of rows, or when some features are highly collinear.
  - but you have to tune two hyperparameters rather than one

Hyperparameters vs. Parameters

- **Parameters**: *internal* to the model whose values can be estimated from the data and we are often trying to estimate them as best as possible
- **hyperparameters**: *external* to the model and cannot be directly learned from the regular training process

$\Rightarrow$ model-specific properties that are *fixed* before the model is trained

Hyperparameters tuning

- Use `GridSearchCV` or `RandomizedSearchCV` to automate search over parameter space.
  - For example: Elastic net hyperparameters should be selected to optimize out-of-sample fit.
  - "Grid search" scans over the hyperparameter space ($\alpha_1 \geq 0$,$\alpha_2 \geq 0$), computes out-of-sample MSE for all pairs (α_1, α_2), and selects the MSE-minimizing model.

Regularized Models Require Standardized Data

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$$\tilde{x}_i = \frac{x_i - \bar{\boldsymbol{x}}}{\mathrm{SD}[\boldsymbol{x}]}$$

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- Taking out the mean will convert sparse data to dense data, you can avoid that by just dividing by the standard deviation:

$$\tilde{x}_i = \frac{x_i}{\mathrm{SD}[\boldsymbol{x}]}$$

  - in sklearn, set `with_mean=False`.

Outline

Data Prep for Machine Learning

- See Geron Chapter 2 for pandas and sklearn syntax:
  - imputing missing values.
  - feature scaling (often helpful/necessary for ML models to work well)
  - encoding categorical variables.
  - see jupyter notebook
- Best practice: **reproducible data pipeline**.

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  - encoding categorical variables.
  - see jupyter notebook
- Best practice: **reproducible data pipeline**.
- **Key point**: all data transformations, feature selection, and hyperparameter tuning must be done **in the training set**.

Cross-Validation

- Use `cross_val_score` method to get model performance across subsets of the training set:
  - split data into K folds.
  - for each fold $k \in \{1, 2, ..., K\}$, train model in rest of data $(-k)$ and evaluate MSE in k.
  - Report mean and s.d. of MSE across folds.

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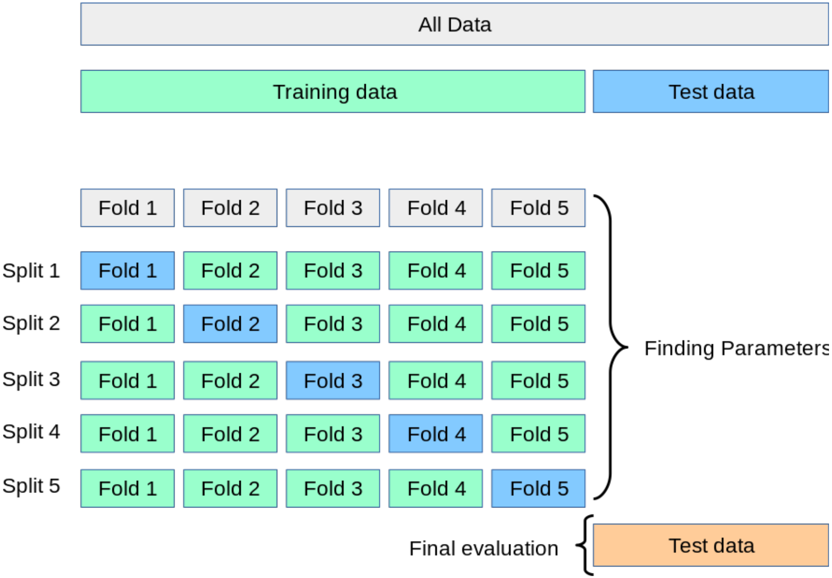
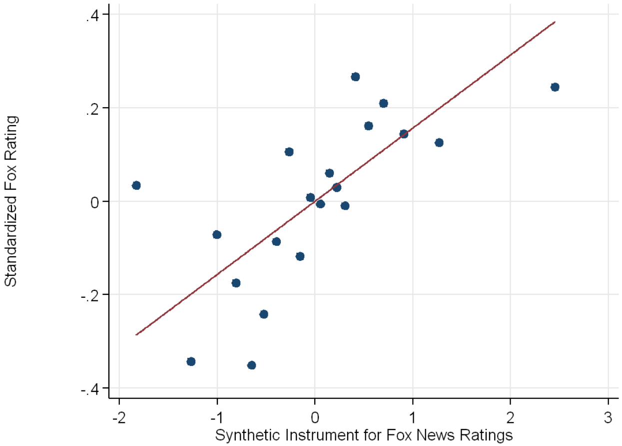


Evaluating Regression Models: R^2

- Mean squared error (MSE) can be used to compare regression models, but the units depend on the outcome variable and therefore are not interpretable.
  - Use R^2 in the test set for a more interpretable evaluation metric.
  - MSE provides same ranking as R^2 and is faster to compute, so it's preferred for model selection.

Evaluating Regression Models: Binscatter Plots

- Binscatters provide visual evidence of regression model performance: Plot Y against $\hat{Y}$ in the test set:



Sample from Ash and Labzina (2019). $R^2 = .03$.

A Machine Learning Project, End-to-End

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5. Select a model and train it.
6. Fine-tune your model:
   6.1 Testing and validating
   6.2 Hyperparameter tuning and model selection.
7. Present your solution.
8. Launch, monitor, and maintain your system.

ML with Python

- Python packages
  - pandas for handling tabular data
  - matplotlib and seaborn for plotting
  - Scikit-Learn (sklearn) for standard (non-deep-learning) ML algorithm
    - scikit-learn is very comprehensive and the online-documentation itself provides a good introducion into ML.
  - TensorFlow, PyTorch and Keras for deep-learning.

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- **Sensible defaults:** Provides reasonable default values for hyperparameters – easy to get a good baseline up and running.