



Data Science With Python

Mosky

Data Science

- = Extract knowledge or insights from data.
- Data Science ⊃
 - Visualization
 - Statistics
 - Machine Learning
 - Big Data
 - Etc.
- ≈ Data Mining

Statistics vs. Machine Learning

- Statistics constructs more solid **inferences**.
- Machine learning constructs more interesting **predictions**.
 - Machine Learning ⊇ Deep Learning
- The models may be the same, but the focuses are different.
- Good **predictions** usually needs good **inferences** on dataset.

Science, Analysis, Scientist, and Engineering

- Data Engineering / Data Engineer
 - Prepare the data infra to enable others to work with.
- Data Analysis / Data Analyst
 - Analyze to help the company's decisions.
- Data Scientist
 - Create software to optimize the company's operations.



Mosky

- Backend Lead at Pinkoi.
- Has spoken at: PyCons in TW, JP, SG, HK, KR, MY, COSCUPs, and TEDx, etc.
- Countless hours on teaching Python.
- Own Python packages: ZIPCodeTW, etc.
- <http://mosky.tw/>

Outline

1. **Exploratory** (EDA, Exploratory Data analysis)
 - Correlation Analysis, PCA, FA, etc.
2. **Inference** (Statistical Inference)
 - Hypothesis Testing, OLS, Logit, etc.
3. **Preprocessing**
 - By pandas, scikit-learn, etc.
4. **Prediction** (Machine Learning Prediction)
 - SVM, Trees, KNN, K-Means, etc.
5. **Models of Models**
 - Cross-Validation & Pipeline, Model Development, etc.

PDF & Notebooks

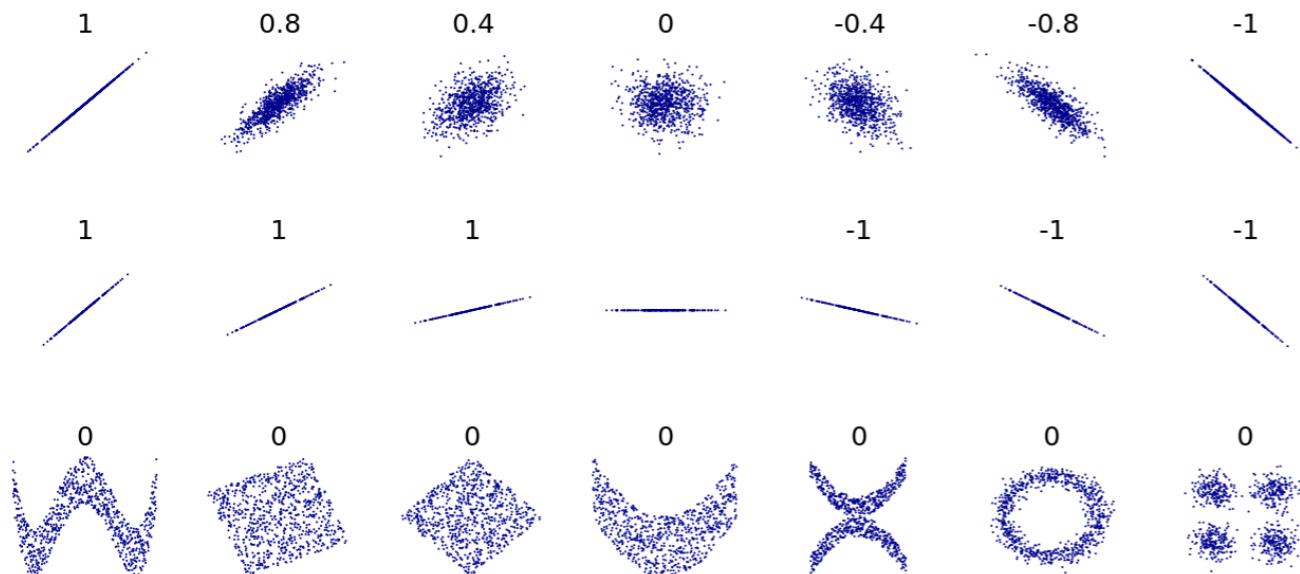
- The PDF and notebooks are available here:
 - <https://github.com/moskytw/data-science-with-python>
- A good notebook reader:
 - <https://nbviewer.jupyter.org/>
- Or run it on your own computer:
 - Prepare Python and Pipenv.
 - `$ pipenv sync`

Datasets

- The handouts are based on:
 - American National Election Survey 1996 (944×10)
- You may play with:
 - Extramarital Affairs Dataset (1978; 6366×9)
 - Star98 Educational Dataset (1998; 303×13)
- Handout: datasets.ipynb
- The context matters:
 - 1970s – Wikipedia, 1990s – Wikipedia.
 - 1996 United States presidential election – Wikipedia.

Exploration

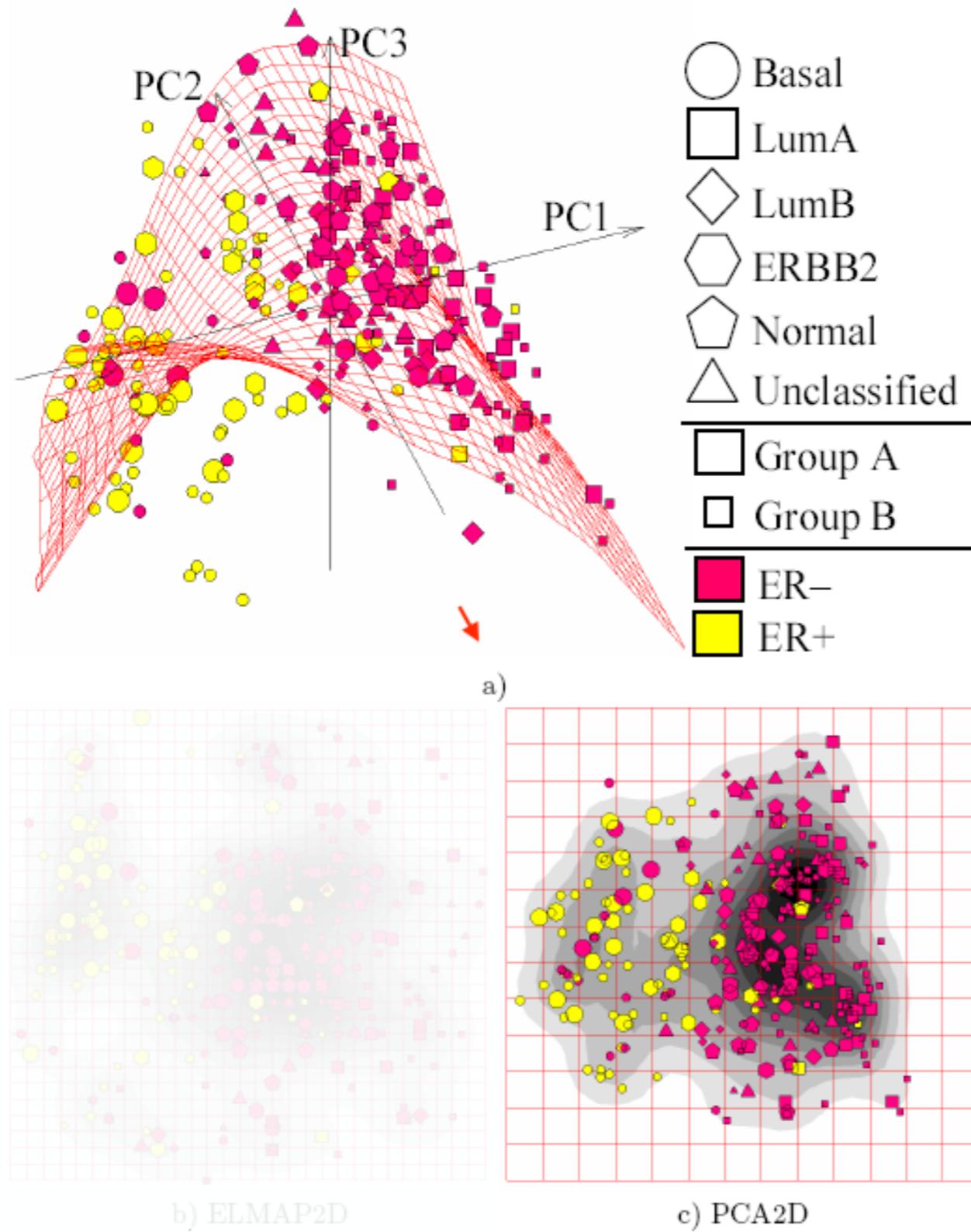
Correlation Analysis



- Measures the bivariate linear “tightness”.
- ← Pearson's Correlation Coefficient (r)
- All pairs → correlation matrix.
- Handout:
correlation_analysis.ipynb

PCA & FA

-
- Maps into a lower-dim space.
 - ← Principal Component Analysis (PCA)
 - Visualize quickly, usually.
 - Factor Analysis (FA)
 - Assume lower-number unobserved variables (factors) exist.
 - Handouts:
 - pca.ipynb, pca_3d.ipynb, ipywidgets.ipynb, fa.ipynb

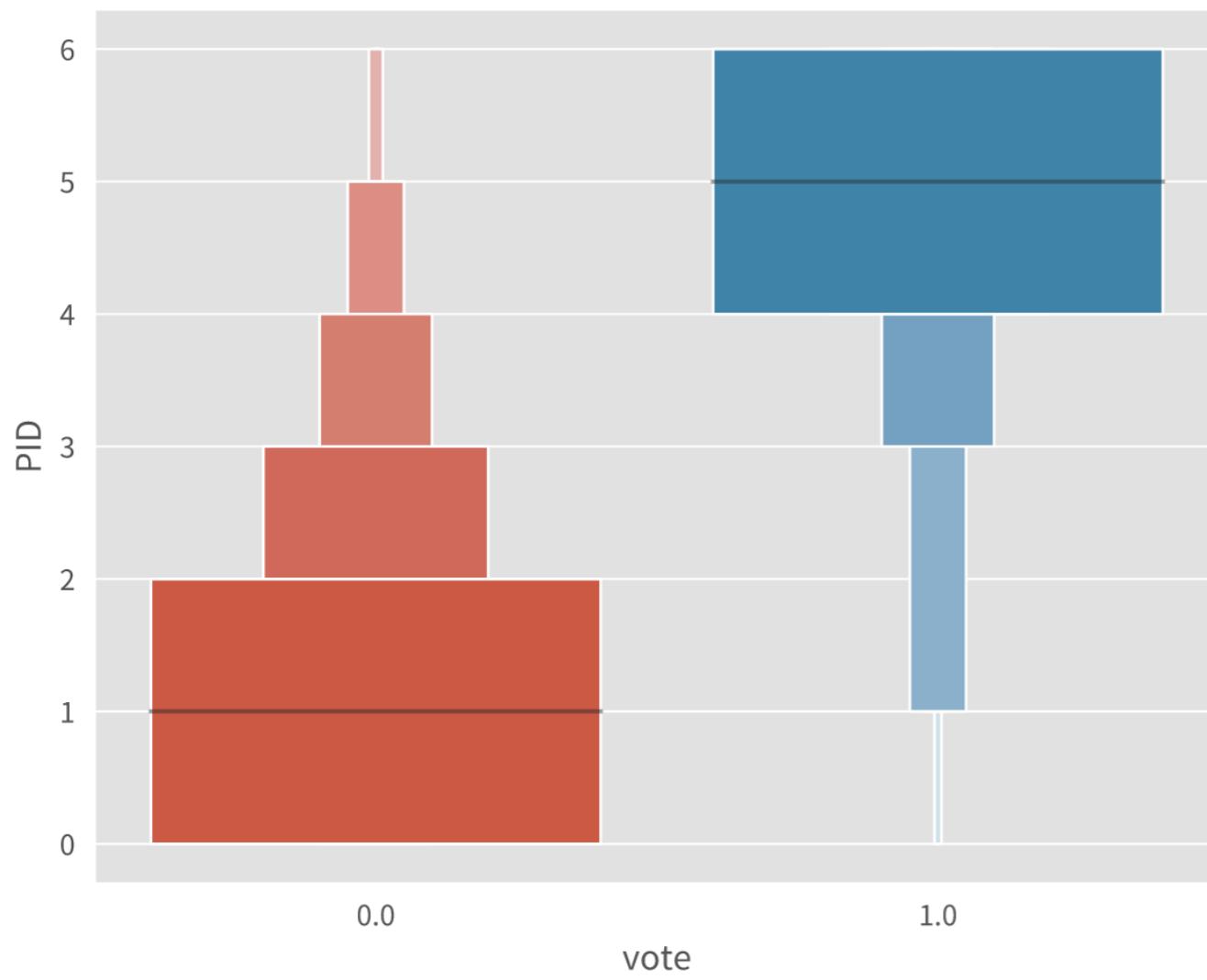


See Also

- seaborn
 - For drawing attractive and informative statistical graphics.
- Plotly
 - Makes interactive graphs.
- pandas.DataFrame.corr
 - Also has **Kendall's τ** (tau) and **Spearman's ρ** (rho).
- Isomap – scikit-learn
 - Seeks a lower-dimensional embedding which maintains geodesic distances between all points.
- Dimensionality reduction – scikit-learn

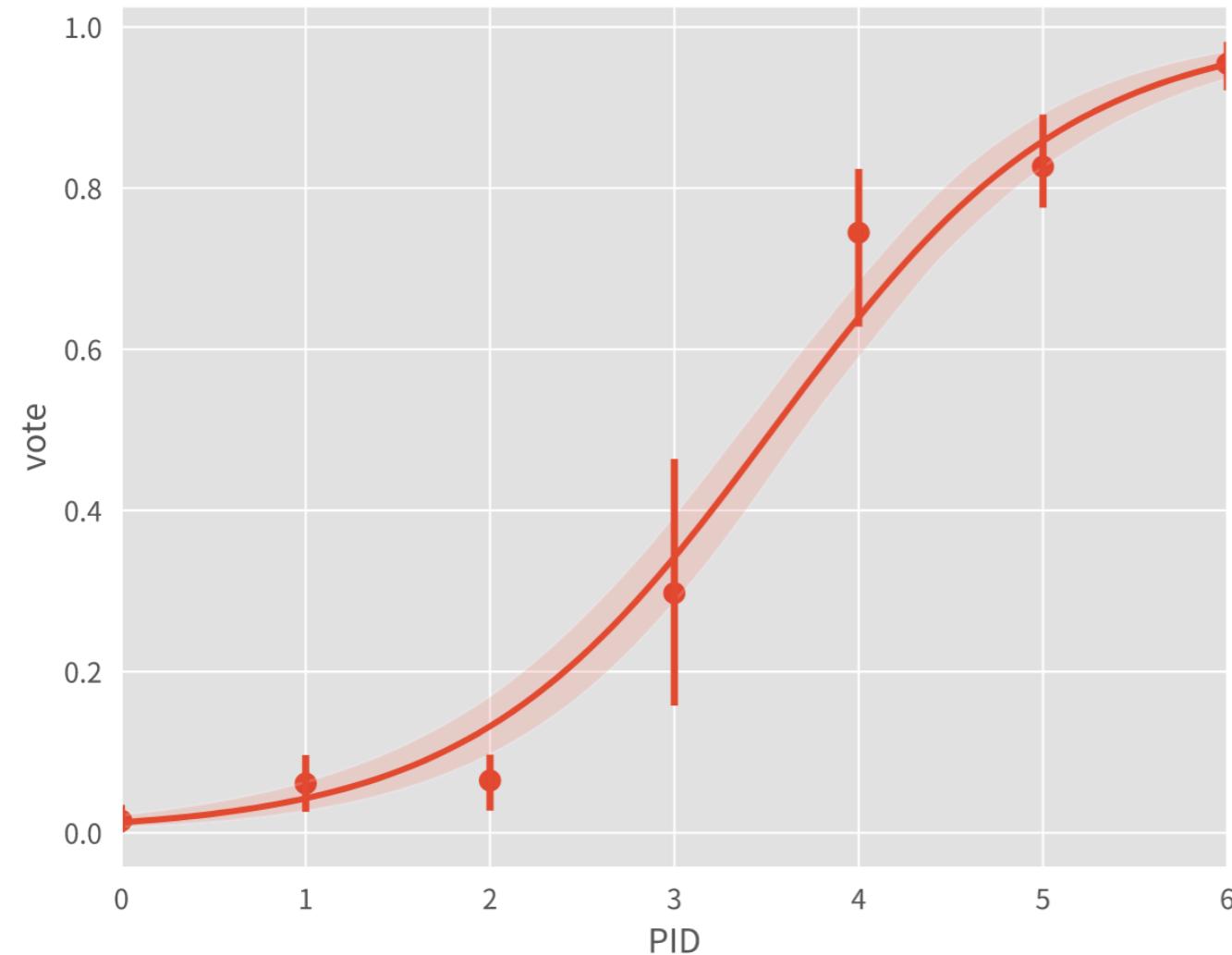
Inference

Hypothesis Testing



- Given a hypothesis, calculate the probability to observe the data.
- The hypothesis may be:
 - “the means are the same”
 - “the medians are the same”
 - “the prop. are the same, e.g., conversion rates”, etc.
- Like testing the performances of the model A and the B.
- Handout:
`hypothesis_testing.ipynb`

OLS & Logit

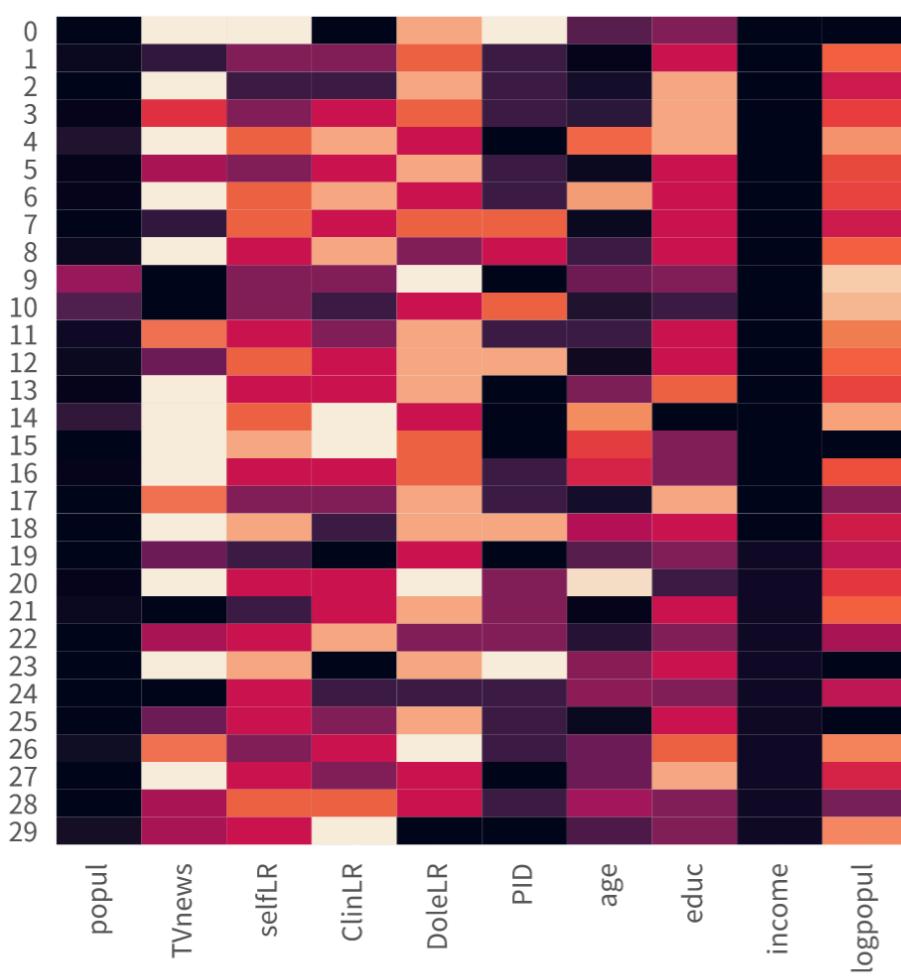
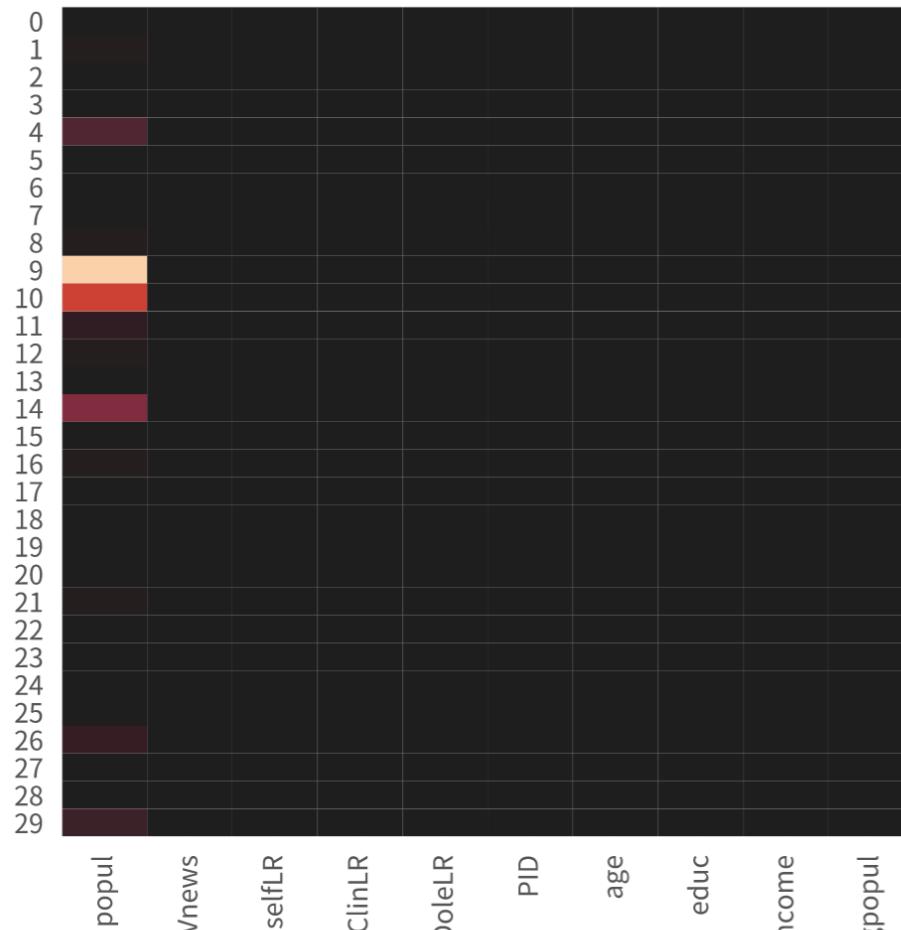


- Measures the “steepness”.
- With various assumptions:
 - Linear: OLS
 - $y \in \{0, 1\}$: Logit
 - $y \in \{0, 1, \dots\}$: Poisson, etc.
- ← Logit Regression
- Like understanding the dataset, or may find the insights directly.
- Handouts:
ols.ipynb, logit.ipynb

See Also

- [Statistical functions – SciPy](#)
 - Includes most of the hypothesis testing functions.
- [User Guide – statsmodels](#)
 - Includes much more models for statistical inference.
- [Hypothesis Testing With Python](#)
 - Answers like “how much sample is enough?”
- [Statistical Regression With Python](#)
 - Answers like “how to understand a regression summary?”

Preprocessing



Preprocessing

- Make the models understand the data by various methods.
- ← MixMinScaler
- Handouts:
pandas_preprocessing.ipynb,
sqlite.ipynb,
sklearn_preprocessing.ipynb

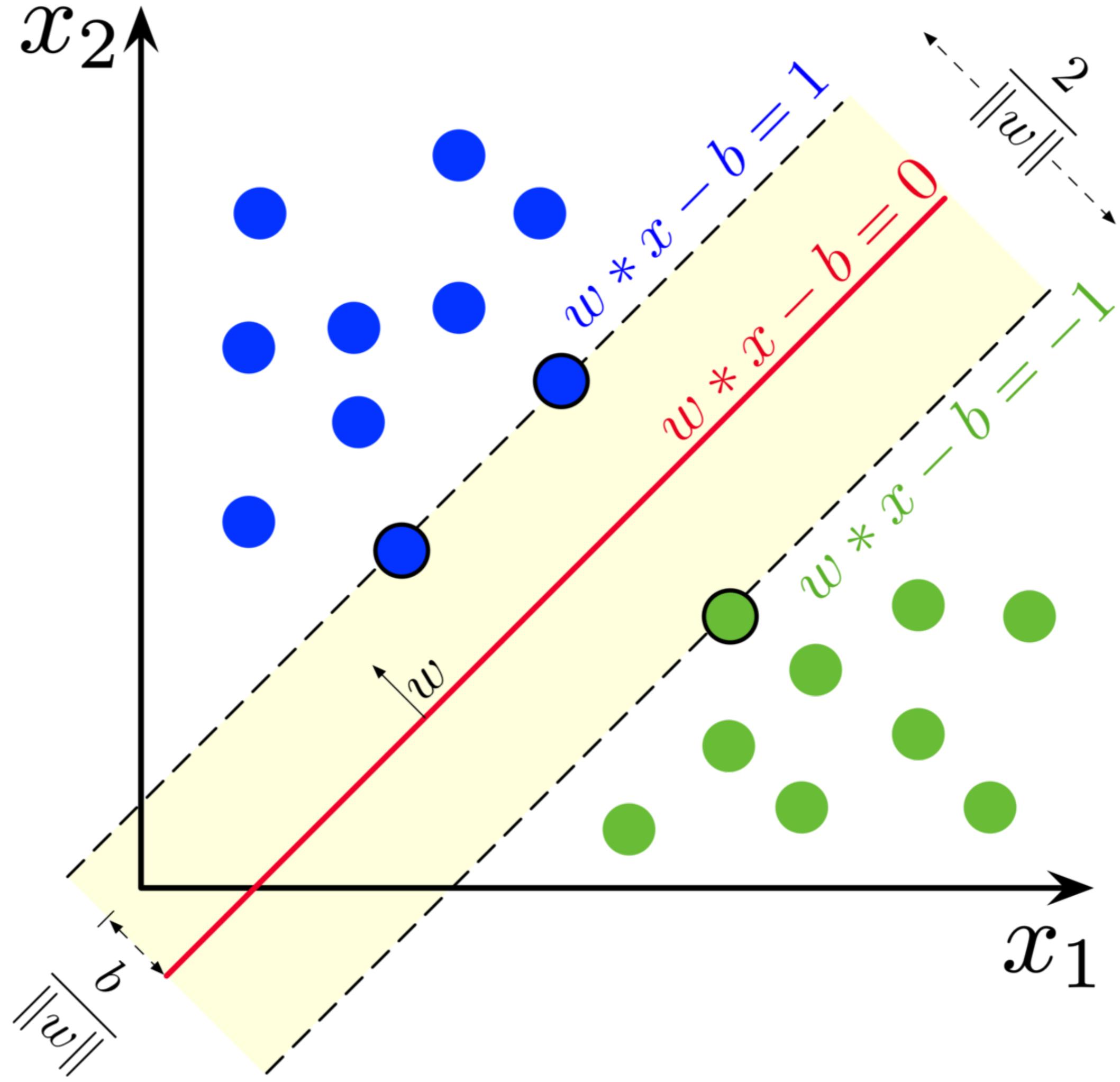
See Also

- [Text feature extraction & Image feature extraction – scikit-learn](#)
- [patsy](#): describes models by formulas, e.g., $y \sim age + C(gender)$.
- [imbalanced-learn](#): balances the classes more carefully.
 - The `class_weight='balanced'` in scikit-learn may be also helpful.
- Rather than pandas:
 - [Polars](#): faster.
 - [Spark](#): more scalable.
 - [Database-like ops benchmark – H2O.ai](#)
- [Feature Engineering](#): create features by domain knowledge.

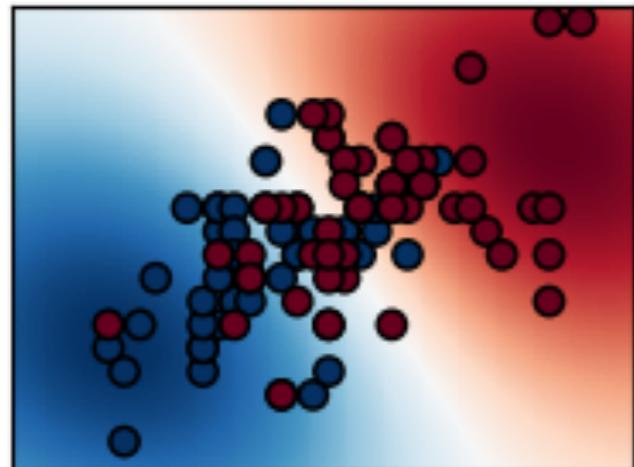
Prediction

Prediction

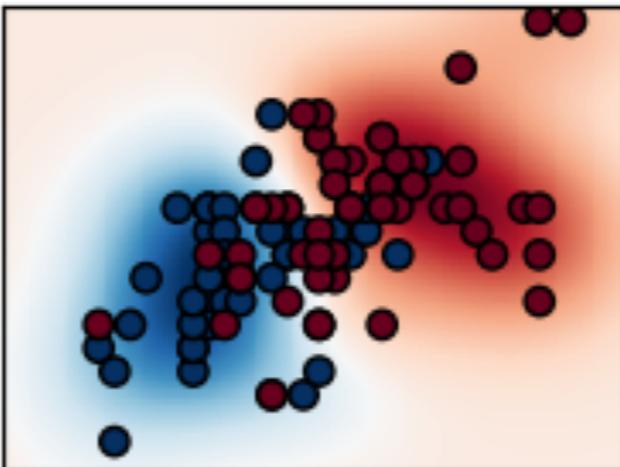
Support-Vector Machines (SVM)



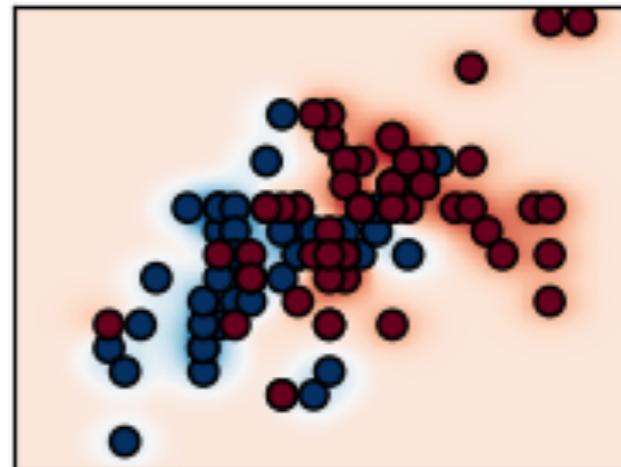
$\text{gamma}=10^{-1}, C=10^{-2}$



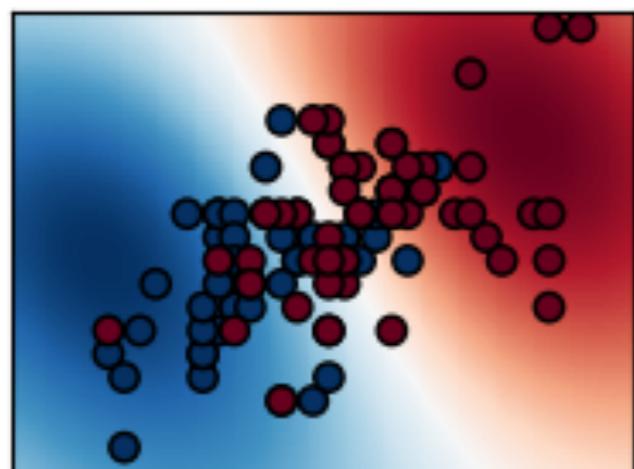
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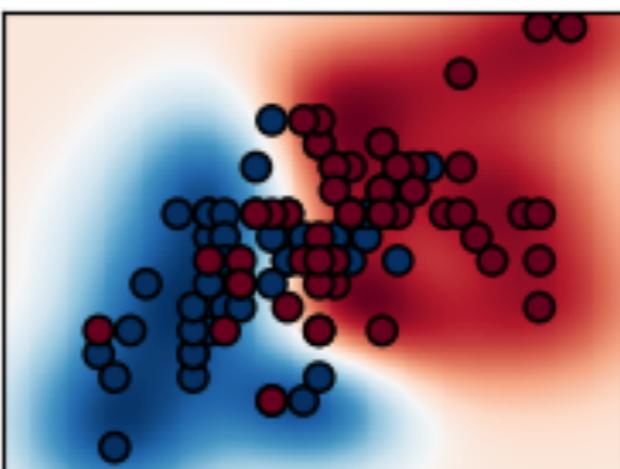
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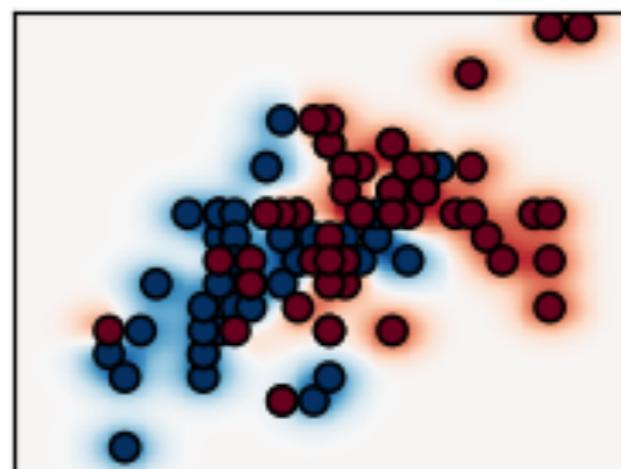
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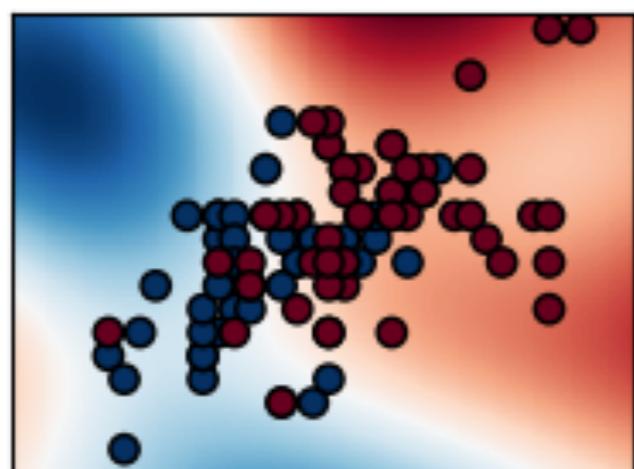
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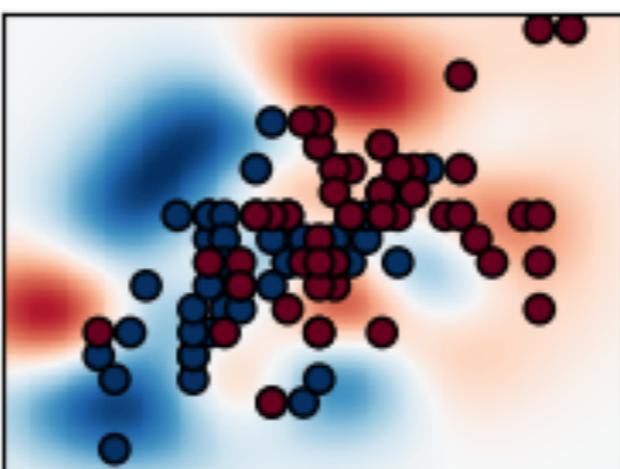
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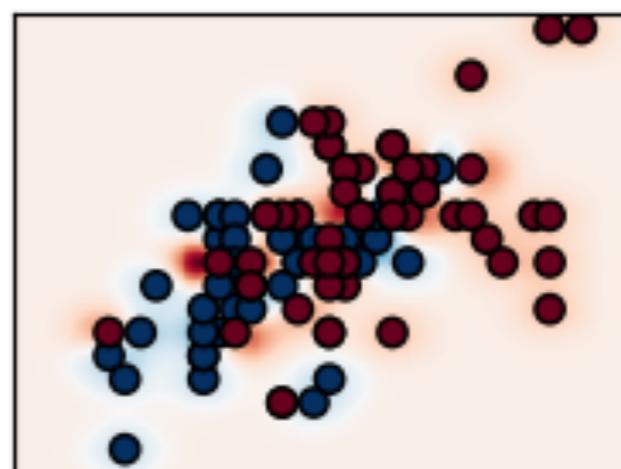
$\text{gamma}=10^{-1}, C=10^2$



$\text{gamma}=10^0, C=10^2$



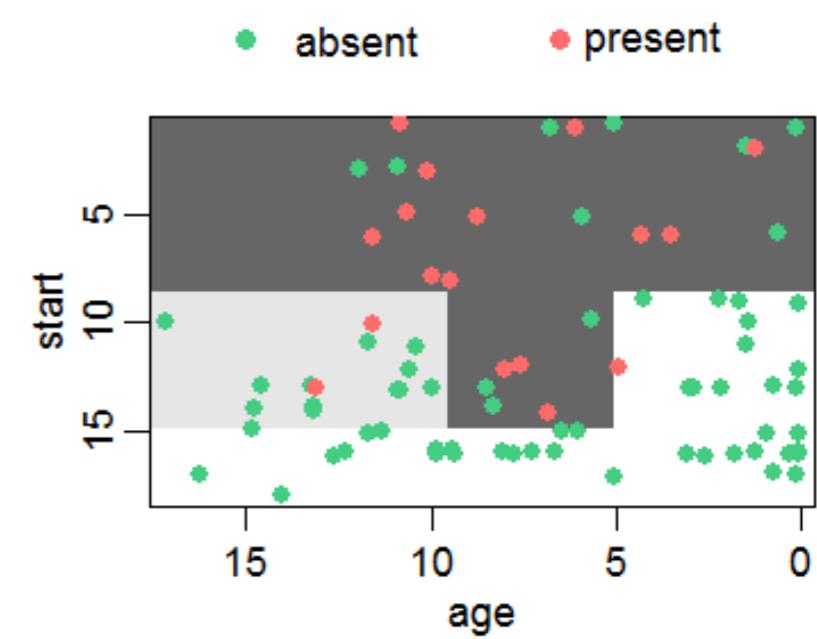
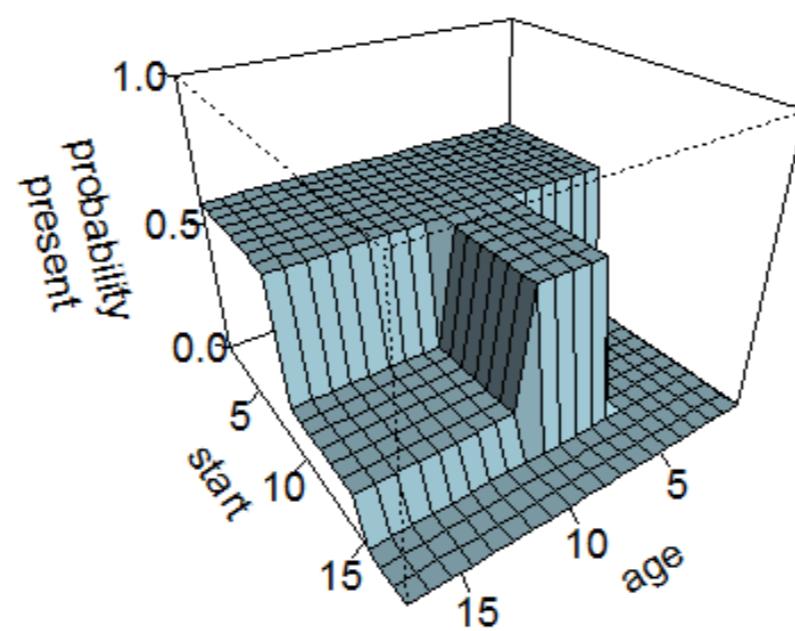
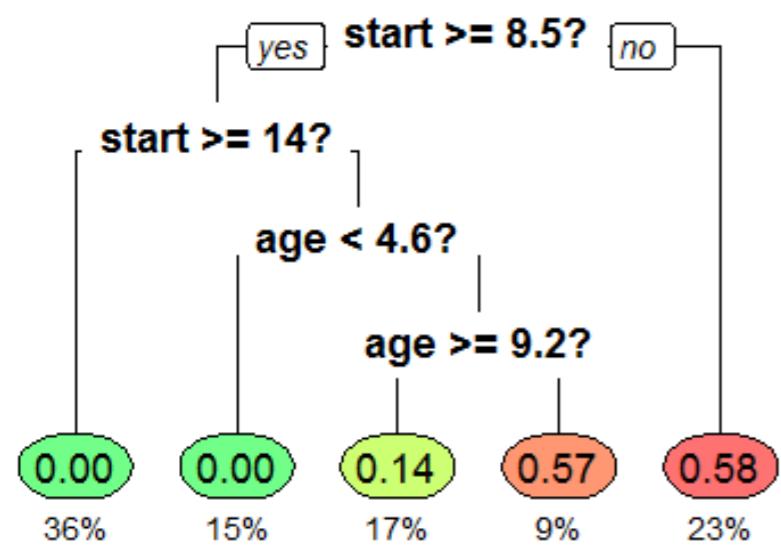
$\text{gamma}=10^1, C=10^2$



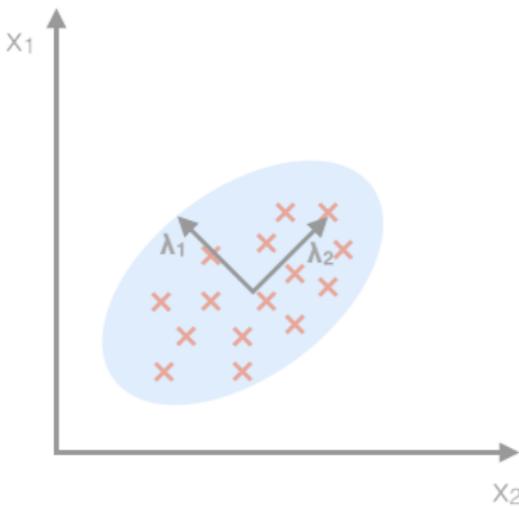
SVM With Radial Basis Function (RBF) Kernel

Prediction

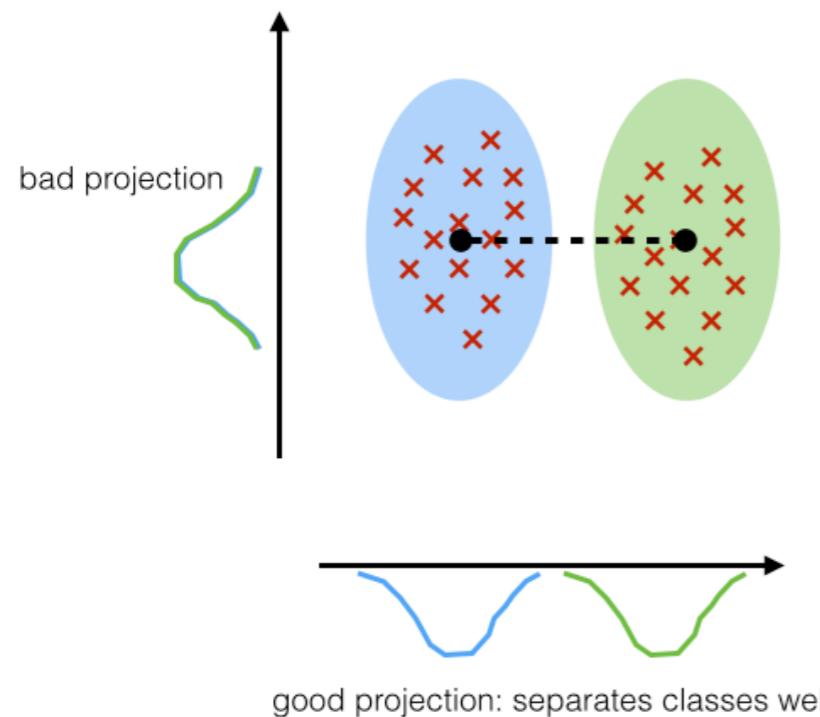
Decision Tree



PCA:
component axes that
maximize the variance



LDA:
maximizing the component
axes for class-separation



Prediction

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- Predict the category or continuous value.
- By various models:
 - ↑ SVM
 - ↑ Tree
 - ← Linear Discriminant Analysis (LDA)
- KNN & K-Means
- Handouts: svm.ipynb, trees.ipynb, logistic_and_lda.ipynb, knn.ipynb, kmeans.ipynb

See Also

- [LightGBM](#): the most popular choice in Kaggle in 2019 [[ref](#)].
- [Approximate Nearest Neighbor \(ANN\) Benchmark](#)
- [Recommender Systems in Practice – Towards Data Science](#)
- [Association Rules – mlxtend](#)
- [Voting & Stacking – scikit-learn](#)

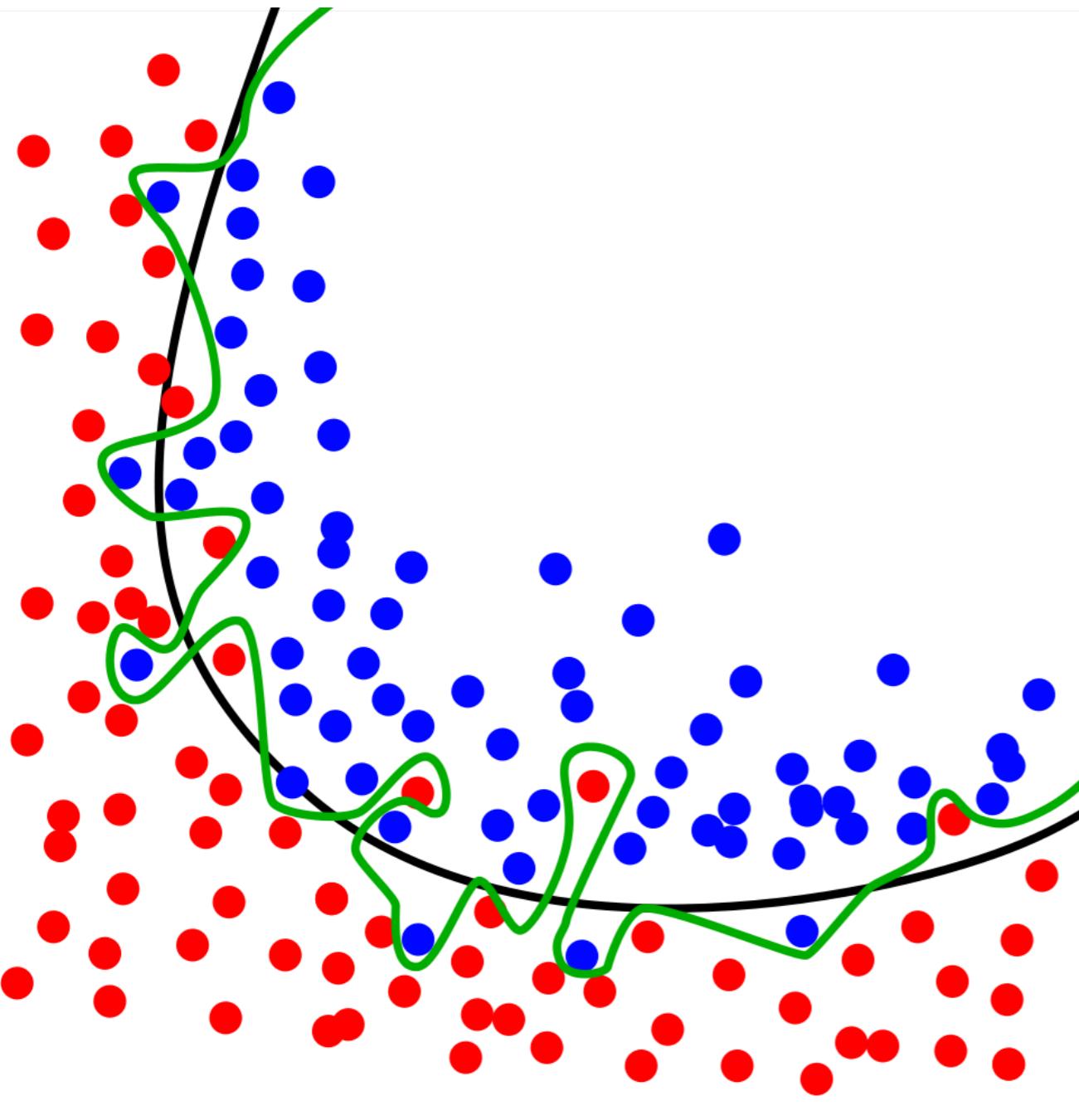
Models of Models

Data Leakage



- The training data which **leads a high performance** is **not available when prediction**. Not the “data breach” in the security area.
- Two major types: [ref]
 - **Train-Test Contamination:** like backfilling train by test.
 - **Target Leakage:** like *diseased* is y , and *treated* in X .
- Solutions:
 - Pipeline
 - Explanation
(+ Domain Knowledge)

Overfitting



- A model **fits the training data too well**, and then fails to predict.
- It happens because of the natural of models, like trees, or over-tuning the hyperparameters.
- ← Green may be an **overfit**.
- Solutions:
 - *train_score / test_score* should be around 1.
 - **Train-Test Split**
 - **Cross-Validation**



Spurious Relationship

- The model **uses a false relationship to predict.**
- ← Get the 90% accuracy by “the background is snowy, so the animal is Husky.” [ref]
- Solution:
 - Explanation
(+ Domain Knowledge)



Model-Market Fit

- Like “Product-Market Fit”.
- “Hey, this house is super similar to the one you just bought, buy one more?”
- “I build this model by ten years, please buy one!”
- Solution:
- Model Development



Pipeline

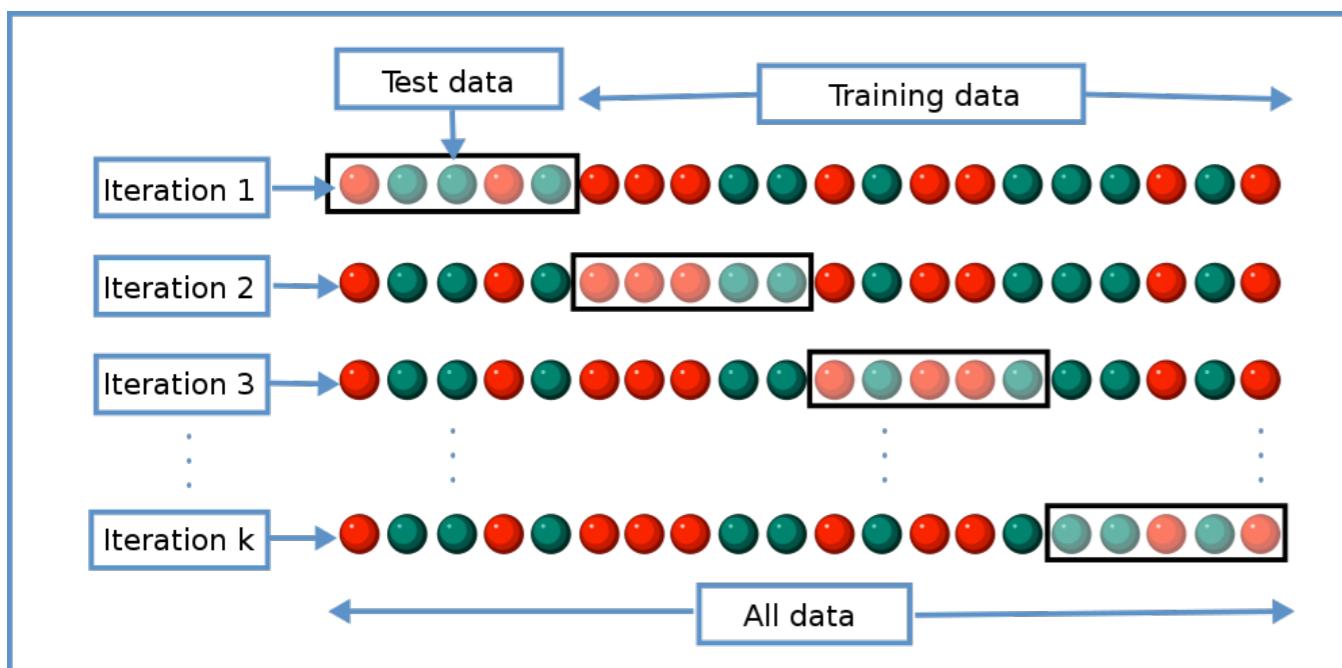
- Predefine the steps and run the *fit / transform* (*predict*) separately to avoid data leakage.

Cross-Validation

.....

- Train-Test Split is simple, but can't use the data fully.
- Use the data fully by various strategies.

← K-Fold Cross-Validation
(K-Fold CV)



- **Train-Test Split?** Keep **a set clean from fitting** to evaluate the performance correctly.
- **Cross-Validation?** Also rotate the 2 sets to cover all of the data.
- **Train-Valid-Test Split?** Keep **another set clean from the model selection**, e.g., selecting from Logistics, SVM, Random Forest.
- **Nested Cross-Validation?** Also rotate the 3 sets.
- **Handout:** pipe_and_cv.ipynb

See Also

- [Cross validation iterators – scikit-learn](#)
 - Choose by the data generating process like groups.
- [Exhaustive Grid Search – scikit-learn](#)
 - Search the best hyperparameters automatically.
- [AWS Data Pipeline](#)
 - It's a different “pipeline”, but it's also important in the data engineering.



Model Development

- Like “Software Development”.
- How to “model-market fit”?
Delight people with fast release!
- People must like your model:
 - Domain experts.
 - Colleagues.
 - Users.
- Release faster; then learn faster,
ideally 1–2 weeks.

See Also

- The Analysis Steps
 - A suggested method to make an analysis, may be an analysis for building models or reviewing models.
- The Study Designs
 - Besides the A/B testing, some not costly methods.
- The Mini-Scrum
 - How to work with a team efficiently.

Time Series

- A Spurious Relationship happens between independent non-stationary variables naturally, like the mean varies by time.
- The methods and libraries for time series.
 - plot_acf & plot_pacf – statsmodels
 - tsa & statespace – statsmodels
 - ADF test – statsmodels
 - pmdarima: brings R's auto.arima to Python.
 - Prophet: using Bayesian-based method.
 - Cross validation of time series data – scikit-learn

Recap

- Exploratory like PCA helps to understand the data.
- Inference like statistical regressions finds the insights out.
- Preprocessing is for feeding easy-to-digest data to models.
- Inference helps prediction.
- Delight people with fast release! 😊

Image Credits

- “Linear PCA vs. Nonlinear Principal Manifolds”: https://en.wikipedia.org/wiki/Principal_component_analysis#/media/File:Elmap_breastcancer_wiki.png
- “SVM”: https://en.wikipedia.org/wiki/Support_vector_machine#/media/File:SVM_margin.png
- “SVM With RBF Kernel”: https://scikit-learn.org/stable/auto_examples/svm/plot_rbf_parameters.html
- “Tree”: https://en.wikipedia.org/wiki/Decision_tree_learning#/media/File:Cart_tree_kyphosis.png
- “PCA vs. LDA”: https://sebastianraschka.com/Articles/2014_python_lda.html
- “Overfitting”: <https://en.wikipedia.org/wiki/Overfitting#/media/File:Overfitting.svg>
- “Data Leakage”: <https://www.kaggle.com/dansbecker/data-leakage>
- “Husky”: <https://en.wikipedia.org/wiki/Husky>
- “Wolf”: https://en.wikipedia.org/wiki/Wolf#/media/File:Front_view_of_a_resting_Canis_lupus_ssp.jpg
- “Houses”: <https://unsplash.com/photos/vZEPXDQHR4s>
- “K-Fold Cross-Validation”: [https://en.wikipedia.org/wiki/Cross-validation_\(statistics\)#/media/File:K-fold_cross_validation_EN.svg](https://en.wikipedia.org/wiki/Cross-validation_(statistics)#/media/File:K-fold_cross_validation_EN.svg)
- “Pipeline”: <https://unsplash.com/photos/KP6XQIEjjPA>
- “Smile”: <https://unsplash.com/photos/g1Kr4Ozfoac>