

Building a Robot Judge: Data Science for Decision-Making

3. Machine Learning Essentials

Notes

- ▶ Intuition on colliders – ask ChatGPT.
- ▶ First homework due tomorrow, submit if you want to continue participating in the class.
- ▶ Critical presentations:
 - ▶ Sign-up by tomorrow or be randomly assigned.
 - ▶ Template: <https://eash.cc/BRJ-pres-template>
 - ▶ First presentation video due this Saturday – any additional volunteers?

Outline

Essentials

Regression / Regularization

Binary Classification

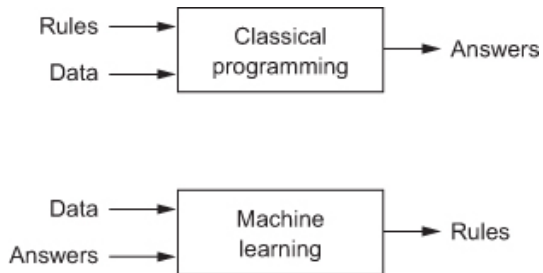
ML Applications

Activity on Causal Graphs

Learning Objectives

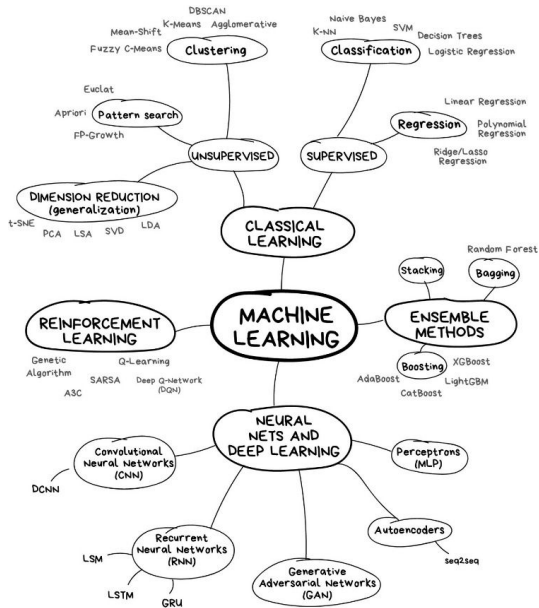
1. **Implement and evaluate machine learning pipelines.**
 - **Evaluate (find problems in) existing machine learning pipelines.**
 - **Design a pipeline to solve a given ML problem.**
 - **Implement some standard pipelines in Python.**
2. Implement and evaluate causal inference designs.
3. Understand how (not) to use data science tools (ML and CI) to support expert decision-making.

What is machine learning?

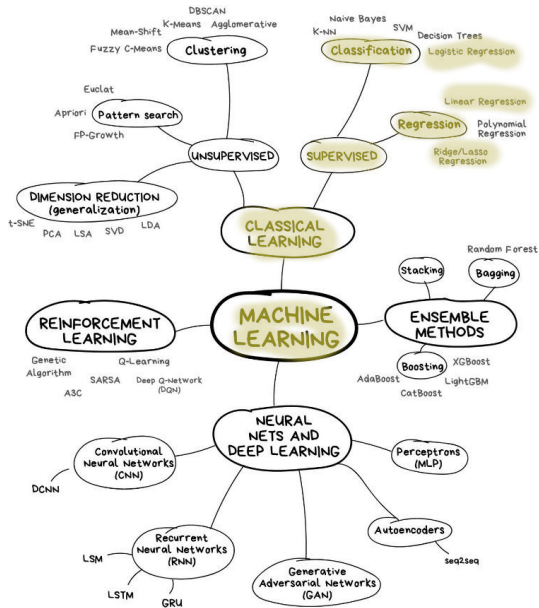


- ▶ In classical computer programming, humans input the rules and the data, and the computer provides answers.
- ▶ In machine learning, humans input the data and the answers, and the computer learns the rules.

The Machine Learning Landscape



What we will do today



A Machine Learning Project, End-to-End

Aurelien Geron, *Hands-on machine learning with Scikit-Learn, Keras, & TensorFlow*, Chapter 2:

1. Look at the big picture.
2. Get the data.
3. Discover and visualize the data to gain insights.
4. Prepare the data for Machine Learning algorithms.
5. Select a model and train it.
6. Fine-tune your model.
7. Present your solution.
8. Launch, monitor, and maintain your system.

Three Types of (Standard) Machine Learning Problems

Determined by the data type of the outcome variable (or label):

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- ▶ **Regression:** a one-dimensional, continuous, real-valued outcome.
 - ▶ e.g., number of days of prison assigned
- ▶ **Multinomial Classification:** Three or more discrete, un-ordered outcomes.
 - ▶ e.g., predict what judge is assigned to a case: Alito, Breyer, or Cardozo

What type of ML Problem is this?

- ▶ Based on defendant characteristics and the facts of the case, predict which charges the prosecutor will bring:
 - ▶ third degree murder (manslaughter)
 - ▶ second degree murder (crime of passion)
 - ▶ first degree murder (premeditated)

{binary classification, regression, or multinomial classification}
- ▶ **write down your answer (30 secs)**

What do ML Algorithms do? Minimize a cost function

What do ML Algorithms do? Minimize a cost function

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

$$\text{MSE}(\theta) = \frac{1}{n_D} \sum_{i=1}^{n_D} (h(x_i; \theta) - y_i)^2$$

- ▶ n_D , the number of rows/observations
- ▶ x , the matrix of predictors, with row x_i
- ▶ y , the vector of outcomes, with item y_i
- ▶ $h(x_i; \theta) = \hat{y}$ the model prediction (hypothesis)

Loss functions, more generally

- ▶ The loss function $L(\hat{\mathbf{y}}, \mathbf{y})$ assigns a score based on prediction and truth:
 - ▶ Should be bounded from below, with the minimum attained only for cases where the prediction is correct.
- ▶ The average loss for the test set is

$$\mathcal{L}(\theta) = \frac{1}{n_D} \sum_{i=1}^{n_D} L(h(\mathbf{x}_i; \theta), \mathbf{y}_i)$$

- ▶ The estimated parameter matrix θ solves

$$\hat{\theta} = \arg \min_{\theta} \mathcal{L}(\theta)$$

↪ optimizes over parameter space; treats the data as constants.

OLS Regression is Machine Learning

- ▶ Ordinary Least Squares Regression (OLS), also called simple linear regression, assumes the functional form $h(x; \theta) = x_i' \theta$ and minimizes the mean squared error (MSE)

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- ▶ This minimand has a closed form solution

$$\hat{\theta} = (\mathbf{x}'\mathbf{x})^{-1} \mathbf{x}'\mathbf{y}$$

- ▶ most machine learning models do **not** have a closed form solution \rightarrow use numerical optimization (gradient descent).

$$\text{MSE}(\theta) = \frac{1}{n_D} \sum_{i=1}^{n_D} (h(\theta; \mathbf{x}_i) - y_i)^2$$

- The partial derivative for feature $j \in \{1, \dots, n_x\}$ is

$$\frac{\partial \text{MSE}}{\partial \theta_j} = \frac{2}{n_D} \sum_{i=1}^{n_D} \underbrace{(h(\theta; \mathbf{x}_i) - y_i)}_{\text{error for this obs}} \underbrace{\frac{\partial h(\theta; \mathbf{x}_i)}{\partial \theta_j}}_{\text{how } \theta_j \text{ shifts } h(\cdot)}$$

- → estimates how changing θ_j would reduce the error across the whole dataset.

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- ▶ The **gradient** ∇ gives the vector of these partial derivatives for all features:

$$\nabla_{\theta} \text{MSE} = \begin{bmatrix} \frac{\partial \text{MSE}}{\partial \theta_1} \\ \frac{\partial \text{MSE}}{\partial \theta_2} \\ \vdots \\ \frac{\partial \text{MSE}}{\partial \theta_{n_x}} \end{bmatrix}$$

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$$\theta_{t+1} = \theta_t - \eta \nabla_{\theta} \text{MSE}$$

- ▶ η = learning rate
- ▶ keep nudging until convergence.

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- ▶ **Stochastic gradient descent (SGD)**: Compute gradient for single random instance (rather than whole dataset) at each iteration. Much faster, still works.

Data Prep for Machine Learning

- ▶ Data Pre-Processing: See Geron Chapter 2 for pandas and sklearn syntax:
 - ▶ imputing missing values.
 - ▶ feature scaling (often helpful/necessary for ML models to work well)
 - ▶ if predictors are sparse (e.g. bag-of-words), use `StandardScaler(with_mean=False)`.
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- ▶ Don't touch the data manually: use code for a reproducible data pipeline.
- ▶ Train/Test Split:
 - ▶ ML models can achieve arbitrarily high accuracy in-sample, so performance should be evaluated out-of-sample.
 - ▶ standard approach: randomly sample 80% training dataset to learn parameters, form predictions in 20% testing dataset for evaluating performance.

Use Cross-Validation During Model Training

- ▶ Within the training set:
 - ▶ Use cross-validation with grid search to get model performance metrics across subsets of data using different hyperparameter specs.
 - ▶ Find the best hyperparameters for out-of-fold prediction in the training set.
- ▶ Then evaluate model performance in the test set using these hyperparameters.

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- ▶ Then evaluate model performance in the test set using these hyperparameters.
- ▶ Cross-validation is less common in deep learning, where training multiple models can be too computationally expensive.
 - ▶ instead, use dropout and early stopping.

Model Evaluation in Test Set

Evaluating a “good” model is context-dependent. Here are some basics.

Regression:

- ▶ mean squared error (MSE)
- ▶ R-squared (same ranking as MSE, but units are more interpretable)
- ▶ mean absolute error (MAE, $\sum |\hat{y}(\theta) - y|$) is less sensitive to outliers.

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accuracy = ($\#$ correct test-set predictions) / ($\#$ of test-set observations)
- ▶ What if one of the outcomes is over-represented – e.g., 19 out of 20? Then I can guess the modal class and get 95% accuracy.
 - ▶ Some alternative classifier metrics designed to address class imbalance (more below and in week 5).

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Regression / Regularization

Binary Classification

ML Applications

Activity on Causal Graphs

Regression models \leftrightarrow Continuous outcome

- ▶ If the outcome is continuous (e.g., Y = tax revenues collected, or criminal sentence imposed in months of prison):
 - ▶ Need a regression model. Problems with OLS:
 - ▶ tends to over-fit training data.
 - ▶ cannot handle multicollinearity.

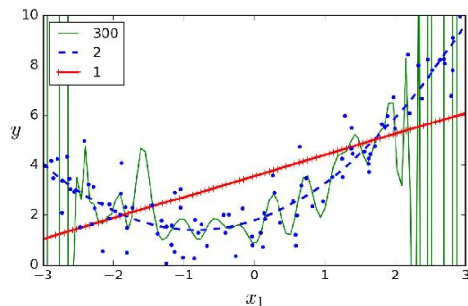


Figure 4-14. High-degree Polynomial Regression

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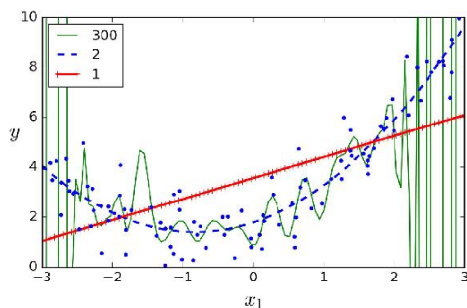


Figure 4-14. High-degree Polynomial Regression

- ▶ Machine learning models are evaluated by the fit in held-out data (the test set)
 - ▶ “Regularization” refers to ML model training methods designed to reduce/prevent over-fitting of the training set
 - ▶ (and hopefully better fit in the test set).

Regularization

- ▶ Minimizing the loss L directly usually results in over-fitting. It is standard to add **regularization**:

$$\hat{\theta} = \arg \min_{\theta} \frac{1}{n_D} \sum_{i=1}^{n_D} L(h(\mathbf{x}_i; \theta), \mathbf{y}_i) + \lambda R(\theta)$$

- ▶ $R(\theta)$ is a “regularization function” or “regularizer”, designed to reduce over-fitting.
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“Ridge” and “Lasso” penalize larger coefficients, shrinking them toward zero:

- ▶ Ridge (or L2) penalty:

$$R_2 = \|\theta\|_2^2 = \sum_{j=1}^{n_x} (\theta_j)^2$$

- ▶ also helps select between collinear predictors.

- ▶ Lasso (or L1) penalty:

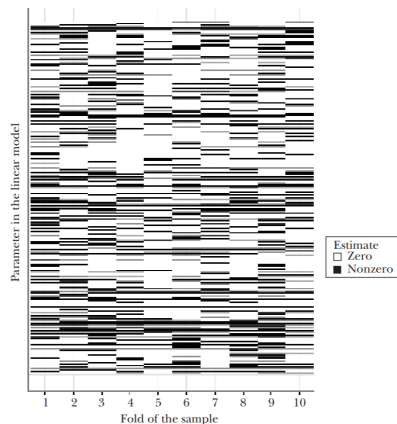
$$R_1 = \|\theta\|_1 = \sum_{j=1}^{n_x} |\theta_j|$$

- ▶ also performs feature selection and outputs a sparse model.

Does lasso pick the “true” model?

Lasso prediction of house prices with 150 variables – which variables are “selected” (non-zero coefficients) by lasso, in ten models trained on separate data subsamples (Mullainathan and Spiess 2017):

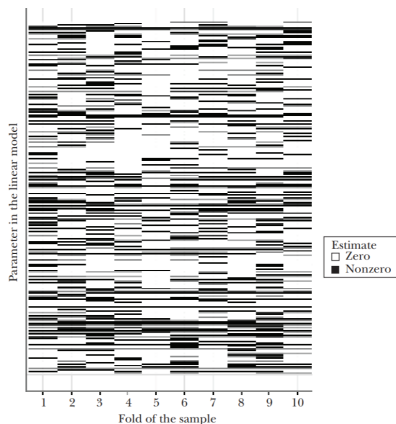
Selected Coefficients (Nonzero Estimates) across Ten LASSO Regressions



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Selected Coefficients (Nonzero Estimates) across Ten LASSO Regressions



- ▶ The set of lasso-selected variables changes across folds in the data
- ▶ → Lasso does not pick the “correct” predictors.
 - ▶ It just learns the correct $\hat{h}(X)$
 - ▶ when predictors are correlated with each other, they are substitutable.

Elastic Net = Lasso + Ridge

The Elastic Net cost function is:

$$\begin{aligned} L(\theta) &= \text{MSE}(\theta) + \lambda_1 R_1 + \lambda_2 R_2 \\ &= \text{MSE}(\theta) + \lambda_1 \sum_{j=1}^{n_x} |\theta_j| + \lambda_2 \sum_{j=1}^{n_x} (\theta_j)^2 \end{aligned}$$

- ▶ λ_1, λ_2 = strength of L1 (Lasso) penalty and L2 (Ridge) penalty, respectively.
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In scikit-learn, e-net penalties are parametrized as “alpha” = total penalty, and “l1_ratio” = proportion of penalty to L1.

```
from sklearn.linear_model import ElasticNet
enet = ElasticNet(alpha=2.0, l1_ratio = .75) # L1 = 1.5, L2 = 0.5
enet.fit(X,y)
```

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Binary Outcome \leftrightarrow Binary Classification

- ▶ Binary classifiers try to match a boolean outcome $y \in \{0, 1\}$.
 - ▶ The standard approach is to apply a transformation (e.g. sigmoid/logit) to normalize $\hat{y} \in [0, 1]$.
 - ▶ Prediction rule is 0 for $\hat{y} < .5$ and 1 otherwise.

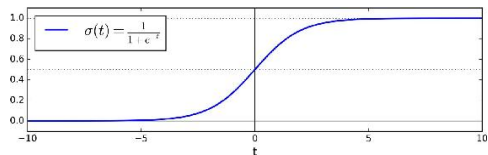
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- ▶ The binary cross-entropy (or log loss) is:

$$L(\theta) = \underbrace{-\frac{1}{n_D}}_{\text{negative}} \sum_{i=1}^{n_D} \left[\underbrace{y_i}_{y_i=1} \underbrace{\log(\hat{y}_i)}_{\log \text{ prob}_{y_i=1}} + \underbrace{(1-y_i)}_{y_i=0} \underbrace{\log(1-\hat{y}_i)}_{\log \text{ prob}_{y_i=0}} \right]$$

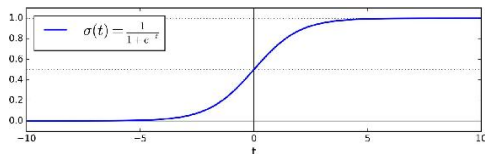
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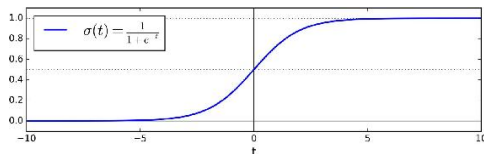
- Plugging into the binary-cross entropy loss gives the logistic regression cost objective:

$$\min_{\theta} \sum_{i=1}^{n_D} -y_i \log(\text{sigmoid}(\mathbf{x}_i \cdot \theta)) - [1 - y_i] \log(1 - \text{sigmoid}(\mathbf{x}_i \cdot \theta))$$

- does not have a closed form solution, but it is convex (guaranteeing that gradient descent will find the global minimum).

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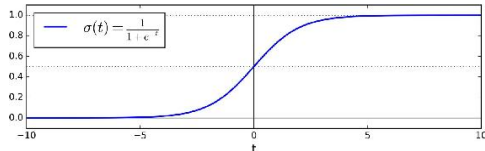
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- ▶ Like linear regression, logistic regression can be regularized with L1 or L2 penalties.

```
from sklearn.linear_model import LogisticRegression
logit = LogisticRegression(penalty='l2', C = 2.0) # lambda = 1/2
logit.fit(X,y)
```

A **Confusion Matrix** is a nice way to visualize classifier performance:

		Predicted Class	
		Negative	Positive
True Class	Negative	# True Negatives	# False Positives
	Positive	# False Negatives	# True Positives

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- ▶ Precision decreases with false positives. “When I guess this outcome, I tend to guesses correctly.”

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- ▶ Precision decreases with false positives. “When I guess this outcome, I tend to guesses correctly.”

$$\text{Recall (for positive class)} = \frac{\text{True Positives}}{\text{True Positives} + \text{False Negatives}}$$

- ▶ Recall decreases with false negatives. “When this outcome occurs, I don’t miss it.”

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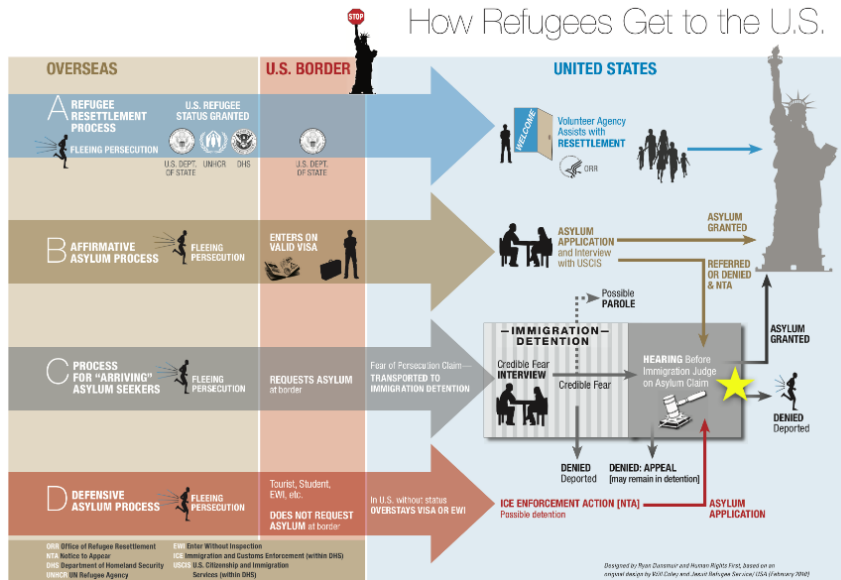
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Binary Classification

ML Applications

Activity on Causal Graphs

Asylum in the U.S.



Dunn, Sagun, Sirin, and Chen (2017): Asylum Courts

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 - ▶ universe of asylum court cases, 1981-2013
 - ▶ 492,903 decisions, 336 courts, 441 judges

Dunn, Sagun, Sirin, and Chen (2017): Asylum Courts

- ▶ Data:
 - ▶ universe of asylum court cases, 1981-2013
 - ▶ 492,903 decisions, 336 courts, 441 judges
- ▶ High stakes: denial of asylum results in deportation.
- ▶ Average grant rate: 35%.
- ▶ What type of ML problem is this?

Predicting U.S. Asylum Court Decisions

		Predicted	
		Denied	Granted
True	Denied	195,223	65,798
	Granted	73,269	104,406

Accuracy = 68.3%, F1 = 0.60

- predictions made using logistic regression with L2 regularization, penalty selected by cross-validation grid search.

Judge Identity is Most Predictive Factor

Model	Accuracy	ROC AUC
Judge ID	0.71	0.74
Judge ID & Nationality	0.76	0.82
Judge ID & Opening Date	0.73	0.77
Judge ID & Nationality & Opening Date	0.78	0.84
Full model at case completion	0.82	0.88

- ▶ Predictions from random forest classifier, with parameters selected by cross-validated grid search.
 - ▶ Training/test split 482K/120K.

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Judge Variation in Predictability

- ▶ Some judges are highly predictable, always granting or rejecting.
 - ▶ suggests they use heuristics or stereotypes rather than considering cases carefully.
- ▶ There is significant variation in predictability by judge, conditional on grant rate.
 - ▶ suggests disagreement about circumstances contributing to asylum decision.

Outline

Essentials

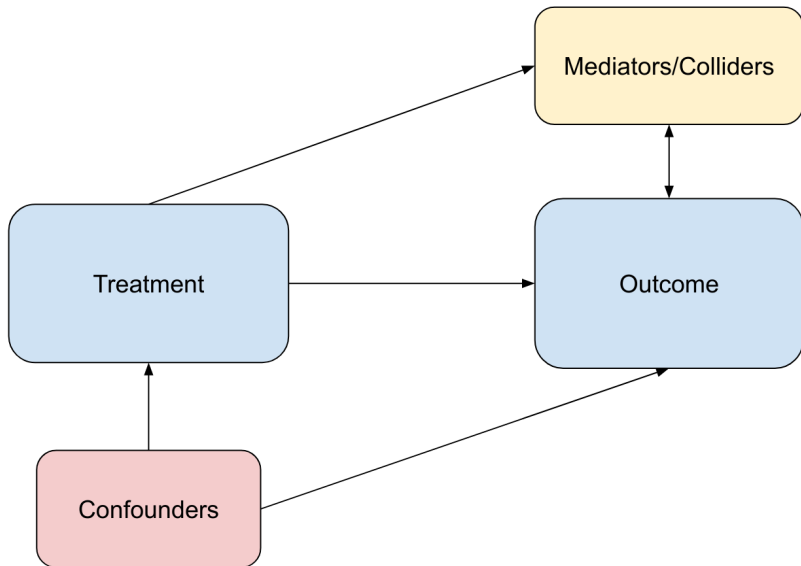
Regression / Regularization

Binary Classification

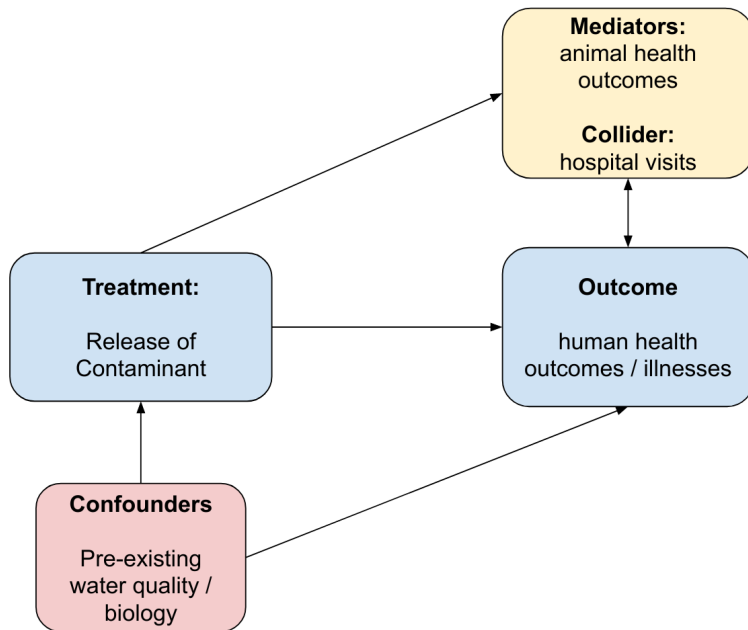
ML Applications

Activity on Causal Graphs

Causal Graphs: Review



Causal Graph Example: Pollution of a River

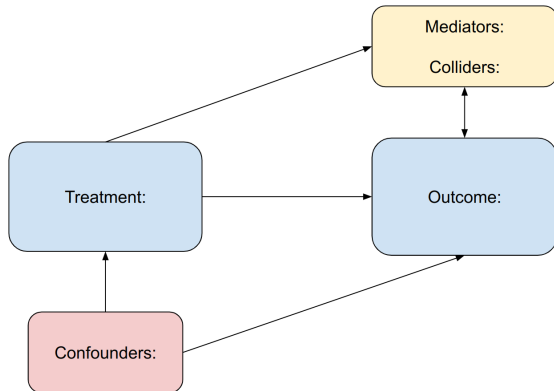


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 - ▶ a research question from your field
 - ▶ a policy you are interested in
 - ▶ a mystery you are fascinated by

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Causal graph template

(also at <http://bit.ly/BRJ-W5A2a>):



- ▶ Draw this template on a piece of paper (recommended), or save a copy of the template
- ▶ Fill in on paper or electronically.
- ▶ Share with neighbors.