Introduction to Machine Learning

Greg Mori - CMPT 419/726

Bishop PRML Ch. 1

Outline

Administrivia

- We will cover techniques in the standard ML toolkit 

    - maximum likelihood, regularization, neural networks, stochastic gradient descent, principal components analysis (PCA), Markov random fields (MRF), graphical models, belief propagation, Markov Chain Monte Carlo (MCMC), hidden Markov models (HMM), particle filters, recurrent neural networks (RNNs), long short-term memory (LSTM), generative adversarial networks (GANs), variational auto-encoders (VAEs), ...
- There will be 3 assignments
- Exam in class on Dec. 2

Administrivia

- Recommend doing associated readings from Bishop, *Pattern Recognition and Machine Learning* (PRML) after each lecture
    - Reference books for alternate descriptions
        - *The Elements of Statistical Learning*, Trevor Hastie, Robert Tibshirani, and Jerome Friedman
        - *Information Theory, Inference, and Learning Algorithms*, David MacKay (available online)
        - *Deep Learning*, Ian Goodfellow, Yoshua Bengio and Aaron Courville (available online)
    - Online courses
        - Coursera, Udacity

Administrivia - Assignments

- Assignment late policy
  - 3 *grace days*, use at your discretion (not on project)
- Programming assignments use Python

Administrivia - Project

- Project details
  - Practice doing research
  - Ideal project – take problem from your research/interests, use ML (properly)
  - Other projects fine too ($1 million project: `http://netflixprize.com`)
    - Too late :(
    - Others on `http://www.kaggle.com`

Administrivia - Project

- Project details
  - Work in groups (up to 5 students)
  - Produce (short) research paper
  - Graded on proper research methodology, not just results
    - Choice of problem / algorithms
    - Relation to previous work
    - Comparative experiments
    - Quality of exposition
  - Details on course webpage
    - Poster session Dec. 8, 4-7pm Downtown Vancouver (tentative)
    - Report due Dec. 13 at 11:59pm

Administrivia - Office Hours

- Blocks (sections)
  - Block 1: Grad students, CMPT MSc/PhD thesis, other
  - Block 2: Grad students, CMPT Prof. MSc (last name A-L)
  - Block 3: Grad students, CMPT Prof. MSc (last name M-Z)
- See schedule on course website
- Please attend office hours for your block, priority given to corresponding students
- Will have separate, bookable office hours for project groups

Administrivia - Background

- Calculus:
$$E = mc^2 \Rightarrow \frac{\partial E}{\partial c} = 2mc$$
- Linear algebra:
$$\boldsymbol{A}\boldsymbol{u}_i = \lambda_i \boldsymbol{u}_i; \ \frac{\partial}{\partial \boldsymbol{x}}(\boldsymbol{x}^T \boldsymbol{a}) = \boldsymbol{a}$$
  - See PRML Appendix C
- Probability:
$$p(X) = \sum_Y p(X, Y); \ p(x) = \int p(x, y)dy; \ \mathbb{E}_x[f] = \int p(x)f(x)dx$$
  - See PRML Ch. 1.2

PARENTAL ADVISORY EXPLICIT LYRICS — It will be possible to refresh, but if you've never seen these before this course will be **very** difficult.

What is Machine Learning (ML)?

- Algorithms that automatically improve performance through experience
- Often this means define a model by hand, and use data to fit its parameters

Why ML?

- The real world is complex – difficult to hand-craft solutions.
- ML is the preferred framework for applications in many fields:
  - Computer Vision
  - Natural Language Processing, Speech Recognition
  - Robotics
  - ...

Hand-written Digit Recognition

Belongie et al. PAMI 2002

- Difficult to hand-craft rules about digits

Hand-written Digit Recognition

$x_i =$  $t_i = (0, 0, 0, 1, 0, 0, 0, 0, 0, 0)$

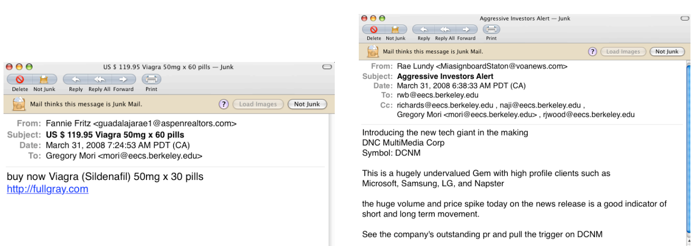
- Represent input image as a vector $x_i \in \mathbb{R}^{784}$.
- Suppose we have a target vector t_i
  - This is supervised learning
  - Discrete, finite label set: perhaps $t_i \in \{0, 1\}^{10}$, a classification problem
- Given a training set $\{(x_1, t_1), \ldots, (x_N, t_N)\}$, learning problem is to construct a "good" function $y(x)$ from these.
  - $y : \mathbb{R}^{784} \to \mathbb{R}^{10}$

Face Detection

Schneiderman and Kanade, IJCV 2002

- Classification problem
- $t_i \in \{0, 1, 2\}$, non-face, frontal face, profile face.

Spam Detection



- Classification problem
- $t_i \in \{0, 1\}$, non-spam, spam
- x_i counts of words, e.g. `Viagra`, `stock`, `outperform`, `multi-bagger`

Caveat - Horses (source?)

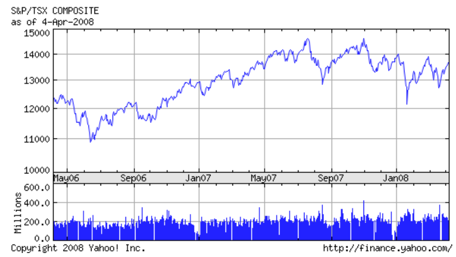
- Once upon a time there were two neighboring farmers, Jed and Ned. Each owned a horse, and the horses both liked to jump the fence between the two farms. Clearly the farmers needed some means to tell whose horse was whose.
- So Jed and Ned got together and agreed on a scheme for discriminating between horses. Jed would cut a small notch in one ear of his horse. Not a big, painful notch, but just big enough to be seen. Well, wouldn't you know it, the day after Jed cut the notch in horse's ear, Ned's horse caught on the barbed wire fence and tore his ear the exact same way!
- Something else had to be devised, so Jed tied a big blue bow on the tail of his horse. But the next day, Jed's horse jumped the fence, ran into the field where Ned's horse was grazing, and chewed the bow right off the other horse's tail. Ate the whole bow!

Caveat - Horses (source?)

- Finally, Jed suggested, and Ned concurred, that they should pick a feature that was less apt to change. Height seemed like a good feature to use. But were the heights different? Well, each farmer went and measured his horse, and do you know what? The brown horse was a full inch taller than the white one!

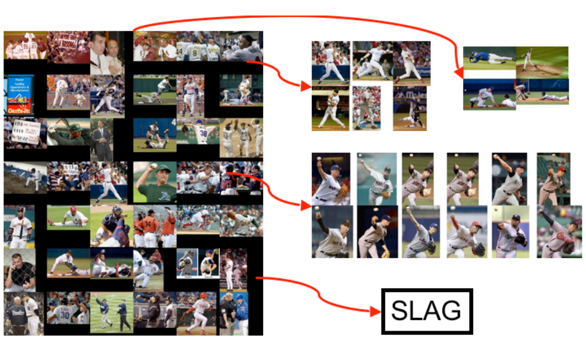
Moral of the story: ML provides theory and tools for setting parameters. Make sure you have the right model and inputs.

Stock Price Prediction



- Problems in which t_i is continuous are called regression
- E.g. t_i is stock price, x_i contains company profit, debt, cash flow, gross sales, number of spam emails sent, . . .

Clustering Images



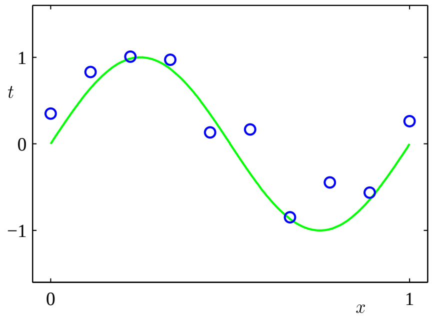
Wang et al., CVPR 2006

- Only x_i is defined: unsupervised learning
- E.g. x_i describes image, find groups of similar images

Types of Learning Problems

- Supervised Learning
  - Classification
  - Regression
- Unsupervised Learning
- Reinforcement Learning
  - maybe just a little

An Example - Polynomial Curve Fitting



- Suppose we are given training set of N observations $(x_1, \ldots, x_N)$ and $(t_1, \ldots, t_N)$, $x_i, t_i \in \mathbb{R}$
- Regression problem, estimate $y(x)$ from these data

Polynomial Curve Fitting

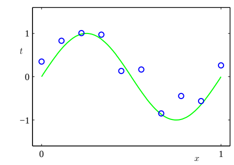
- What form is $y(x)$?
  - Let's try polynomials of degree M:

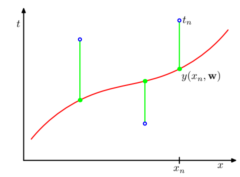
$$y(x, \boldsymbol{w}) = w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M$$

    - This is the hypothesis space.
- How do we measure success?
  - Sum of squared errors:

$$E(\boldsymbol{w}) = \frac{1}{2} \sum_{n=1}^{N} \{y(x_n, \boldsymbol{w}) - t_n\}^2$$

- Among functions in the class, choose that which minimizes this error





Polynomial Curve Fitting

- Error function

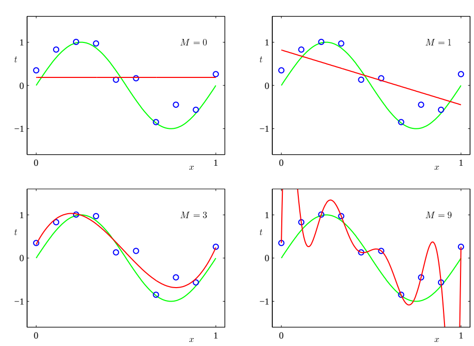
$$E(\boldsymbol{w}) = \frac{1}{2} \sum_{n=1}^{N} \{y(x_n, \boldsymbol{w}) - t_n\}^2$$

- Best coefficients

$$\boldsymbol{w}^* = \arg\min_{\boldsymbol{w}} E(\boldsymbol{w})$$

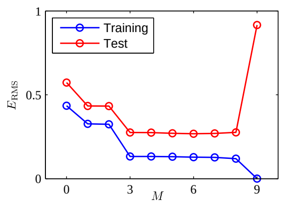
- Found using pseudo-inverse (more later)

Which Degree of Polynomial?



- A model selection problem
- $M = 9 \rightarrow E(\boldsymbol{w}^*) = 0$: This is over-fitting

Generalization

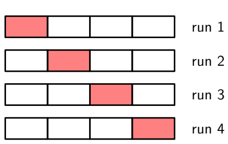


- Generalization is the holy grail of ML
  - Want good performance for new data
- Measure generalization using a separate set
  - Use root-mean-squared (RMS) error: $E_{RMS} = \sqrt{2E(\mathbf{w}^*)/N}$

Validation Set

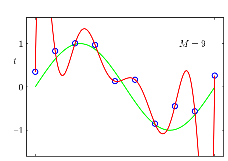
- Split training data into training set and validation set
- Train different models (e.g. diff. order polynomials) on training set
- Choose model (e.g. order of polynomial) with minimum error on validation set

Cross-validation



- Data are often limited
- Cross-validation creates S groups of data, use $S-1$ to train, other to validate
  - Extreme case leave-one-out cross-validation (LOO-CV): S is number of training data points
- Cross-validation is an effective method for model selection, but can be slow
  - Models with multiple complexity parameters: exponential number of runs

Controlling Over-fitting: Regularization

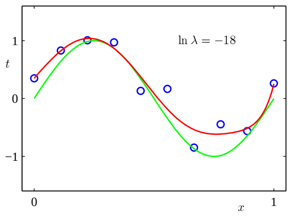


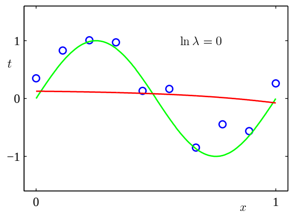
	$M=0$	$M=1$	$M=3$	$M=9$
$w_0^\star$	0.19	0.82	0.31	0.35
$w_1^\star$		-1.27	7.99	232.37
$w_2^\star$			-25.43	-5321.83
$w_3^\star$			17.37	48568.31
$w_4^\star$				-231639.30
$w_5^\star$				640042.26
$w_6^\star$				-1061800.52
$w_7^\star$				1042400.18
$w_8^\star$				-557682.99
$w_9^\star$				125201.43

- As order of polynomial M increases, so do coefficient magnitudes
- Penalize large coefficients in error function:

$$\tilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n, \mathbf{w}) - t_n\}^2 + \frac{\lambda}{2}||\mathbf{w}||^2$$

Controlling Over-fitting: Regularization

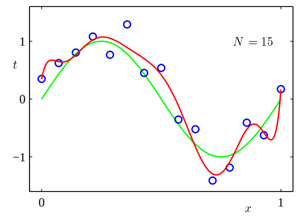


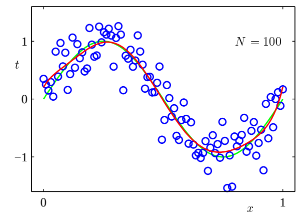


	$\ln \lambda = -\infty$	$\ln \lambda = -18$	$\ln \lambda = 0$
$w_0^\star$	0.35	0.35	0.13
$w_1^\star$	232.37	4.74	-0.05
$w_2^\star$	-5321.83	-0.77	-0.06
$w_3^\star$	48568.31	-31.97	-0.05
$w_4^\star$	-231639.30	-3.89	-0.03
$w_5^\star$	640042.26	55.28	-0.02
$w_6^\star$	-1061800.52	41.32	-0.01
$w_7^\star$	1042400.18	-45.95	-0.00
$w_8^\star$	-557682.99	-91.53	0.00
$w_9^\star$	125201.43	72.68	0.01

Fits for $M = 9$

Over-fitting: Dataset size





- With more data, more complex model ($M = 9$) can be fit
- Rule of thumb: 10 datapoints for each parameter

Summary

- Want models that generalize to new data
  - Train model on training set
  - Measure performance on held-out test set
    - Performance on test set is good estimate of performance on new data

Summary - Model Selection

- Which model to use? E.g. which degree polynomial?
  - Training set error is lower with more complex model
    - Can't just choose the model with lowest training error
  - Peeking at test error is unfair. E.g. picking polynomial with lowest test error
    - Performance on test set is no longer good estimate of performance on new data

Summary - Solutions I

- Use a validation set
  - Train models on training set. E.g. different degree polynomials
  - Measure performance on held-out validation set
  - Measure performance of that model on held-out test set
- Can use cross-validation on training set instead of a separate validation set if little data and lots of time
  - Choose model with lowest error over all cross-validation folds (e.g. polynomial degree)
  - Retrain that model using all training data (e.g. polynomial coefficients)

Summary - Solutions II

- Use regularization
  - Train complex model (e.g high order polynomial) but penalize being "too complex" (e.g. large weight magnitudes)
  - Need to balance error vs. regularization (λ)
    - Choose λ using cross-validation
- Get more data

Bayesianity

- Frequentist view – probabilites are frequencies of random, repeatable events
- Bayesian view – probability quantifies uncertain beliefs
- Important distinction for us: Bayesianity allows us to discuss probability distributions over parameters (such as $\boldsymbol{w}$)
  - Include priors (e.g. $p(\boldsymbol{w})$) over model parameters
- Later, we will see Bayesian approaches to combatting over-fitting and model selection for curve fitting
- For now, an illustrative example . . .

Coin Tossing

- Let's say you're given a coin, and you want to find out $P(heads)$, the probability that if you flip it it lands as "heads".
- Flip it a few times: $H\ H\ T$
- $P(heads) = 2/3$, no need for CMPT726
- Hmm... is this rigorous? Does this make sense?

Coin Tossing - Model

- Bernoulli distribution $P(heads) = \mu$, $P(tails) = 1 - \mu$
- Assume coin flips are independent and identically distributed (i.i.d.)
  - i.e. All are separate samples from the Bernoulli distribution
- Given data $\mathcal{D} = \{x_1, \ldots, x_N\}$, heads: $x_i = 1$, tails: $x_i = 0$, the likelihood of the data is:

$$p(\mathcal{D}|\mu) = \prod_{n=1}^{N} p(x_n|\mu) = \prod_{n=1}^{N} \mu^{x_n}(1-\mu)^{1-x_n}$$

Maximum Likelihood Estimation

- Given $\mathcal{D}$ with h heads and t tails
- What should μ be?
- Maximum Likelihood Estimation (MLE): choose μ which maximizes the likelihood of the data

$$\mu_{ML} = \arg\max_{\mu} p(\mathcal{D}|\mu)$$

- Since $\ln(\cdot)$ is monotone increasing:

$$\mu_{ML} = \arg\max_{\mu} \ln p(\mathcal{D}|\mu)$$

Maximum Likelihood Estimation

- Likelihood:

$$p(\mathcal{D}|\mu) = \prod_{n=1}^{N} \mu^{x_n}(1-\mu)^{1-x_n}$$

- Log-likelihood:

$$\ln p(\mathcal{D}|\mu) = \sum_{n=1}^{N} x_n \ln \mu + (1-x_n)\ln(1-\mu)$$

- Take derivative, set to 0:

$$\frac{d}{d\mu} \ln p(\mathcal{D}|\mu) = \sum_{n=1}^{N} x_n \frac{1}{\mu} - (1-x_n)\frac{1}{1-\mu} = \frac{1}{\mu}h - \frac{1}{1-\mu}t$$

$$\Rightarrow \mu = \frac{h}{t+h}$$

Bayesian Learning

- Wait, does this make sense? What if I flip 1 time, heads? Do I believe μ=1?
- Learn μ the Bayesian way:

$$P(\mu|\mathcal{D}) = \frac{P(\mathcal{D}|\mu)P(\mu)}{P(\mathcal{D})}$$

$$\underbrace{P(\mu|\mathcal{D})}_{posterior} \propto \underbrace{P(\mathcal{D}|\mu)}_{likelihood}\underbrace{P(\mu)}_{prior}$$

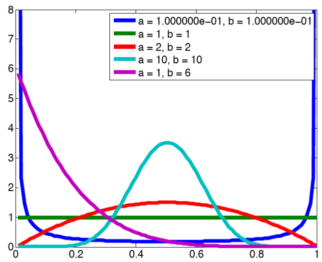
- Prior encodes knowledge that most coins are 50-50
- Conjugate prior makes math simpler, easy interpretation
  - For Bernoulli, the beta distribution is its conjugate

Beta Distribution

- We will use the Beta distribution to express our prior knowledge about coins:

$$Beta(\mu|a,b) = \underbrace{\frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}}_{normalization} \mu^{a-1}(1-\mu)^{b-1}$$

- Parameters a and b control the shape of this distribution



Posterior

$$\begin{aligned} P(\mu|\mathcal{D}) &\propto P(\mathcal{D}|\mu)P(\mu) \\ &\propto \underbrace{\prod_{n=1}^{N} \mu^{x_n}(1-\mu)^{1-x_n}}_{likelihood} \underbrace{\mu^{a-1}(1-\mu)^{b-1}}_{prior} \\ &\propto \mu^h(1-\mu)^t \mu^{a-1}(1-\mu)^{b-1} \\ &\propto \mu^{h+a-1}(1-\mu)^{t+b-1} \end{aligned}$$

- Simple form for posterior is due to use of conjugate prior
- Parameters a and b act as extra observations
- Note that as $N = h + t \to \infty$, prior is ignored

Maximum A Posteriori

- Given posterior $P(\mu|\mathcal{D})$ we could compute a single value, known as the Maximum a Posteriori (MAP) estimate for μ:

$$\mu_{MAP} = \arg\max_{\mu} P(\mu|\mathcal{D})$$

  - Known as point estimation

Bayesian Learning

- However, correct Bayesian thing to do is to use the full distribution over μ
  - i.e. Compute

$$\mathbb{E}_{\mu}[f] = \int p(\mu|\mathcal{D})f(\mu)d\mu$$

  - This integral is usually hard to compute

Conclusion

- Readings: Ch. 1.1-1.3, 2.1
- Types of learning problems
  - Supervised: regression, classification
  - Unsupervised
- Learning as optimization
  - Squared error loss function
  - Maximum likelihood (ML)
  - Maximum a posteriori (MAP)
- Want generalization, avoid over-fitting
  - Cross-validation
  - Regularization
  - Bayesian prior on model parameters