Learning Machine Learning with Kaggle Challenges

(2) Classification

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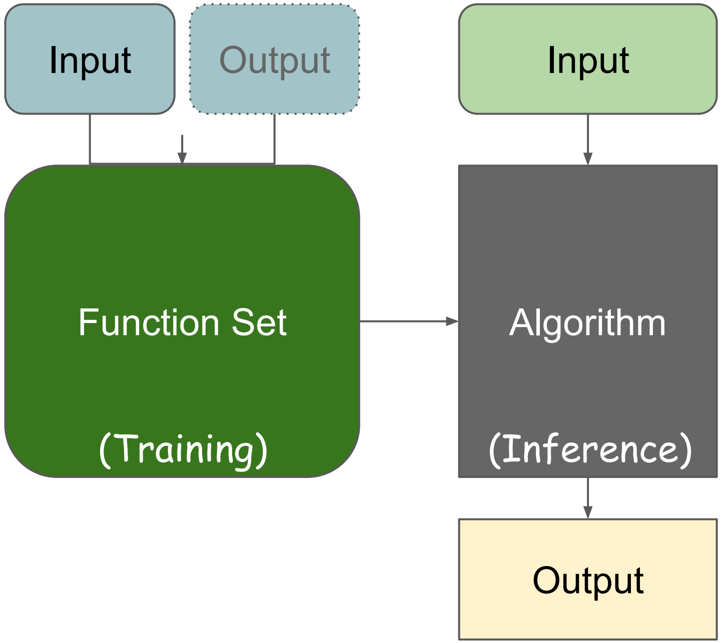
Quick Recap

The Series's Github Repo

https://github.com/huqy/idre_learning_machine_learning

Machine Learning



Before running the colab demos in this series

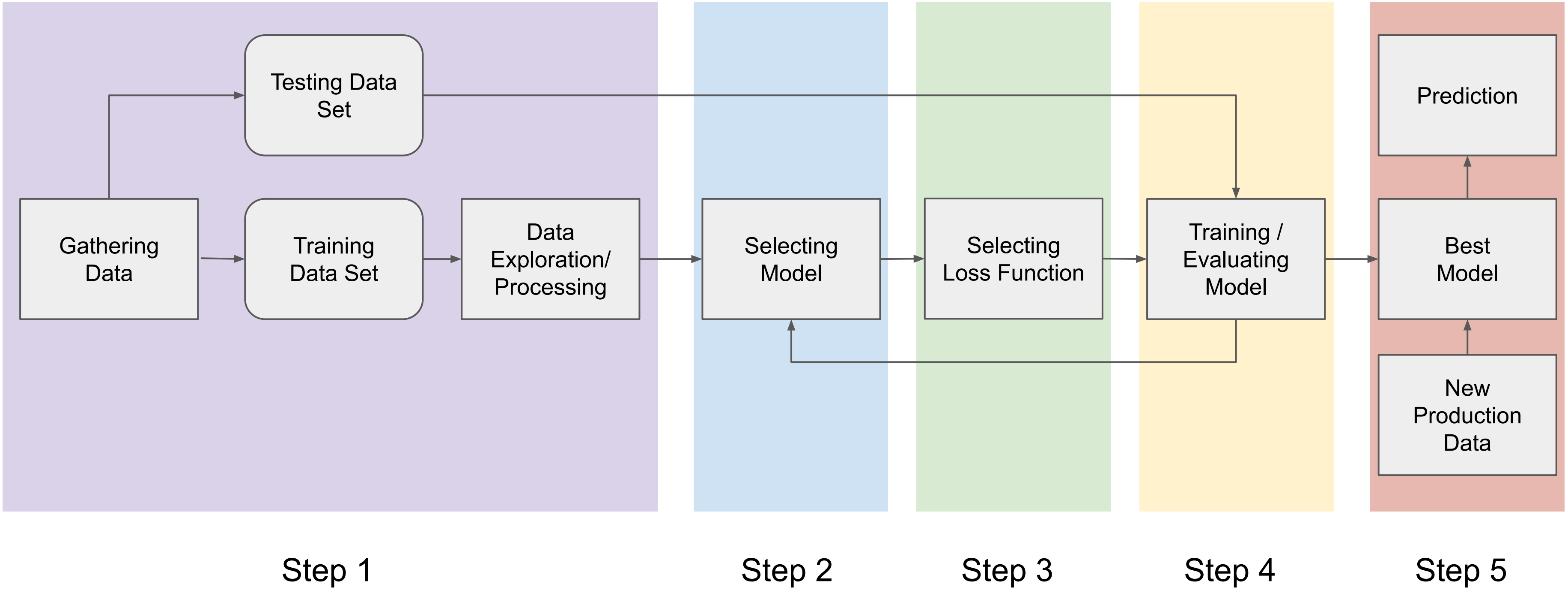
1. Register a Kaggle account
    a. Kaggle.com → "Register"
    b. You can email me your kaggle username so that I can add you to a team for challenges.
2. Create Kaggle API token and download json file
    a. Sign in → Your Profile → "My Account" → "Create New API Token"
3. Join the 2 competitions → "Join Competition"
    a. Titantic Challenge
    b. Dogs-vs-Cats Challenge
4. Get/run the colab files
    a. Just follow the links in the github repo readme page.

Titanic Kaggle Challenge

To predict the survival or the death of a given passenger in Titanic

- Titanic Facts:
  - Survivors
    - 492 passagers
    - 214 crews
  - Victims
    - 832 passagers
    - 685 crews
    - Death causes: drowning, hypothermia, injury, suicide, …
    - [List of deaths](#)

Workflow for a machine learning project



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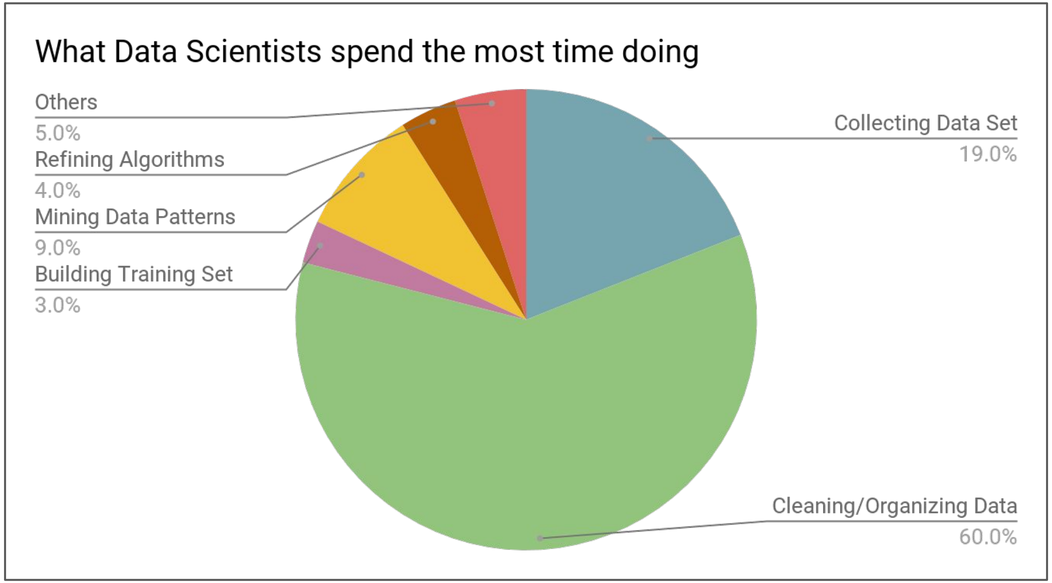
Step 1. Data Prep:

- The most time-consuming but the most creative job
  - Take > 80% time
  - Require experience
  - May need domain expertise
- Determines the upper limit for the goodness of ML
  - Models/Algorithms:
    just approach the upper limit



Survey from Forbes in 2017 (Data Source)

What we will do in Step 1

1. Get the data
2. Know the data (Exploratory Data Analysis)
3. Feature Engineering
4. Feature Selection (use the feature importance property of the model)

In Kaggle's training dataset: 891 passengers, 12 columns (features)

	PassengerId	Survived	Pclass	Name	Sex	Age	SibSp	Parch	Ticket	Fare	Cabin	Embarked
0	1	0	3	Braund, Mr. Owen Harris	male	22.0	1	0	A/5 21171	7.2500	NaN	S
1	2	1	1	Cumings, Mrs. John Bradley (Florence Briggs Th...	female	38.0	1	0	PC 17599	71.2833	C85	C
2	3	1	3	Heikkinen, Miss. Laina	female	26.0	0	0	STON/O2. 3101282	7.9250	NaN	S
3	4	1	1	Futrelle, Mrs. Jacques Heath (Lily May Peel)	female	35.0	1	0	113803	53.1000	C123	S
4	5	0	3	Allen, Mr. William Henry	male	35.0	0	0	373450	8.0500	NaN	S

Feature Engineering

- Transforming raw data into features with a good representation
- Techniques used in our work:
    - Imputation (almost every column)
    - One-hot encoding (embarked, cabin, pclass, ticket, etc)
    - Label binarization (sex)
    - Binning and grouping (family info)
    - Scaling: standardization and normalization (age, fare, family size)
    - Splitting the features (title from name, etc)

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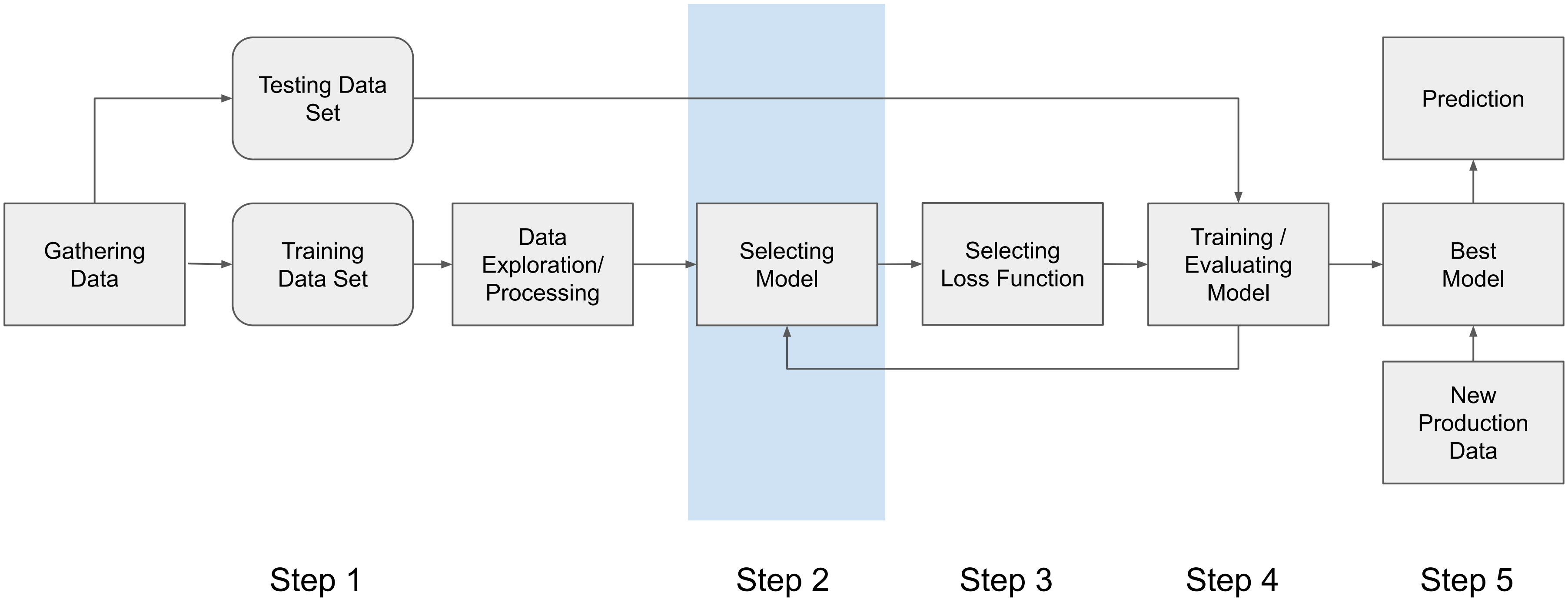

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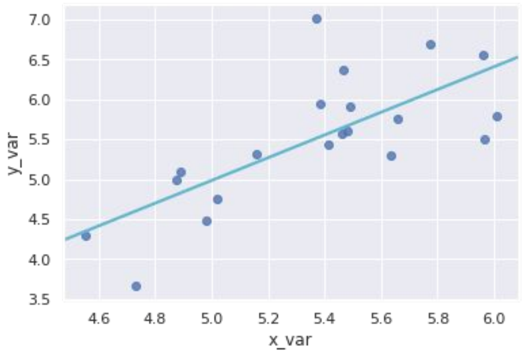
Regression: linear models

- Regression: model output as continuous variable(s)
  - For estimating or predicting a response
  - Real problems: predicting prices, controlling self-driving car, etc.

- Linear Regression:
  - Fitting the data into a straight line $$y = \sum_i w_i x_i + b$$
  - In Scikit learn:
    - sklearn.linear_model.LinearRegression



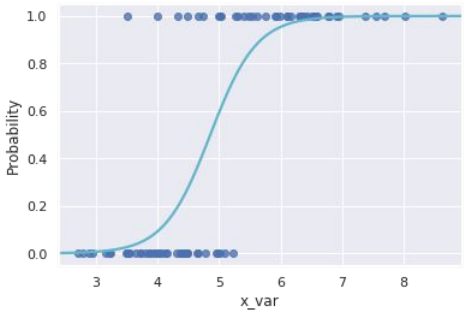
- Polynomial Regression:
  - Treated as linear regression
  - In Scikit Learn:
    - sklearn.preprocessing.PolynomialFeatures
    - sklearn.pipeline.make_pipeline

Classification: linear models from logistic regression

- Classification: model output as discrete variable (class labels)
  - For identifying group membership(s)
  - Examples: handwritten recognition, spam filtering, disease diagnosis
- Logistic Regression:
  - Fitting the data linearly separable
  - Linear model + Sigmoid function

$$y = \sigma(z) = \frac{1}{1 + e^{-z}} = \sigma\left(\sum_i w_i x_i + b\right)$$

  - Scikit Learn:
    - [sklearn.linear_model.LogisticRegression]

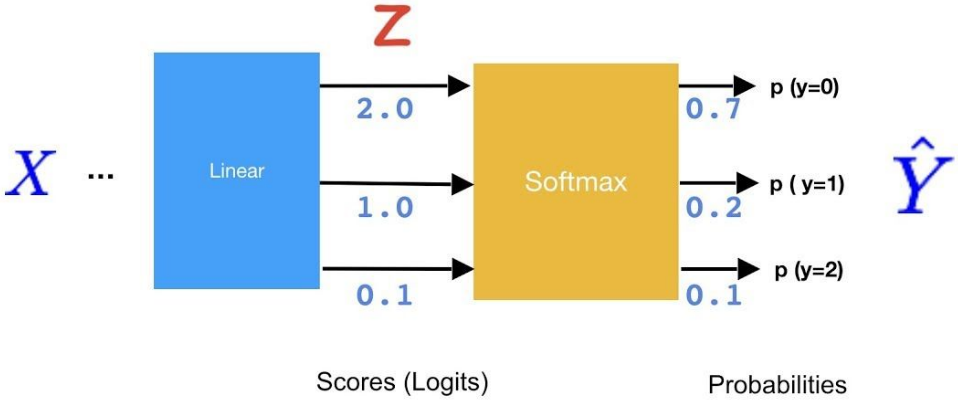


- Binary classification: defining a threshold to map logistic regression
  - Logistic regression give probability

Multi-class Classification

- Multinomial logistic regression (Softmax Regression):
  - Softmax to amplify
  - Different from Sigmoid
  - Mathematically it gives the posterior probabilities that represents a categorical distribution.
  - Commonly used as the last layer in neural networks

$$y_i = \frac{e^{z^{(i)}}}{\sum_{j=0}^{K} e^{z^{(j)}}}$$



Screenshot From the youtube [clip]

Other Classification methods

- Naive Bayes

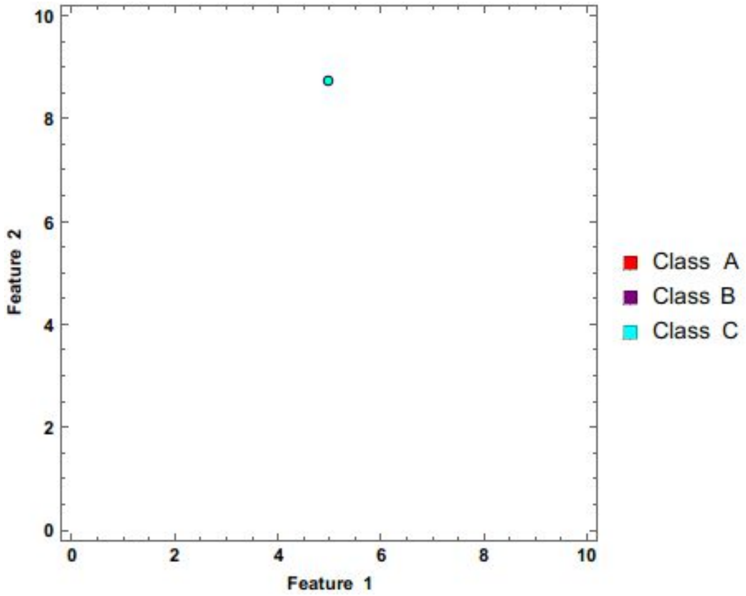


Figure from Wikimedia

- K Nearest Neighbor

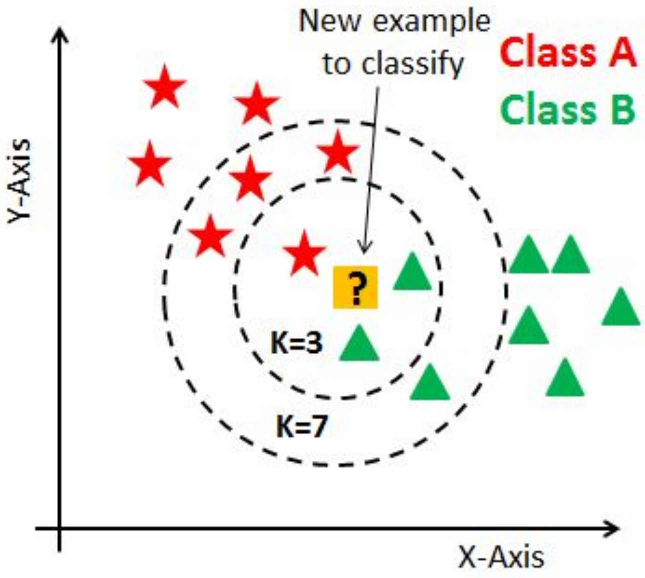


Figure from post

Other Classification methods

- Decision Tree

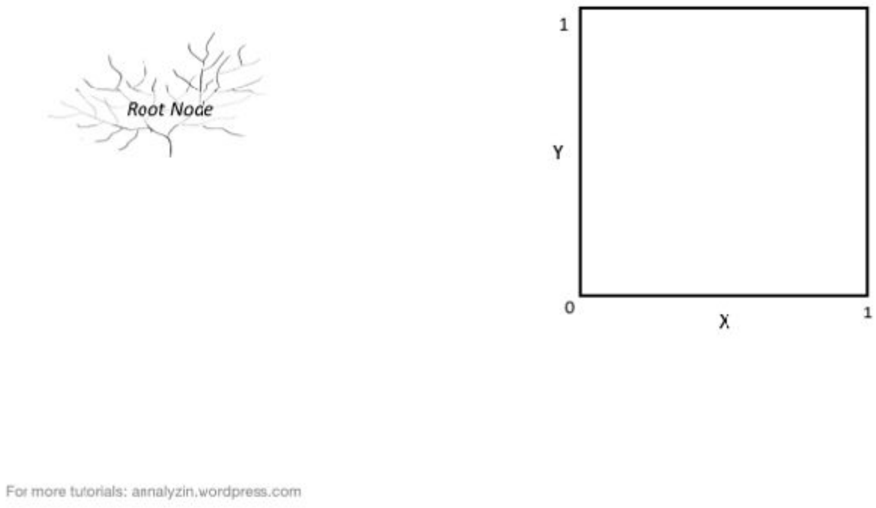


Figure [source]

- Support Vector Machine

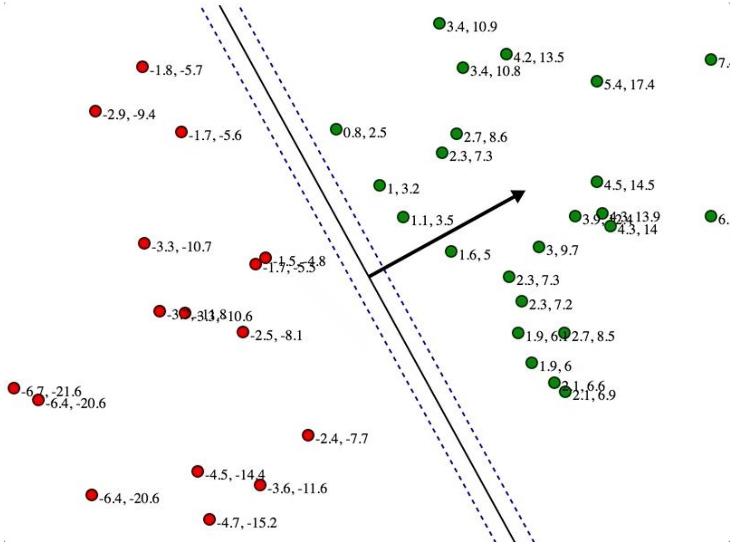


Figure [source]

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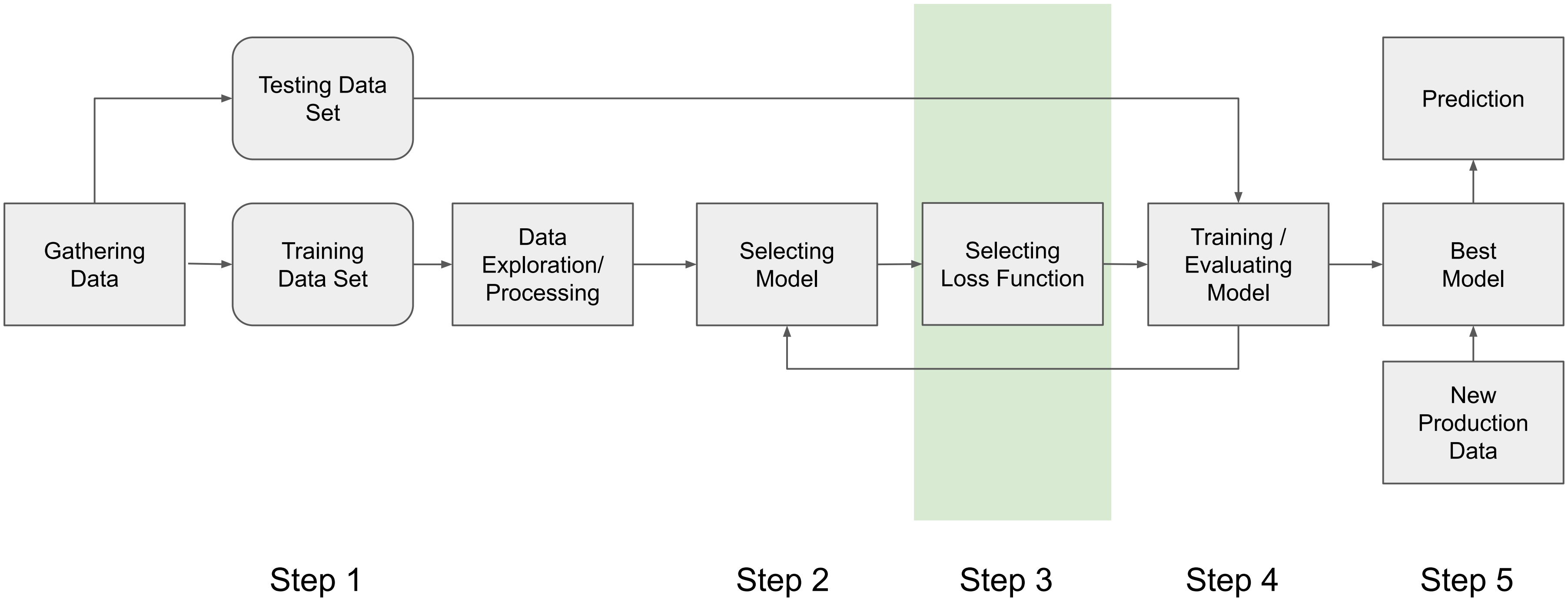

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How to measure the performance of the model?

- General name: objective function

- Measure the misfit of the model as a function of parameters
  - Criterion is to *minimize* the error functions
  - Loss Function: for a single training example
  - Cost Function: over the entire or mini-batch training set

- Evaluate the probability of generating training set
  - Criterion is to *maximize* the distribution likelihood as a function of parameters
  - Maximum (log)-likelihood estimation

- Regression losses and classification losses

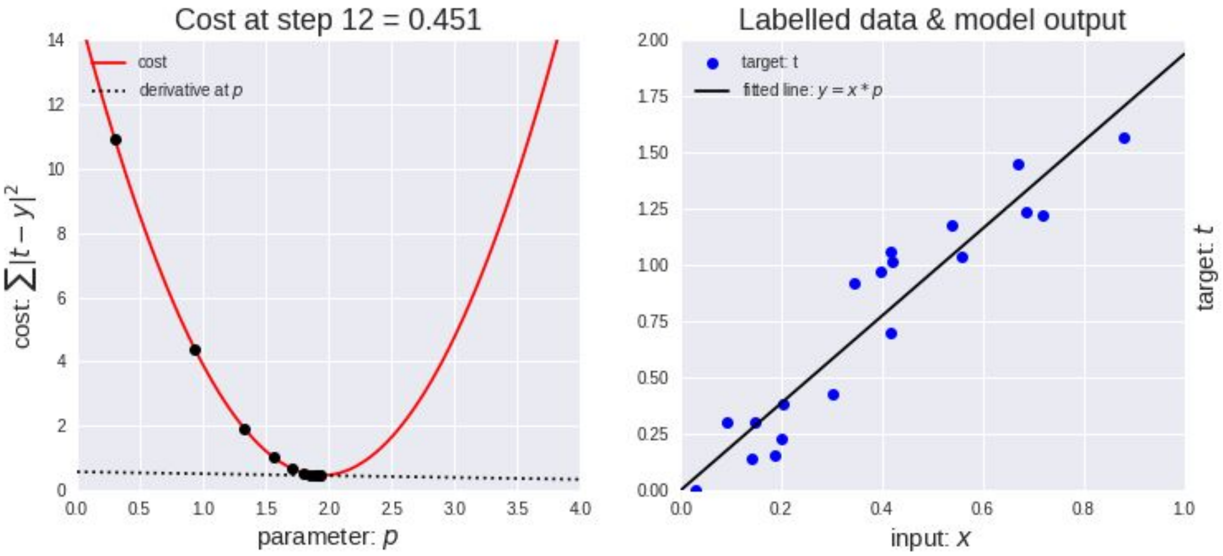
Common loss functions

- Regression Loss
  - Mean Square Error / Quadratic Loss / L2 Loss: $L_{MSE} = \frac{\Sigma_{i=1}^{n}(y_i - \hat{y}_i)^2}{n}$
  - Mean Absolute Error / L1 Loss: $L_{MAE} = \frac{\Sigma_{i=1}^{n}|y_i - \hat{y}_i|}{n}$
- Classification Loss
  - Hinge Loss / Multi class SVM Loss: $L_{Hinge} = \Sigma_{j \neq y_i} \max(0, 1 + s_j - s_{y_i})$
  - Cross Entropy Loss / Log Loss / Negative Log Likelihood:

$$L_{CEL} = -[y_i \log \hat{y}_i + (1 - y_i)\log(1 - \hat{y}_i)]$$

ML Optimization Algorithm

- Gradient Descent (a 1st-order approach) $\theta \longleftarrow \theta - \alpha \nabla J(\theta)$
  - Most popular algorithm
    - Pros: simple and fast
    - Cons: sometimes hard to tune



Source Link

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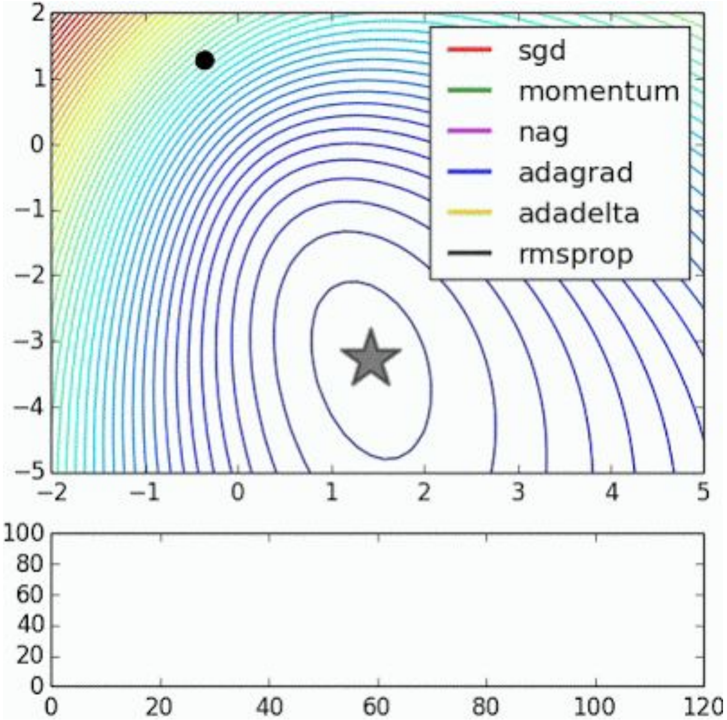
Many Gradient Descent Variations

- Stochastic GD / Mini-Batch GD
- Classical Momentum (CM)
- Nesterov's Accelerated Gradient (NAG)
- AdaGrad
- AdaDelta
- RMSprop (animation source) →
- ADAM (as default in many libs)
- AdaBound/AmsBound (ICLR 2019)



Higher Order Optimization Algorithm

- Newton-like methods (2nd-order methods)

$$\theta \longleftarrow \theta - \frac{\ell'(\theta)}{\ell''(\theta)}$$

  - Prons:
    - Fewer iterations (quadratic convergence)
    - Fewer hyperparameters
  - Cons:
    - Much more **costly** in each iteration
    - Need more storing
  - BFGS/L-BFGS: a quasi-newton one
    - Good for low dimensional models
  - CG (Conjugate gradient)
    - moderately high dimensional models

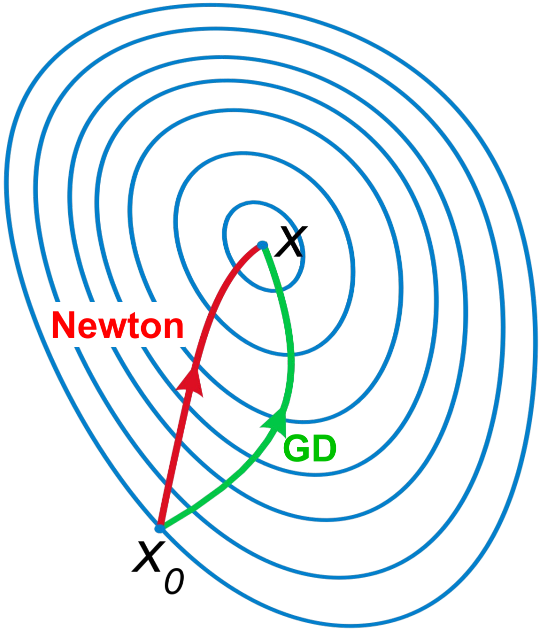


Figure from Wikipedia

Workflow for a machine learning project

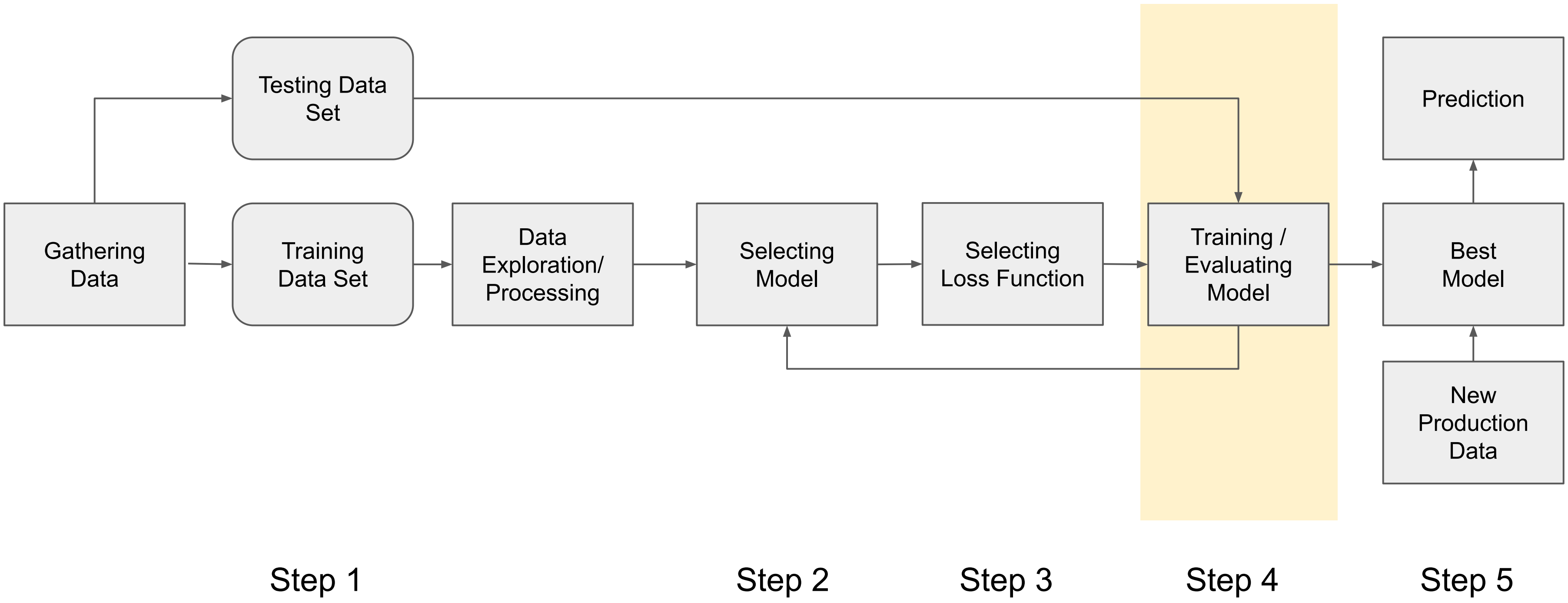


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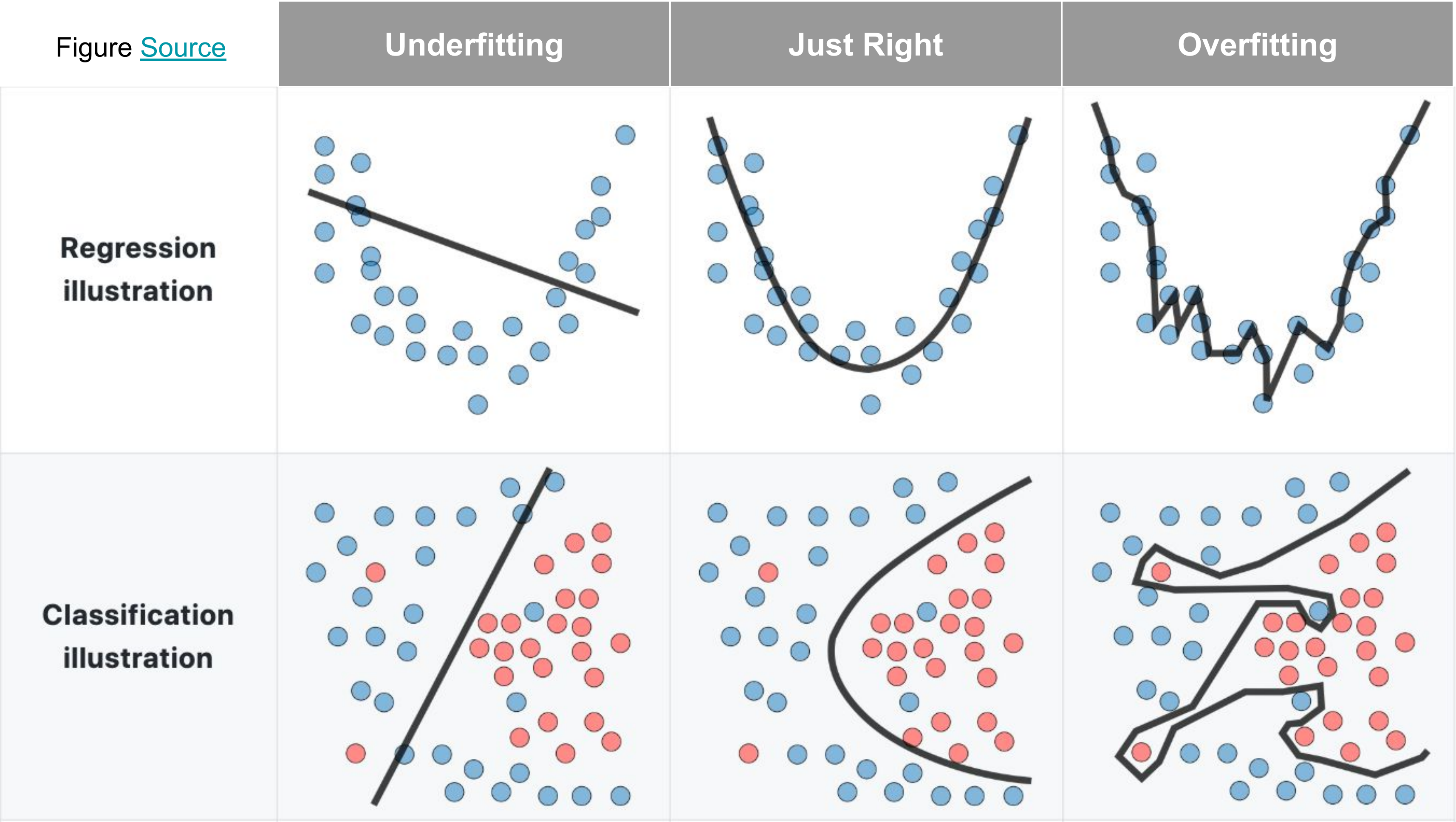
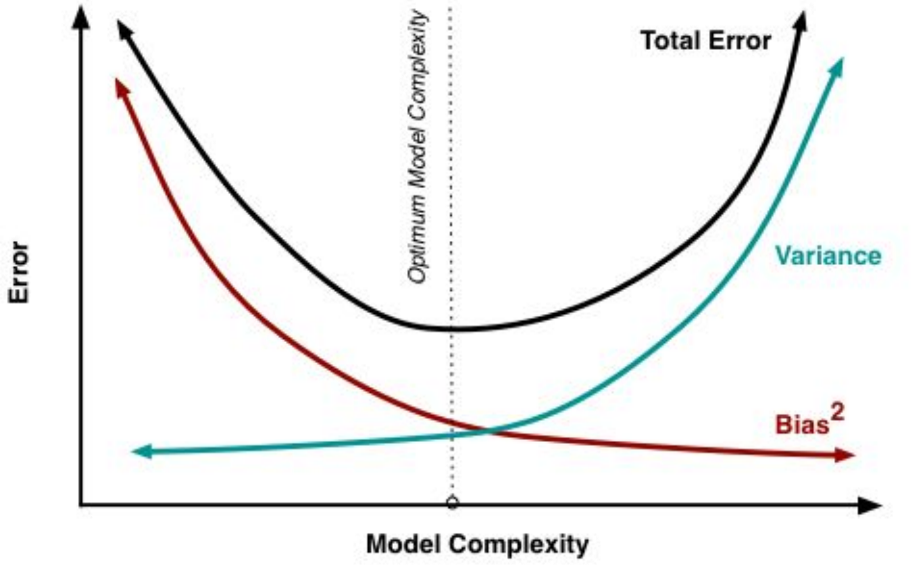
Figure Source



Underfitting and Overfitting

- Underfitting: model too simple:
  - Diagnose:
    - cannot even fit the training data
    - training error ~ testing error
  - Ignore the variance in training data
  - Higher prediction bias

- Overfitting: model too complex
  - Diagnose:
    - well-fit for training data
    - large error for testing data
  - Over-interpret training data
  - More deviation from new data



How to prevent underfitting?

- Redesign the model
- Increase model’s complexity
- Add more features as input
- Training longer
- More data will <u>not</u> help

How to prevent overfitting?

- Get more data
  - Collect more data
  - Data augmentation

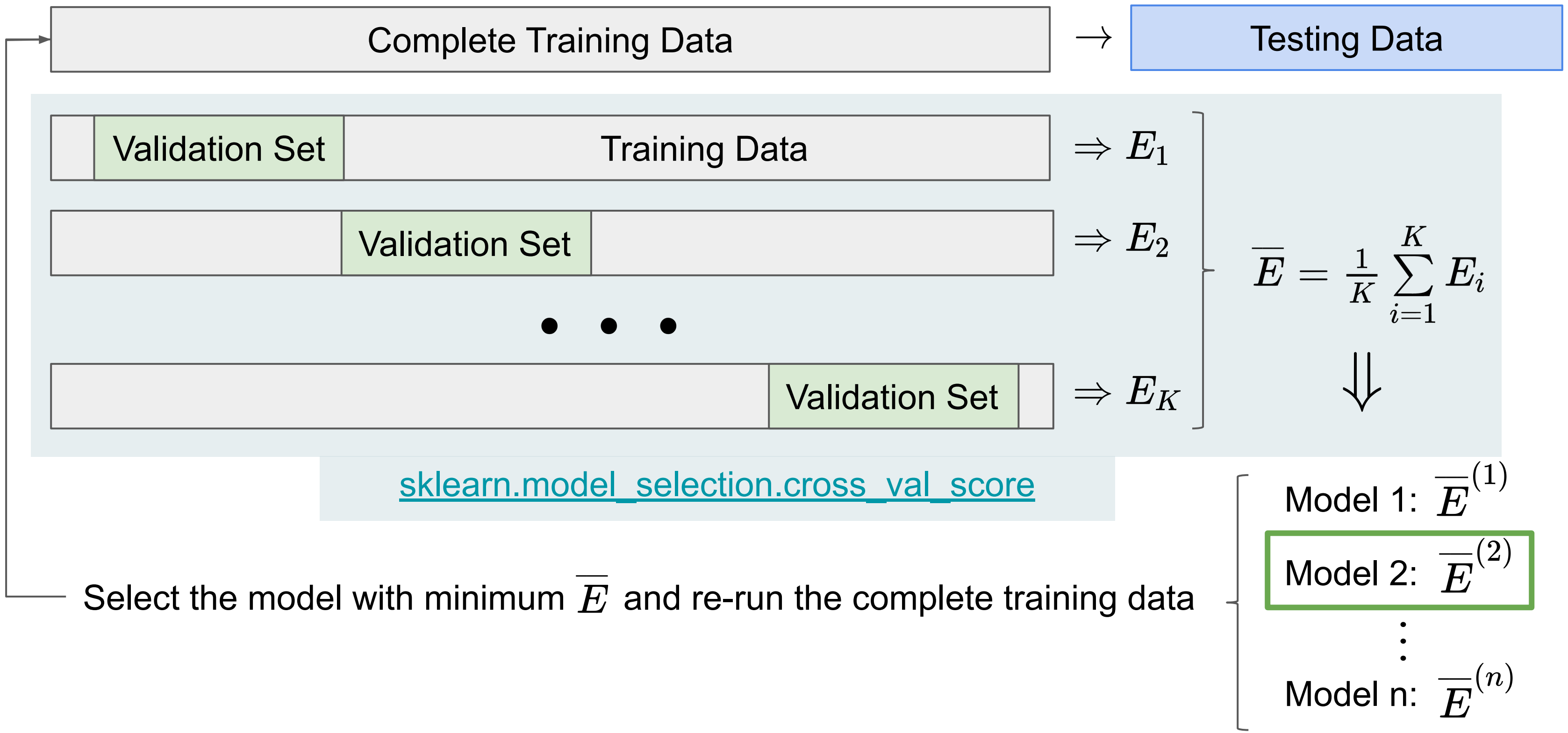
- Reduce the model’s complexity

- Regularization
  - Weight Regularization to make the model smoother (L1, L2, Elastic net)

$$\hat{L}(x, y) = L(x, y) + \lambda \sum_{i=1}^{n} \theta_i^2$$

  - Dropout
  - Early stopping

Model Selection: K-fold Cross Validation



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Errors/scores in practice

Public | Private

Training Set	Validation Set		Testing Set	Testing Set

Error: $E^{val} < E^{Pub} < E^{Pri}$

Score: $S^{val} > S^{Pub} > S^{Pri}$

Ensemble Methods: *wisdom of crowd*

- Bagging (bootstrap aggregating)
  - To decrease the bias to avoid overfitting for “strong” models
    - Decision tree -> Random Forest
  - Partitioning the data randomly to have *parallel* ensemble: each model is built independently
  - Out-of-Bag evaluation for validation
- Boosting (hypothesis boosting)
  - To decrease the bias to avoid underfitting for “weak” models
  - *Sequential* ensemble: try to add new models that do well where previous models lack
  - 3 major methods:
    - AdaBoost, Gradient Boost, XGBoost
- Stacking
  - Add a higher-level of classifier to decide weights between strong and weak models

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- Sign in your info to the class
  - To get the email notifications
- Email me your Kaggle username
  - For joining the IDRE_LML team
- Contact me
  for questions or discussions
  - huqy@idre.ucla.edu
  - Office: Math Sci #3330
  - Phone: 310-825-2011
- Fill out the survey for comments:
  - https://forms.gle/t3f8CztFQpeFFksy6