CS6375: Machine Learning

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Mid-Term Review

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Machine Learning

- Data is identically and independently distributed
- Goal is to learn a function $\hat{f}$ that maps $\boldsymbol{x}$ to y
- Data is generated using an unknown function f
- Learn a hypothesis h that minimizes some notion of distance/error w.r.t f
- New **test example** is classified using the learned h

blood glucose	body mass idx	diastolic blood pr.	age	Diabetes?
30	120	79	32	NO
22	160	80	63	NO
40	160	93	63	YES
22	160	80	18	NO
45	180	95	49	YES
21	140	99	37	YES
d **data features** (aka attributes, variables)				NO
46	153	110	55	YES

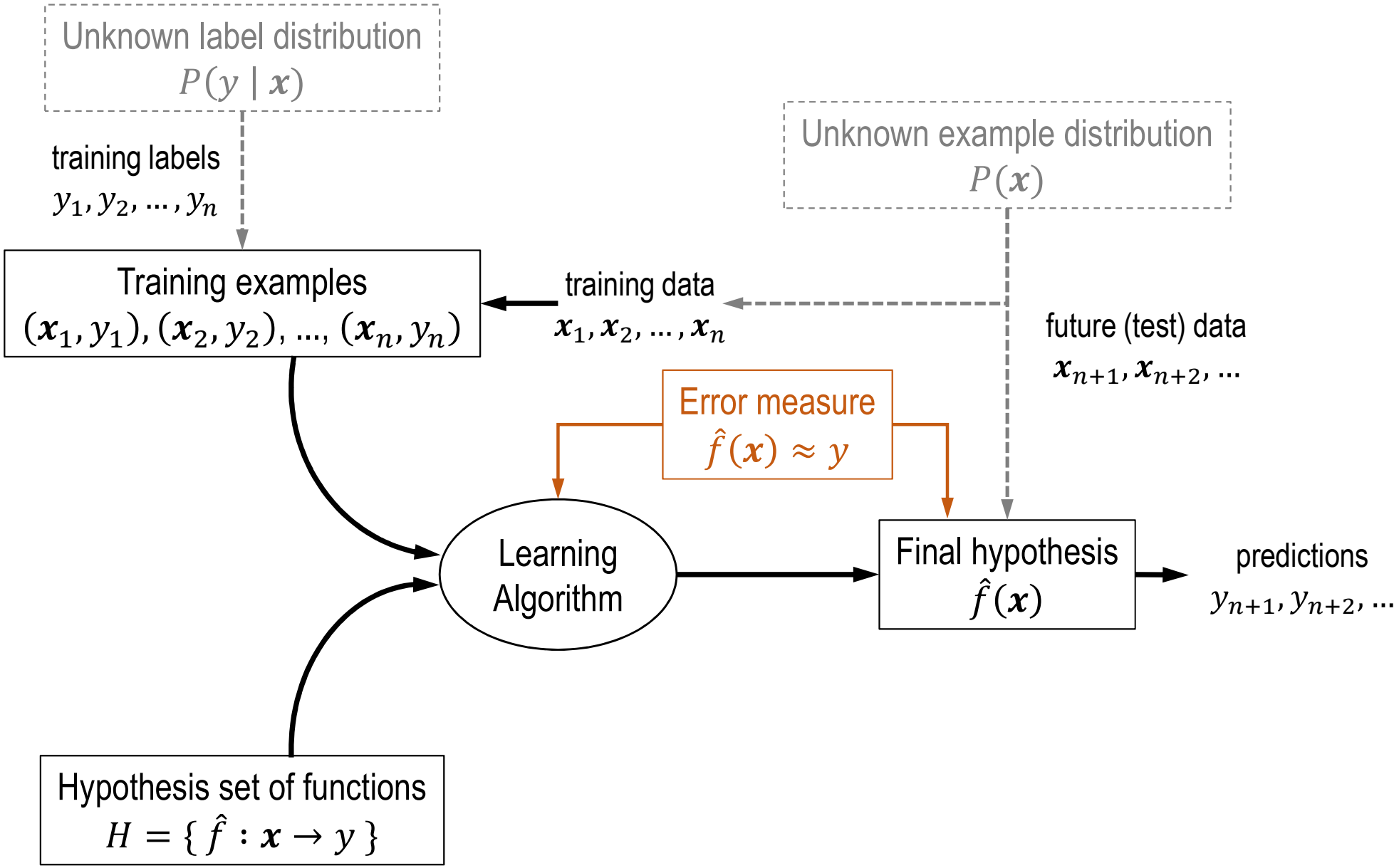
n data examples

attributes and descriptors for each patient are the **features** or **independent variables**
for the i^{th} patient, the k^{th} feature is denoted x_i^k

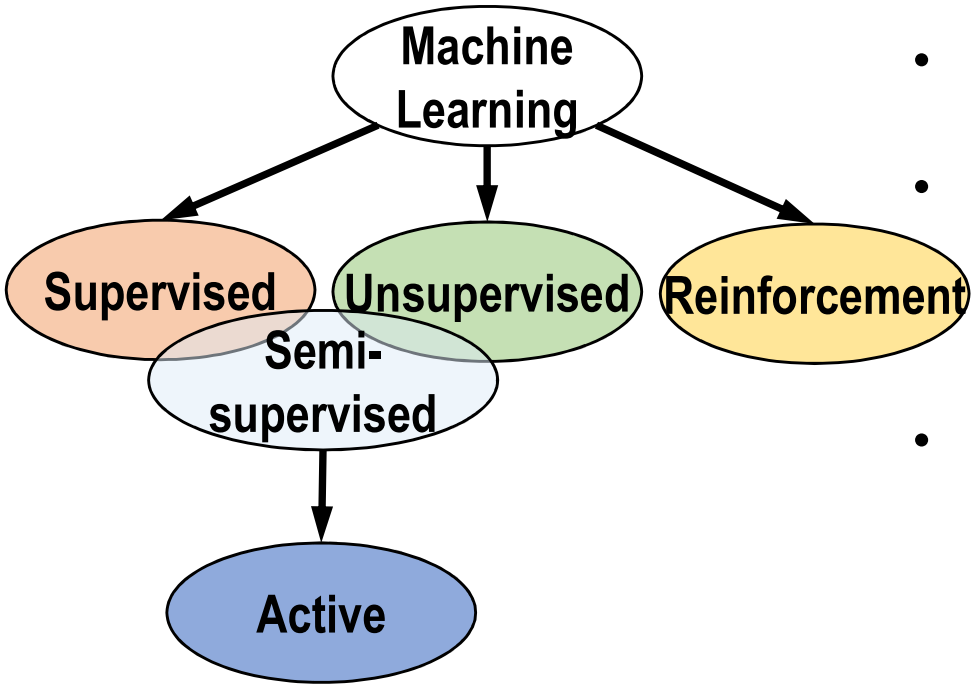
the diagnosis or the **prediction** is the target or the (training) **label**
for the i^{th} patient, denoted y_i

patient features are collected to form a (training) **example**
for the i^{th} patient, denoted $\boldsymbol{x}_i$

Supervised Learning: General Setup



Types of Learning



- **Supervised learning**
  - training data includes desired output
- **Unsupervised learning**
  - training data does not include desired output
- **Semi-supervised learning**
  - some training data comes with desired output
- **Active learning**
  - semi-supervised learning where machine learner can ask for the correct outputs for specific data points
- **Reinforcement learning**
  - Machine learner interacts with the world via allowable actions that change the state of the world and result in rewards
  - learner attempts to maximize rewards through repeated trial and error (*practice makes perfect*)

Discriminative vs. Generative Learning

- **Generative**: Create something that generates ex's
- Can create complete input feature vectors
  - Describes probability distributions for all features
  - Stochastically create a plausible feature vector
  - Example: Naïve Bayes
- Make a model that *generates* positives, negatives
- Classify a test example based on which is more likely to generate it

- **Discriminative**: What differentiates class A from class B?
- Don't try to model all the features, instead focus on the task of categorizing
  - Captures differences between categories
  - May not use all features in models
  - Examples: decision trees, SVMs, neural nets, logistic regression
- Typically more efficient and simpler

Assume some **functional form for P(X|Y), P(Y)**
–Estimate parameters of P(X|Y), P(Y) directly from training data
–Use Bayes rule to calculate P(Y|X= x)
–This is a **'*generative*' model**
•**Indirect** computation of P(Y|X) through Bayes rule
•As a result, **can also generate a sample of the data**, $P(X) = \sum_y P(y)\, P(X|y)$

Discriminative classifiers, e.g., Logistic Regression:
–Assume some **functional form for P(Y|X)**
–Estimate parameters of P(Y|X) directly from training data
–This is the **'*discriminative*' model**
•Directly learn P(Y|X)
•But **cannot obtain a sample of the data**, because P(X) is not available

Linear Regression

Problem Setup: Given data $(\boldsymbol{x}_i)$ and real-valued labels (y_i), find the best model that **fits current data and predicts future data**

Problem: Given n training examples $(\boldsymbol{x}_i, y_i)$, $i = 1, \ldots, n$, find the best model $\boldsymbol{w}$ by solving

$$\underset{\boldsymbol{w}}{\text{minimize}} \ \frac{1}{n}(\boldsymbol{y}^T\boldsymbol{y} - 2\boldsymbol{y}^T X\boldsymbol{w} + \boldsymbol{w}^T X^T X\boldsymbol{w})$$

The solution to this problem is the **ordinary least squares estimator**

$$w = (X^T X)^{-1} X^T \boldsymbol{y}$$

*solution depends on the inverse of the **covariance matrix** $C = X^T X$, which can be **ill-conditioned***

***unique closed-form solution**, provided that number of data points (n) exceeds data dimension (d)*

$(X^T X)^{-1} X^T = X^+$ is called the **pseudo-inverse**

Ridge regression adds L_2 regularization

$$\underset{\boldsymbol{w}}{\text{minimize}} \ \frac{1}{n}(\boldsymbol{y} - X\boldsymbol{w})^T(\boldsymbol{y} - X\boldsymbol{w}) + \lambda \boldsymbol{w}^T\boldsymbol{w}$$

$\boldsymbol{w}^T\boldsymbol{w}$ is a **regularization term** that is used to overcome ill-conditioning, $\lambda > 0$ is the **regularization parameter**, which is **tunable**

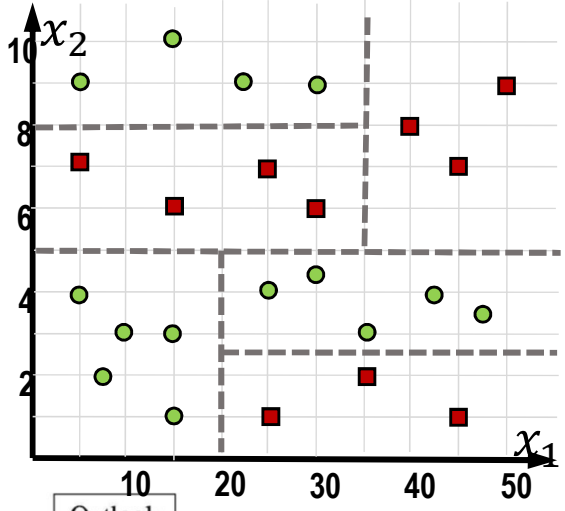
The solution to this problem is the **regularized least squares estimator**

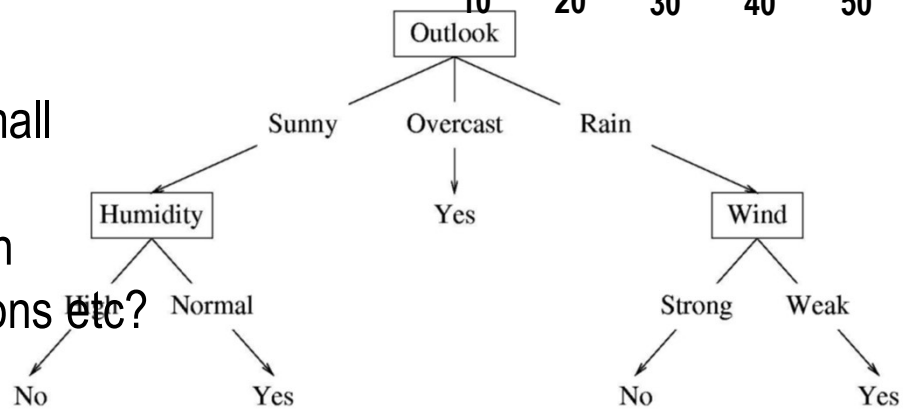
$$w = (X^T X + \lambda I_d)^{-1} X\boldsymbol{y}$$

for $\lambda > 0$, *inverse is can always be computed, algorithm more **robust***

Decision Trees

- Recursively split the features based on some statistical measure – information gain, Mutual Information, gini index p(1-p)
- Splits are binary in general – can you make multi-way split? What will information gain favor? Binary or multi-way?
- What is a decision stump?
- How does the decision boundary look like?
- Pruning will allow decision trees to have a reduced depth
- When will decision trees overfit? What will you prefer – small depths or a very large depth?
- Expressiveness – Can they represent an arbitrary Boolean function? How about a disjunction of conjunctions, negations etc?
- How can you avoid overfitting?
- When do they have bias? When do they exhibit variance?





Mutual information/information gain is used to select next attribute

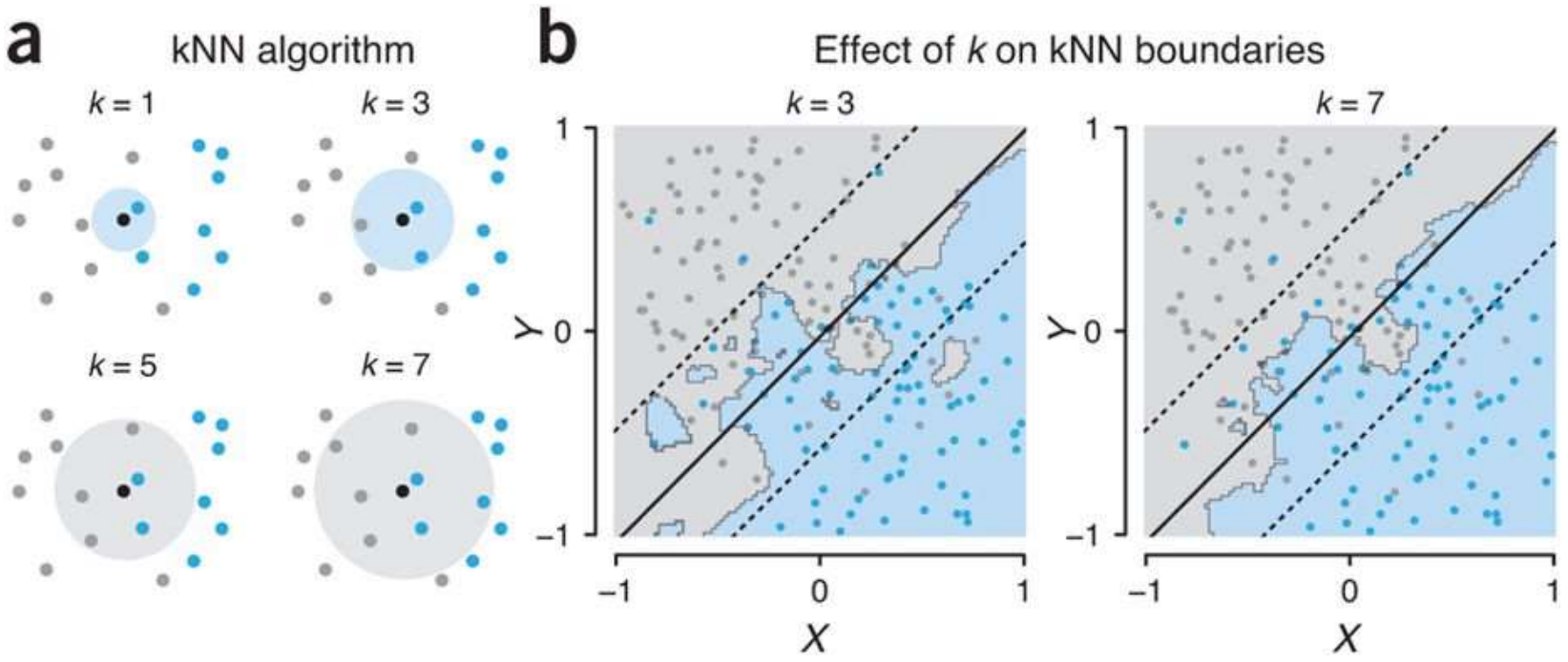
$$H(Y) = -\sum_{y} P(Y = y)\mathbf{log_2}\,\mathrm{P}(Y = y)$$

$$H(Y|X) = -\sum_{x} P(X = x)\sum_{y} P(Y = y \mid X = x)\ \log_2 (Y = y \mid X = x)$$

$$I(X, Y) = H(Y) - H(Y|X)$$

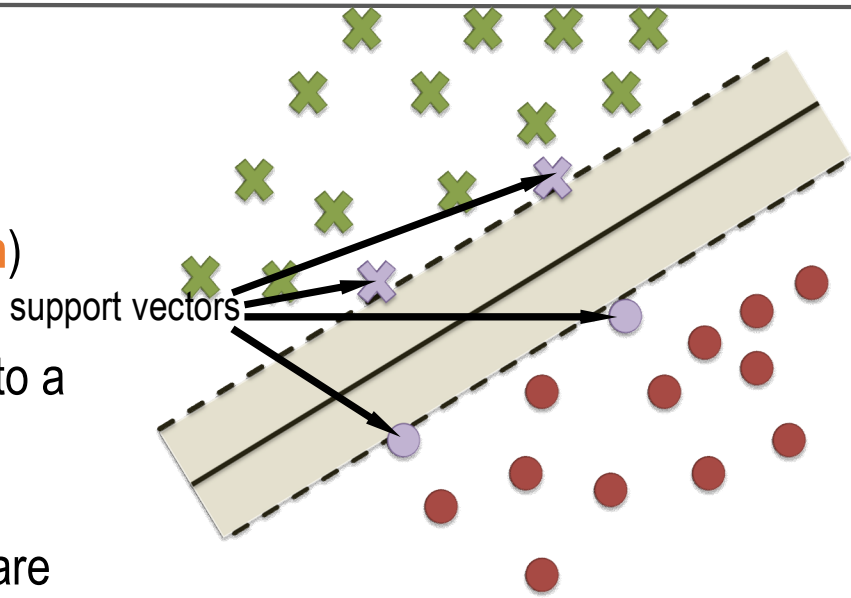
K-Nearest Neighbor

- Lazy algorithm: does not build a classifier from all data. Instead builds as every example comes in
- Decision boundaries are drawn between examples of **opposite** classes. What are distance measures?
- Complex decision boundaries – Voronoi diagram. Small k leads to more complex decision boundaries
- **Choosing k**: increasing k reduces variance, increases bias
- How does noise affect NN? How can their effect be reduced?
- For high-dimensional space, problem that the nearest neighbor may not be very close at all!



Support Vector Machines

- In the simplest case, SVMs search for the hyperplane that maximizes the separation between the two classes (**margin**)
- The minimization problem is a quadratic optimization with linear inequality constraints. The key idea is to convert this to a dual problem with smaller number of constraints
- Hypothesis is a linear combination of training examples
  - only some training examples have non-zero weights, are called **support vectors**
- Can replace the inner product in the dual formulation with a **kernel**; called the **kernel trick**
- What can be represented? When can SVMs overfit? How can you prevent that? (Hint: Think linear SVMs vs non-linear SVMs.)
- When do they have bias? When do they exhibit variance?



soft-margin support vector machine

$$\min \quad \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{n}\xi_i$$

$$\text{s.t.} \quad y_i(\mathbf{w}'\mathbf{x}_i - b) \geq 1 - \xi_i \quad \forall i = 1 \ldots n$$

$$\xi_i \geq 0$$

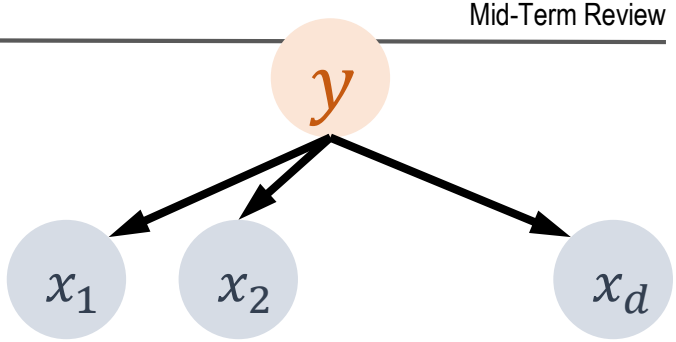
soft-margin svm dual

$$\max \quad -\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j y_i y_j \mathbf{x}_i'\mathbf{x}_j + \sum_{i=1}^{n}\alpha_i$$

$$\text{s.t.} \quad \sum_{i=1}^{n}\alpha_i y_i = 0$$

$$0 \leq \alpha_i \leq C, \quad \forall i = 1 \ldots n$$

Naïve Bayes



- **Generative model** – Learns the joint distribution of the labels and features P(y,**x**)
- **Naïve Bayes assumption**: **features are conditionally independent given** y that is,

$$P(x_1, x_2, \ldots, x_d|y) = \prod_{j=1}^{d} P(x_j|y)$$

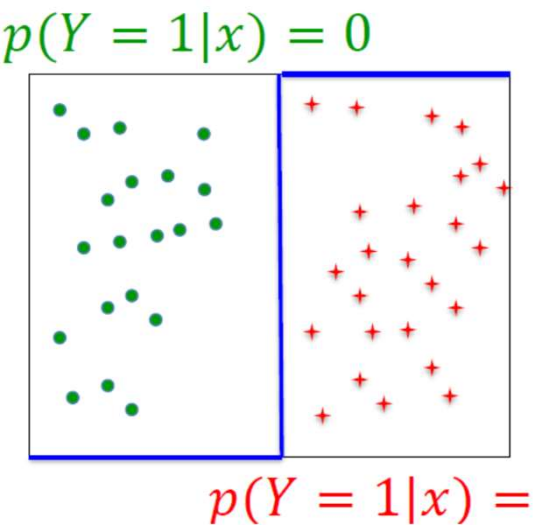
- When is that a good one? When is it a bad assumption?
- Learning is very simple with **maximum likelihood estimation** (MLE).

$$y = \underset{y}{\operatorname{argmax}}\, P(y|\boldsymbol{x}) = \underset{y}{\operatorname{argmax}}\, P(y) \cdot \prod_{j=1}^{d} P(x_j|y)$$

What is the issue with a simple MLE? How can you fix this?

- Can handle a variety of data types. Why?
- First thing to try in most problems – simple yet very efficient
- When do they have bias? When do they exhibit variance?

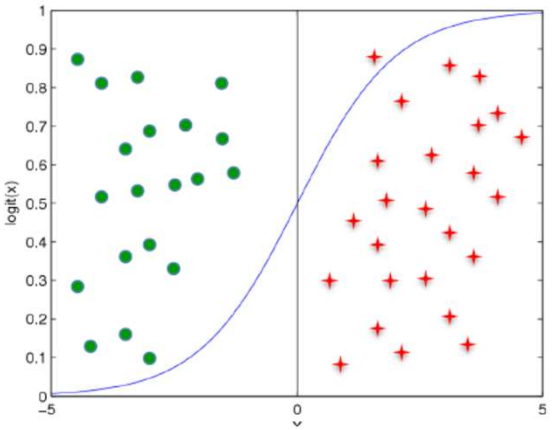
Logistic Regression



Logistic Loss Function: (probabilities from hard classification)
Learn or $p(y|\boldsymbol{x})$ directly from the data

- Assume a functional form, (e.g., a linear classifier $f(\boldsymbol{x}) = \boldsymbol{w}^T\boldsymbol{x} + b$) such that
- $p(y = -1|\,\boldsymbol{x}) = \frac{1}{1+\exp\,(\boldsymbol{w}^T\boldsymbol{x}+b)}$ on one side and
- $p(y = 1|\,\boldsymbol{x}) = \frac{\exp(\boldsymbol{w}^T\boldsymbol{x}+b)}{1+\exp\,(\boldsymbol{w}^T\boldsymbol{x}+b)}$ on the other side

  that is $p(y = -1|\,\boldsymbol{x}) = 1 - p(y = 1|\,\boldsymbol{x})$
- Differentiable, easy to learn, handles noisy labels naturally



Logistic regression **implements a linear classifier** as it maximizes the **log-odds of a training example** belonging to class $y = 1$ are:

$$\log\frac{p(y = 1|\,\boldsymbol{x})}{p(y = -1|\,\boldsymbol{x})} = \boldsymbol{w}^T\boldsymbol{x} + b$$

Consider a **prior distribution** on the weights to prevent overfitting

- assume weights from a normal distribution with zero mean, identity covariance:

$$\mathrm{P}(\boldsymbol{w}) = \frac{1}{\sqrt{2\pi\sigma^2}}\exp\left(-\frac{\|\boldsymbol{w}\|^2}{2\sigma^2}\right)$$

- **maximizing** $\mathrm{P}(\boldsymbol{w})$ pushes weights to zero, which **minimizes the complexity** of classifier; also helps avoid large weights and overfitting

taking the logarithm gives us $\log \mathrm{P}(\boldsymbol{w}) = -\|\boldsymbol{w}\|^2 + \text{const}$

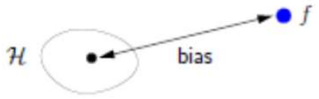
$$\max_{\boldsymbol{w},b}\sum_{i=1}^{n} y_i(\boldsymbol{w}^T\boldsymbol{x}_i + b) - \log(1 + \exp(\boldsymbol{w}^T\boldsymbol{x}_i + b)) \quad -\frac{\lambda}{2}\|\boldsymbol{w}\|^2$$

The Bias-Variance Decomposition

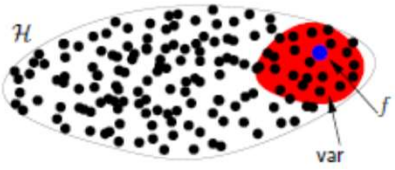
test error *learned model* *true model*

$$
\begin{aligned}
E_{\text{out}}(\mathbf{x}) &= \mathbb{E}_{\mathcal{D}}\left[(g^{\mathcal{D}}(\mathbf{x}) - f(\mathbf{x}))^2\right] \\
&= \mathbb{E}_{\mathcal{D}}\left[g^{\mathcal{D}}(\mathbf{x})^2 - 2g^{\mathcal{D}}(\mathbf{x})f(\mathbf{x}) + f(\mathbf{x})^2\right] \\
&= \mathbb{E}_{\mathcal{D}}\left[g^{\mathcal{D}}(\mathbf{x})^2\right] - 2\bar{g}(\mathbf{x})f(\mathbf{x}) + f(\mathbf{x})^2 \qquad \leftarrow \text{understand this; the rest is just algebra} \\
&= \mathbb{E}_{\mathcal{D}}\left[g^{\mathcal{D}}(\mathbf{x})^2\right] - \bar{g}(\mathbf{x})^2 + \bar{g}(\mathbf{x})^2 - 2\bar{g}(\mathbf{x})f(\mathbf{x}) + f(\mathbf{x})^2 \\
&= \underbrace{\mathbb{E}_{\mathcal{D}}\left[g^{\mathcal{D}}(\mathbf{x})^2\right] - \bar{g}(\mathbf{x})^2}_{\text{var}(\mathbf{x})} + \underbrace{(\bar{g}(\mathbf{x}) - f(\mathbf{x}))^2}_{\text{bias}(\mathbf{x})}
\end{aligned}
$$

$$E_{\text{out}}(\mathbf{x}) = \text{bias}(\mathbf{x}) + \text{var}(\mathbf{x})$$



Very small model

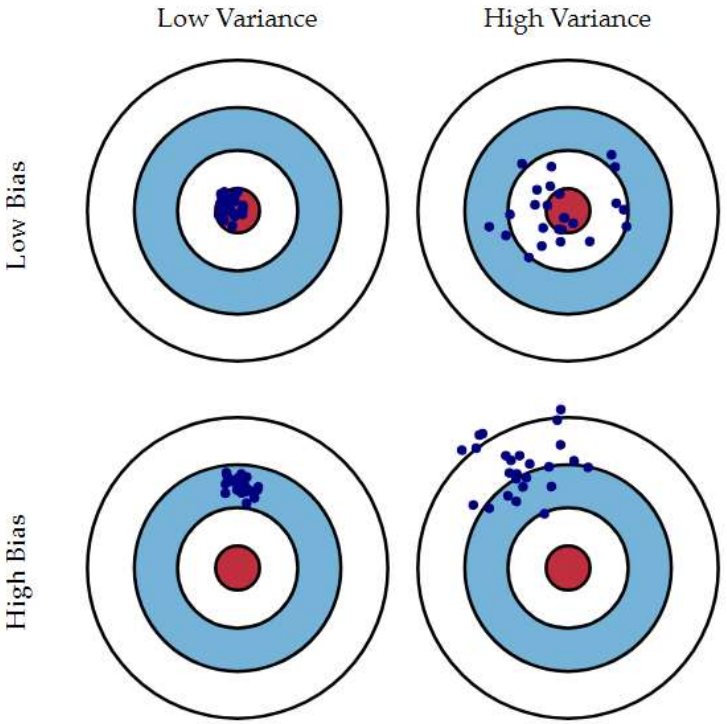


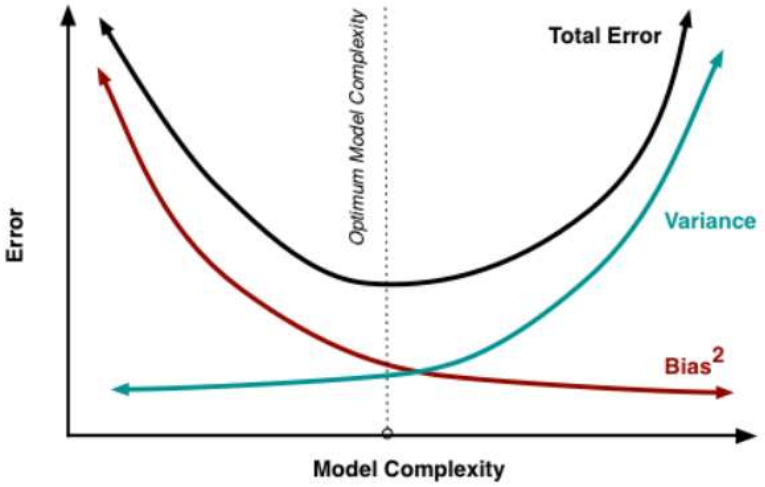
Very large model

If you take average over $\mathbf{x}$: $E_{\text{out}} = \text{bias} + \text{var}$

The Bias-Variance Tradeoff

Logistic regression, linear regression, SVM, neural networks with an $\lambda \|w\|_2^2$ (L2) penalty in the objective	Higher λ means... more/less **variance** more/less **bias**
Logistic regression, linear regression, SVM, neural networks with an $\lambda \|w\|_1$ (L2) penalty in the objective	Higher λ means... more/less **variance** more/less **bias**
Decision tree: n, an upper limit on the number of nodes in the tree	Higher n means... more/less **variance** more/less **bias**
Feature selection with mutual information scoring: include a feature in the model only if its MI(feat, class) is higher than a threshold t	Higher t means... more/less **variance** more/less **bias**
Increasing k in k-nearest neighbor models	Higher k means... more/less **variance** more/less **bias**
Removing all the non-support vectors in an SVM	This means... more/less **variance** more/less **bias**
Dimension reduction as preprocessing: instead of using all features, reduce the training data down to k dimensions	Higher k means... more/less **variance** more/less **bias**



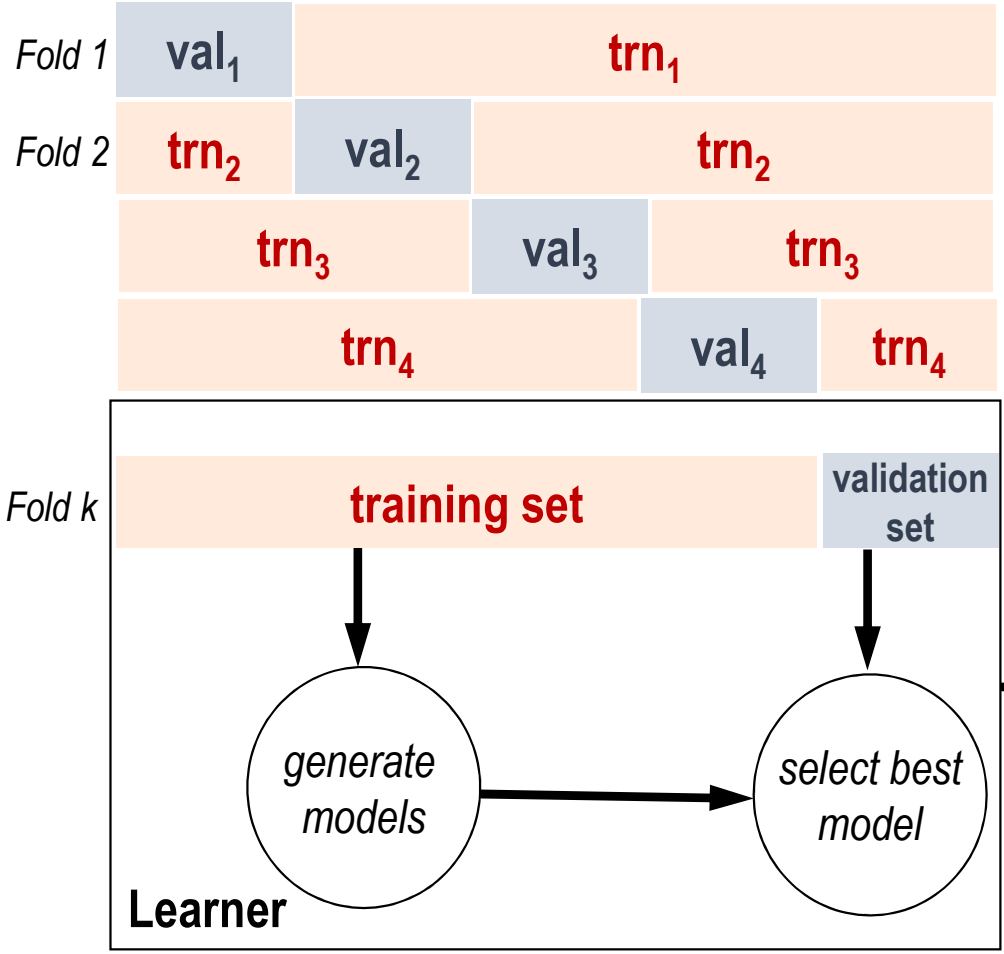


Cross Validation

Using a **single** tuning set can be **unreliable** predictor, plus some data "**wasted**"; cross validation can help with **model selection**:

For each possible set of parameters, θ_p
- Divide training data into k **folds**
- **train** k models using trn_k with θ_p
- score k models using val_k
- average **tuning set score** over the k models

Use **best** set of parameters θ_* and **all (train + tune)** examples to train the best model
Apply resulting model to **test set**



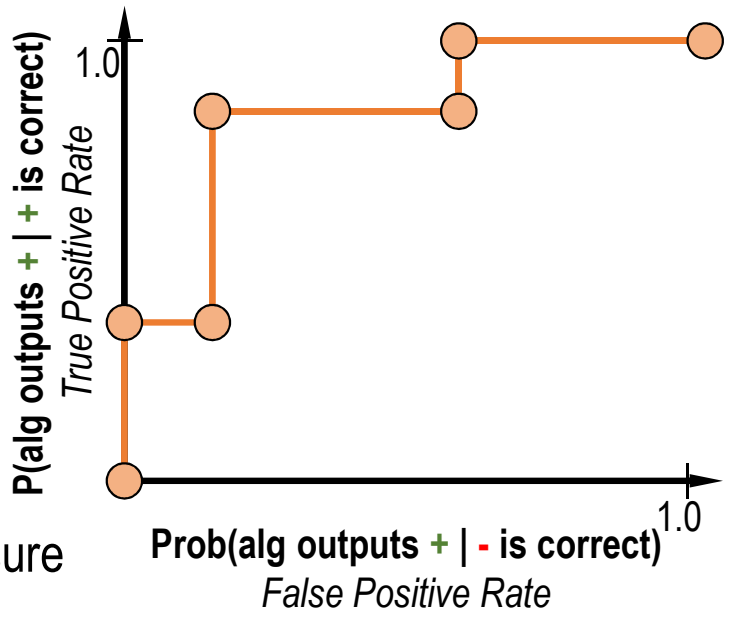
Receiver-Operator Characteristic Curves

An **ROC curve** (receiver operating characteristic curve) is a graph showing the performance of a classification model at **all classification thresholds**.

- judging algorithms on accuracy alone may not be good enough when getting a positive example wrong **costs more** than getting a negative example wrong (**or vice versa**)
- **lowering** the classification **threshold** classifies **more** items as **positive**, thus increasing both False Positives and True Positives

Procedure to construct an ROC curve:

- **sort** predictions on test set
- locate a **threshold** between examples with opposite categories
- **compute** TPR & FPR for each threshold
- **connect** the dots



Area under the ROC Curve (AUC) provides an aggregate measure of performance across all possible classification thresholds

- One way of interpreting AUC is as the **probability** that the model ranks a random **positive example** more **highly** than a random **negative example**
- can compare performance of different algorithms using AUC
- can use AUC/ROC to select a good threshold for classification in order to weight false positives and false negatives differently

Evaluation: Precision and Recall

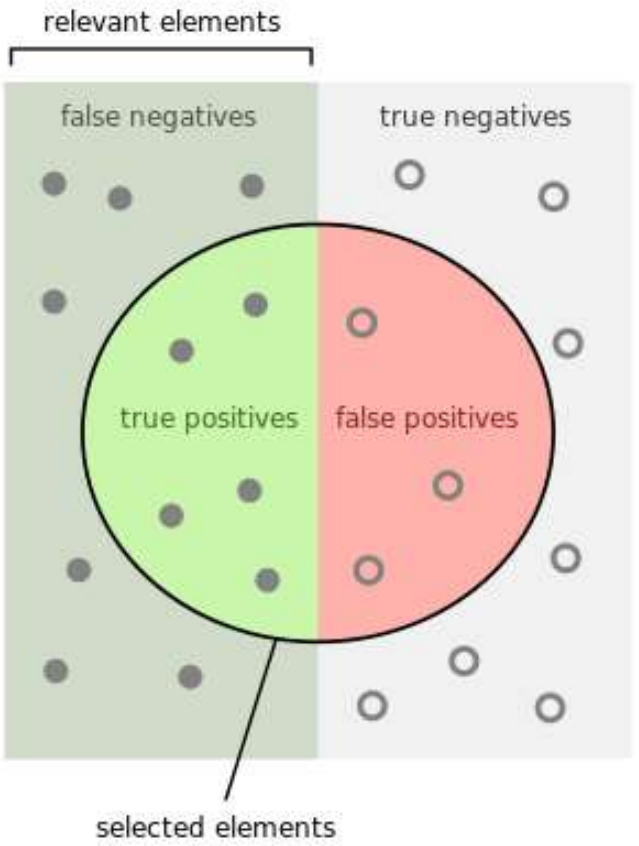
precision $= \frac{\#\ of\ relevant\ items\ retrieved}{total\ \#\ of\ items\ retrieved} = \frac{TP}{TP+FP}$

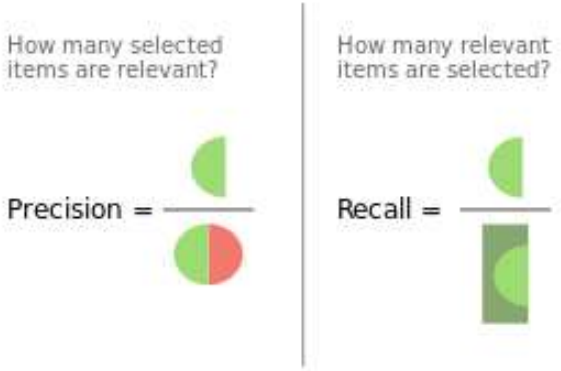
interpretation: Prob(is positive | called positive)

recall $= \frac{\#\ of\ relevant\ items\ retrieved}{total\ \#\ of\ items\ that\ exist} = \frac{TP}{TP+FN}$

interpretation: Prob(called positive | is positive)

Notice that the count of true negatives (TN) is not used in either formula; therefore you get **no credit for filtering out irrelevant items**





Case Study 1: For applications such as **medical diagnosis,** require **high recall to reduce false negatives**

Case Study 2: For applications such as **spam-filtering** and **recommendations systems**, require **high precision to reduce false positives**