CPSC 340: Machine Learning and Data Mining

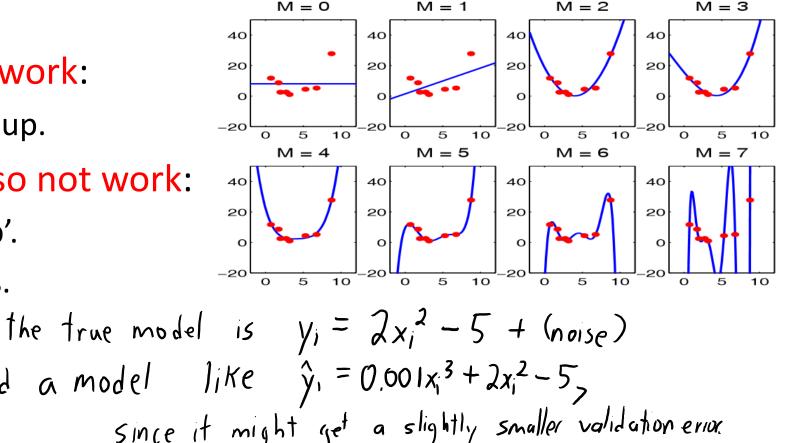
Feature Selection Fall 2018

Admin

- Assignment 3 is due tonight.
 - You can use a "late day" to submit up to 48 hours late.
 - Solutions will be posted Monday.
- Midterm is Thursday of next week.
 - October 18th at 6:30pm (BUCH A102 and A104).
 - 80 minutes.
 - Closed-book.
 - One doubled-sided 'cheat sheet' for midterm.
 - Auditors do not take the midterm.
- There will be two types of questions on the midterm:
 - 'Technical' questions requiring things like pseudo-code or derivations.
 - Similar to assignment questions, and will only be on topics related to those in assignments.
 - 'Conceptual' questions testing understanding of key concepts.
 - All lecture slide material except "bonus slides" is fair game here.

Last Time: Finding the "True" Model

- What if y_i really is a polynomial function of x_i?
 - How can we find the "true" degree 'p' of the polynomial?
- Training error does not work: It goes down as 'p' goes up.
- Cross-validation may also not work:
 - Tends to overestimate 'p'.
 - -20 – Due to optimization bias. 20 10 0 5 5 10 0 For example, imagine that the true model is $y_i = 2x_i^2 - 5 + (noise)$ We might choose d=3 and a model like $\hat{y}_1 = 0.001x_1^3 + 2x_1^2 - 5_2$ ubc.ca/~arnaud/stat535/slides5_revised.pdf since it might get a slightly smaller validation error.



Last Time: Complexity Penalties

- We discussed putting a penalty on the model complexity.
 - Want to fit the data and have a simple model.

Find v' and 'p' minimizing:

$$S(ore(p) = \frac{1}{2} || Z_p v - y ||^2 + \lambda K$$

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- "To increase the degrees of freedom by one, need to decrease error by λ .
- Prefers smaller degrees of freedom, if errors are similar.
 - Can't optimize this using gradient descent, since it's discontinuous in 'p'.
 - Need to search over values of 'p'.

Motivation: Discovering Food Allergies

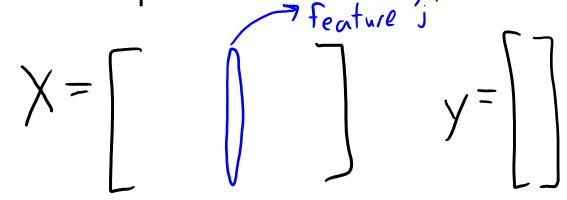
• Recall the food allergy example:

Egg	Milk	Fish	Wheat	Shellfish	Peanuts		Sick?
0	0.7	0	0.3	0	0		1
0.3	0.7	0	0.6	0	0.01		1
0	0	0	0.8	0	0		0
0.3	0.7	1.2	0	0.10	0.01		1

Instead of predicting "sick", we want to do feature selection:
 Which foods are "relevant" for predicting "sick".

Feature Selection

• General feature selection problem:



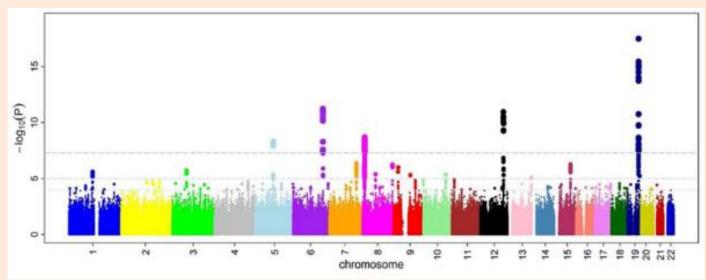
- Find the features (columns) of 'X' that are important for predicting 'y'.
 - "What are the relevant factors?"
 - "Which basis functions should I use among these choices?"
 - "What types of new data should I collect?"
 - "How can I speed up computation?"
- One of most important problems in ML/statistics, but very messy.
 - For now, we'll say a feature is "relevant" if it helps predict y_i from x_i .

"Association" Approach

- A simple/common way to do feature selection:
 - For each feature 'j', compute correlation between feature values x^j and 'y'.
 - Say that 'j' is relevant if correlation is above 0.9 or below -0.9.
- Turns feature selection into hypothesis testing for each feature.
 - There are many other measures of "dependence" (<u>Wikipedia</u>).
- Usually gives unsatisfactory results as it ignores variable interactions:
 - Includes irrelevant variables: "Taco Tuesdays".
 - If tacos make you sick, and you often eat tacos on Tuesdays, it will say "Tuesday" is relevant.
 - Excludes relevant variables: "Diet Coke + Mentos Eruption".
 - Diet coke and Mentos don't make you sick on their own, but together they make you sick.

Genome-Wide Association Studies

- Genome-wide association studies:
 - Measure if there exists a dependency between each individual "singlenucleotide polymorphism" in the genome and a particular disease.



- Has identified thousands of genes "associated" with diseases.

• But by design this has a huge numbers of false positives (and many false negatives).

"Regression Weight" Approach

- A simple/common approach to feature selection:
 - Fit regression weights 'w' based on all features (maybe with least squares).
 - Take all features 'j' where weight $|w_i|$ is greater than a threshold.
- This could recognize that "Tuesday" is irrelevant.
 - If you get enough data, and you sometimes eat tacos on other days.
 (And the relationship is actually linear.)
- This could recognize that "Diet Coke" and "Mentos" are relevant.
 Assuming this combination occurs enough times in the data.

"Regression Weight" Approach

- A simple/common approach to feature selection:
 - Fit regression weights 'w' based on all features (maybe with least squares).
 - Take all features 'j' where weight $|w_i|$ is greater than a threshold.
- Has major problems with collinearity:
 - If the "Tuesday" variable always equals the "taco" variable, it could say that Tuesdays are relevant but tacos are not. $\hat{\gamma}_i = W_1 * f_{\alpha_i \cup j} + W_2 * T_{uesday} = 6 * f_{\alpha_i \cup j} + (w_1 + w_2) * T_{uesday}$
 - If you have two copies of an irrelevant feature,

it could take both irrelevant copies.

 $\hat{\gamma}_i = 0 * irrelevant + 0 * irrelevant = 10000 * irrelevant + (-10000) * irrelevant$

(pause)

Search and Score Methods

- Most common feature selection framework is search and score:
 - 1. Define score function f(S) that measures quality of a set of features 'S'.
 - 2. Now search for the variables 'S' with the best score.
- Example with 3 features:
 - Compute "score" of using feature 1.
 - Compute "score" of using feature 2.
 - Compute "score" of using feature 3.
 - Compute "score" of using features {1,2}.
 - Compute "score" of using features {1,3}.
 - Compute "score" of using features {2,3}.
 - Compute "score" of using features {1,2,3}.
 - Compute "score" of using features {}.
 - Return the set of features 'S' with the best "score".

Which Score Function?

- The score can't be the training error.
 - Training error goes down as you add features, so will select all features.
- A more logical score is the validation error.
 - "Find the set of features that gives the lowest validation error."
 - To minimize test error, this is what we want.
- But there are problems due to the large number of sets of variables:
 - If we have 'd' variables, there are 2^d sets of variables.
 - Optimization bias is high: we're optimizing over 2^d models (not 10).
 - Prone to false positives: irrelevant variables will sometimes help by chance.

"Number of Features" Penalties

• To reduce false positives, we can again use complexity penalties:

$$s_{core}(S) = \frac{1}{2} \sum_{i=1}^{n} (w_s^{T} x_{is} - y_i)^{2} + s_{ize}(S)$$

- E.g., we could use squared error and number of non-zeroes.
- We're using ' x_{is} ' as the features 'S' of example x_i .
- If two 'S' have similar error, this prefers the smaller set.
 It prefers having removing feature 3 instead of having w₃ = 0.00001.

• Instead of "size(S)", we usually write this using the "LO-norm"...

LO-Norm and "Number of Features We Use"

• In linear models, setting w_i = 0 is the same as removing feature 'j':

$$y_{i} = w_{i} x_{i1} + w_{2} x_{i2} + w_{3} x_{i3} + \cdots + w_{d} x_{id}$$

$$\int s_{i1} + w_{2} x_{i2} + w_{3} x_{i3} + \cdots + w_{d} x_{id}$$

$$\hat{y}_{i} = w_{i} x_{i1} + O + w_{3} x_{i3} + \cdots + w_{d} x_{id}$$

$$\lim_{i \neq nore + x_{i2}}$$

• The LO "norm" is the number of non-zero values.

If
$$W = \begin{bmatrix} 1 \\ 0 \\ 3 \end{bmatrix}$$
 then $\|I_W\|_0 = 3$ If $w = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$ then $\|I_W\|_0 = 0$.

- Not actually a true norm.
- If 'w' has a small LO-norm, then it doesn't use many features.

L0-penalty: optimization

• L0-norm penalty for feature selection:

$$f(w) = \frac{1}{2} || X_w - y ||^2 + \frac{1}{2} || w|_0$$

$$\frac{d_{o}grees}{d_{o}grees} of$$

$$\frac{d_{o}grees}{freedom'k'}$$

- Suppose we want to use this to evaluate the features S = {1,2}:
 - First fit the 'w' just using features 1 and 2.
 - Now compute the training error with this 'w' and features 1 and 2.
 - Add λ^* 2 to the training error to get the score.
- We repeat this with other choices of 'S' to find the "best" features.

L0-penalty: interpretation

• L0-norm penalty for feature selection:

$$f(w) = \frac{1}{2} || X_w - y ||^2 + \frac{1}{2} || w|_0$$

- Balances between training error and number of features we use.
 - With λ =0, we get least squares with all features.
 - With $\lambda = \infty$, we must set w=0 and not use any features.
 - With other λ , balances between training error and number of non-zeroes.
 - Larger λ puts more emphasis on having zeroes in 'w' (more feature selection).
 - Different values give AIC, BIC, and so on.

Forward Selection (Greedy Search Heuristic)

- In search and score, it's also just hard to search for the best 'S'.
 There are 2^d possible sets.
- A common greedy search procedure is forward selection:

Forward Selection (Greedy Search Heuristic)

- Forward selection algorithm for variable selection:
 - 1. Start with an empty set of features, S = [].
 - 2. For each possible feature 'j':
 - Compute scores of features in 'S' combined with feature 'j'.
 - 3. If no 'j' improves the score, stop.
 - 4. Otherwise, add the 'j' that improves the score the most to 'S'.
 - Then go back to Step 2.
- Not guaranteed to find the best set, but reduces many problems:
 - Considers O(d²) models: cheaper, ovefits less, has fewer false positives.

Backward Selection and RFE

- Forward selection often works better than naïve methods.
- A related method is **backward selection**:
 - Start with all features, remove the one that most improves the score.
- If you consider adding or removing features, it's called stagewise.
- Stochastic local search is a class of fancier methods.
 - Simulated annealing, genetic algorithms, ant colony optimization, etc.
- Recursive feature elimination is another related method:
 - Fit parameters of a regression model.
 - Prune features with small regression weights.
 - Repeat.

(pause)

• Consider a supervised classification task:

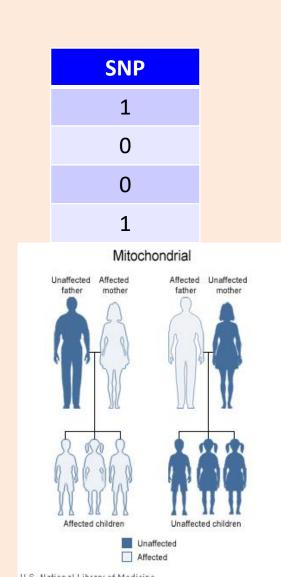
gender	mom	dad	
F	1	0	
М	0	1	
F	0	0	
F	1	1	

- Predict whether someone has particular genetic variation (SNP).
 - Location of mutation is in "mitochondrial" DNA.
 - "You almost always have the same value as your mom".
 - For simplicity we'll assume 1950s-style gender and parentage.

• Consider a supervised classification task:

gender	mom	dad
F	1	0
Μ	0	1
F	0	0
F	1	1

- True model:
 - (SNP = mom) with very high probability.
 - (SNP != mom) with some very low probability.
- What are the "relevant" features for this problem?
 - Mom is relevant and {gender, dad} are not relevant.



• What if "mom" feature is repeated?

gender	mom	dad	mom2	
F	1	0	1	
М	0	1	0	
F	0	0	0	
F	1	1	1	

- Are "mom" and "mom2" relevant?
 - Should we pick them both?
 - Should we pick one because it predicts the other?
- General problem ("dependence", "collinearity" for linear models):

Neither of these is "correct", but not picking either

IS

incorrect.

If features can be predicted from features, don't know one(s) to pick.

• What if we add (maternal) "grandma"?

gender	mom	dad	grandma
F	1	0	1
Μ	0	1	0
F	0	0	0
F	1	1	1

- Is "grandma" relevant?
 - You can predict SNP very accurately from "grandma" alone.
 - But "grandma" is irrelevant if I know "mom".
- General problem (conditional independence):
 - "Relevant" features may be irrelevant given other features.

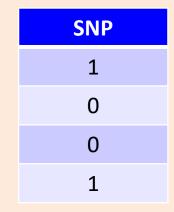
• What if we don't know "mom"?

gender	grandma	dad	SNP
F	1	0	1
Μ	0	1	0
F	0	0	0
F	1	1	1

- Now is "grandma" is relevant?
 - Without "mom" variable, using "grandma" is the best you can do.
- General problem ("taco Tuesday"):
 - Features can be relevant due to missing information.

• What if we don't know "mom" or "grandma"?

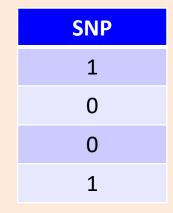
gender	dad
F	0
Μ	1
F	0
F	1



- Now there are no relevant variables, right?
 - But "dad" and "mom" must have some common maternal ancestor.
 - "Mitochondrial Eve" estimated to be ~200,000 years ago.
- General problem (effect size):
 - "Relevant" features may have small effects.

• What if we don't know "mom" or "grandma"?

gender	dad
F	0
Μ	1
F	0
F	1



- Now there are no relevant variables, right?
 - What if "mom" likes "dad" because he has the same SNP as her?
- General problem (confounding):
 - Hidden effects can make "irrelevant" variables "relevant".

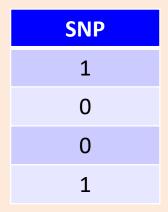
• What if we add "sibling"?

gender	dad	sibling
F	0	1
Μ	1	0
F	0	0
F	1	1

- Sibling is "relevant" for predicting SNP, but it's not the cause.
- General problem (non-causality or reverse causality):
 - A "relevant" feature may not be causal, or may be an effect of label.

• What if don't have "mom" but we have "baby"?

gender	dad	baby
F	0	1
Μ	1	1
F	0	0
F	1	1



- "Baby" is relevant when (gender == F).
 - "Baby" is relevant (though causality is reversed).
 - Is "gender" relevant?
 - If we want to find relevant causal factors, "gender" is not relevant.
 - If we want to predict SNP, "gender" is relevant.
- General problem (context-specific relevance):
 - Adding a feature can make an "irrelevant" feature "relevant".

- Warnings about feature selection:
 - A feature is only "relevant" in the context of available features.
 - Adding/removing features can make features relevant/irrelevant.
 - Confounding factors can make "irrelevant" variables the most "relevant".
 - If features can be predicted from features, you can't know which to pick.
 - Collinearity is a special case of "dependence" (which may be non-linear).
 - A "relevant" feature may have a tiny effect.

- "Relevance" for prediction does not imply a causal relationship.

Is this hopeless?

- We often want to do feature selection we so have to try!
- Different methods are affected by problems in different ways.
 We'll ignore causality and confounding issues (bonus slides).
- These "problems" don't have right answers but have wrong answers:
 - Variable dependence ("mom" and "mom2" have same information).
 - But should take at least one.
 - Conditional independence ("grandma" is irrelevant given "mom").
- These "problems" have application-specific answers:
 - Tiny effects.
 - Context-specific relevance (is "gender" relevant if given "baby"?).

Method\Issue	Dependence	Conditional Independence	Tiny effects	Context-Specific Relevance
Association (e.g., measure correlation between features 'j' and 'y')	Ok (takes "mom" and "mom2")	Bad (takes "grandma", "great-grandma", etc.)	Ignores	Bad (misses features that must interact, "gender" irrelevant given "baby")

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Regression Weight (fit least squares, take biggest w _j)	Bad (can take irrelevant but collinear, can take none of "mom1-3")	Ok (takes "mom" not "grandma", if linear and 'n' large.	lgnores (unless collinear)	Ok (if linear, "gender" relevant give "baby")

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Search and Score w/ Validation Error	Ok (takes at least one of "mom" and "mom2")	Bad (takes "grandma", "great-grandma", etc.)	Allows	Ok ("gender" relevant given "baby")

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Search and Score w/ Validation Error	Ok (takes at least one of "mom" and "mom2")	Bad (takes "grandma", "great-grandma", etc.)	Allows (many false positives)	Ok ("gender" relevant given "baby")
Search and Score w/ LO-norm	Ok (takes exactly one of "mom" and "mom2")	Ok (takes "mom" not grandma if linear-ish).	Ignores (even if collinear)	Ok ("gender" relevant given "baby")

Summary

- Feature selection is task of choosing the "relevant" features.
 Obvious simple approaches have obvious simple problems.
- Search and score: find features that optimize some score.
 - L0-norm penalties are the most common scores.
 - Forward selection is a heuristic to search over a smaller set of features.
- "Relevance" is really hard to define.

• Next time: getting a good test error even with irrelevant features.

Mallow's Cp

• Older than AIC and BIC is Mallow's Cp:

$$f(w) = \frac{\|X_{w} - y\|^{2}}{\|X_{w}^{2} - y\|^{2}} - n + 2\|w\|_{0}$$

$$= \frac{1}{n} \|X_{w}^{2} - y\|^{2}$$

$$= \frac{1}{n} \|X_{w}^{2} - y\|^{2} + y\|^{2}$$

$$= \frac{1}{n} \|X_{w}^{2} - y\|^{2} + y\|$$

• Minimizing this score is equivalent to LO-regularization:

$$f(w) = \frac{1}{2} || \chi_w - \gamma ||^2 + \lambda || w ||_0$$

with $\lambda = \frac{||\chi_w^2 - \gamma||^2}{2}$

• So again, viewing λ as hyper-parameter, this score is special case.

Adjusted R²

• Older than AIC and BIC and Mallow's Cp is adjusted R²:

$$f(w) = \left[- (1 - R^2) \frac{n - 1}{n - 1} \right] \text{ where } R^2 = \left[- \frac{11 \times w - y}{11 \times w - y} \right]^2$$

• Maximizing this score is equivalent to LO-regularization:

$$= \frac{1}{2} || \chi_{w} - \gamma ||^{2} + \lambda || w ||_{0}$$

with $\lambda = \frac{||\chi_{w} - \gamma ||^{2}}{Z(n-1)}$

• So again, viewing λ as hyper-parameter, this score is special case.

ANOVA

• Some people also like to compute this "ANOVA" quantity:

ullet

 $f(w) = \frac{\|X_w - y\|^2}{\|y - y\|^2}$ This is based on the decomposition of "total squared error" as: $\|y - y\|^2 = \|y\| = \|y\|$

$$\frac{\|y - y\|^2}{\|y - y\|^2} = \frac{\|\chi_w - y\|^2}{\|y\|^2} + \frac{\|\chi_w - y\|^2}{\|y\|^2}$$

"total" error "explained" error "residual" (usual) error.

- Notice that "explained error" goes up as our usual ("residual") error goes down.
- Trying to find the 'k' features that maximize 'f' ("explain the most variance") is equivalent to LO-regularization with a particular λ (so another special case).

Information Criteria with Noise Variance

• We defined AIC/BIC for feature selection in least squares as:

$$f(w) = \frac{1}{2} || \chi_w - \gamma ||^2 + \frac{1}{2} || w|_0$$

- The first term comes from assuming y_i = w^Tx_i + ε, where ε comes from a normal distribution with a variance of 1.
 We'll discuss why when we discuss MLE and MAP estimation.
- If you treat variance as a parameter, then after some manipulation:

$$f(w) = \frac{n}{2} \log (||Xw - y||^2) + \frac{1}{2} ||w||_0$$

- However, this is again equivalent to just changing λ .
- If you aren't doing least squares, replace first term by "log-likelihood".

Complexity Penalties for Other Models

- Scores like AIC and BIC can also be used in other contexts:
 - When fitting a decision tree, only split a node if it improves BIC.
 - This makes sense if we're looking for the "true tree", or maybe just a simple/interpretable tree that performs well.
- In these cases we replace "LO-norm" with "degrees of freedom".
 - In linear models fit with least squares, degrees of freedom is number of non-zeroes.
 - Unfortunately, it is not always easy to measure "degrees of freedom".

Alternative to Search and Score: good old p-values

- Hypothesis testing ("constraint-based") approach:
 - Generalization of the "association" approach to feature selection.
 - Performs a sequence of conditional independence tests.

- If they are independent (like "p < .05"), say that 'j' is "irrelevant".
- Common way to do the tests:
 - "Partial" correlation (numerical data).
 - "Conditional" mutual information (discrete data).

Testing-Based Feature Selection

- Hypothesis testing ("constraint-based") approach:
- Two many possible tests, "greedy" method is for each 'j' do:
 First test if xij L y;
 If still dependent test xij L y, l xis where 's' has one feature feature features to minimize
 If still dependent test xij L y, l xis where 's' now has two features dependence.
 If still dependent test xij L y, l xis where 's' now has two features dependence.
- "Association approach" is the greedy method where you only do the first test (subsequent tests remove a lot of false positives).

Hypothesis-Based Feature Selection

- Advantages:
 - Deals with conditional independence.
 - Algorithm can explain why it thinks 'j' is irrelevant.
 - Doesn't necessarily need linearity.
- Disadvantages:
 - Deals badly with exact dependence: doesn't select "mom" or "mom2" if both present.
 - Usual warning about testing multiple hypotheses:
 - If you test p < 0.05 more than 20 times, you're going to make errors.
 - Greedy approach may be sub-optimal.
- Neither good nor bad:
 - Allows tiny effects.
 - Says "gender" is irrelevant when you know "baby".
 - This approach is sometimes better for finding relevant factors, not to select features for learning.

Causality

- None of these approaches address causality or confounding:
 - "Mom" is the only relevant direct causal factor.
 - "Dad" is really irrelevant.
 - "Grandma" is causal but is irrelevant if we know "mom".

- Other factors can help prediction but aren't causal:
 - "Sibling" is predictive due to confounding of effect of same "mom".
 - "Baby" is predictive due to reverse causality.
 - "Gender" is predictive due to common effect on "baby".

We can sometimes address this using interventional data...

Interventional Data

- The difference between observational and interventional data:
 - If I see that my watch says 10:45, class is almost over (observational).
 - If I set my watch to say 10:45, it doesn't help (interventional).
- The intervention can help discover causal effects:
 - "Watch" is only predictive of "time" in observational setting (so not causal).
- General idea for identifying causal effects:
 - "Force" the variable to take a certain value, then measure the effect.
 - If the dependency remains, there is a causal effect.
 - We "break" connections from reverse causality, common effects, or confounding.

Causality and Dataset Collection

- This has to do with the way you collect data:
 - You can't "look" for variables taking the value "after the fact".
 - You need to manipulate the value of the variable, then watch for changes.
- This is the basis for randomized control trial in medicine:
 - Randomly assigning pills "forces" value of "treatment" variable.
 - Include a "control" as a value to prevent placebo effect as confounding.
- See also Simpson's Paradox:
 - <u>https://www.youtube.com/watch?v=ebEkn-BiW5k</u>

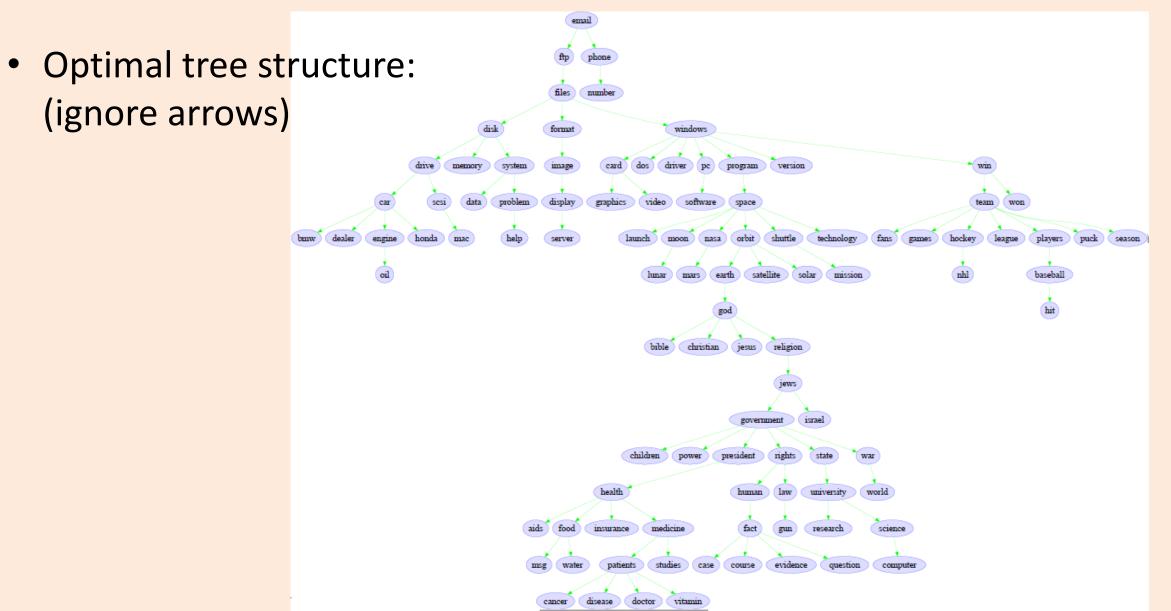
Structure Learning: Unsupervised Feature Selection

• "News" data: presence of 100 words in 16k newsgroup posts:

car	drive	files	hockey	mac	league	рс	win
0	0	1	0	1	0	1	0
0	0	0	1	0	1	0	1
1	1	0	0	0	0	0	0
0	1	1	0	1	0	0	0
0	0	1	0	0	0	1	1

- Which words are related to each other?
- Problem of structure learning: unsupervised feature selection.

Structure Learning: Unsupervised Feature Selection



Naïve Approach: Association Networks

- A naïve approach to structure learning ("association networks"):
 - For each pair of variables, compute a measure of similarity or dependence.
- Using these n² similarity values either:
 - Select all pairs whose similarity is above a threshold.
 - Select the "top k" most similar features to each feature 'j'.
- Main problems:
 - Usually, most variables are dependent (too many edges).
 - "Sick" is getting connected to "Tuesdays" even if "tacos" are a variable.
 - "True" neighbours may not have the highest dependence.
 - "Sick" might get connected to "Tuesdays" before it gets connected to "milk".
- (Variation: best tree can be found as minimum spanning tree problem.)

Example: Vancouver Rain Data

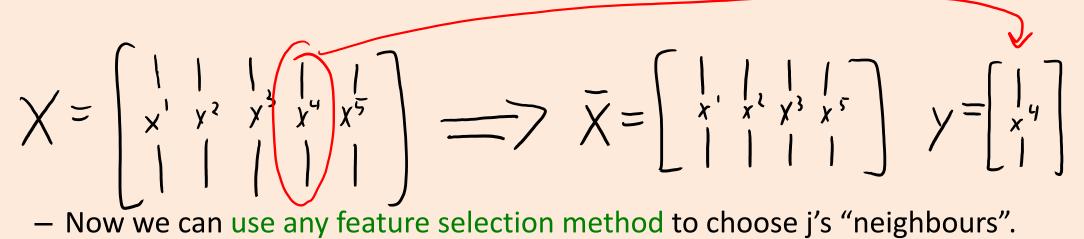
• Consider modeling the "Vancouver rain" dataset.

	Day 1	Day 2	Day 3	Day 4	Day 5	Day 6	Day 7	Day 8	Day 9	
Month 1	0	0	0	1	1	0	0	1	1	
Month 2	1	0	0	0	0	0	1	0	0	
Month 3	1	1	1	1	1	1	1	1	1	
Munilh 4	1	1	1	1	0	0	1	1	1	
Munilh 4 Month J	0	0	0	0	1	1	0	0	0	
Murith 6	0	1	1	0	0	0	0	1	1	

- The strongest signal in the data is the simple relationship:
 - If it rained yesterday, it's likely to rain today (> 50% chance that $x^{t-1} = x^t$).
 - But an "association network" might connect all days (all dependent).

Dependency Networks

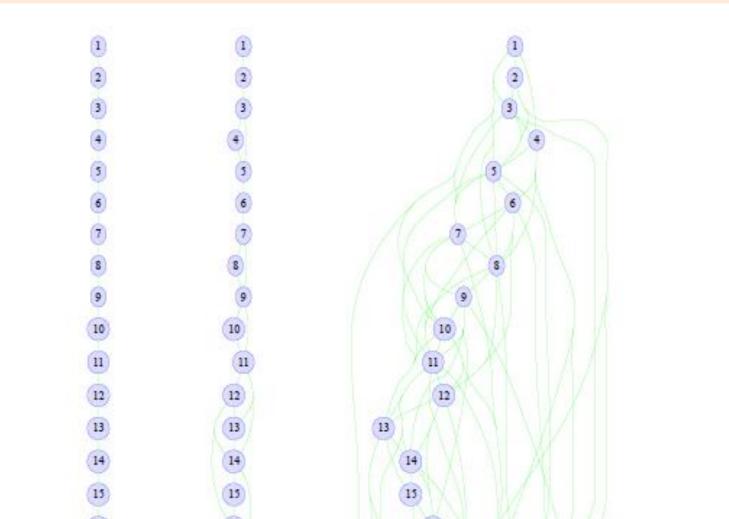
- A better approach is dependency networks:
 - For each variable 'j', make it the target in a supervised learning problem.



- Forward selection, L1-regularization, ensemble methods, etc.
- Can capture conditional independence:
 - Might connect "sick" to "tacos", and "tacos" to "Tuesdays" (w/o sick-tacos).

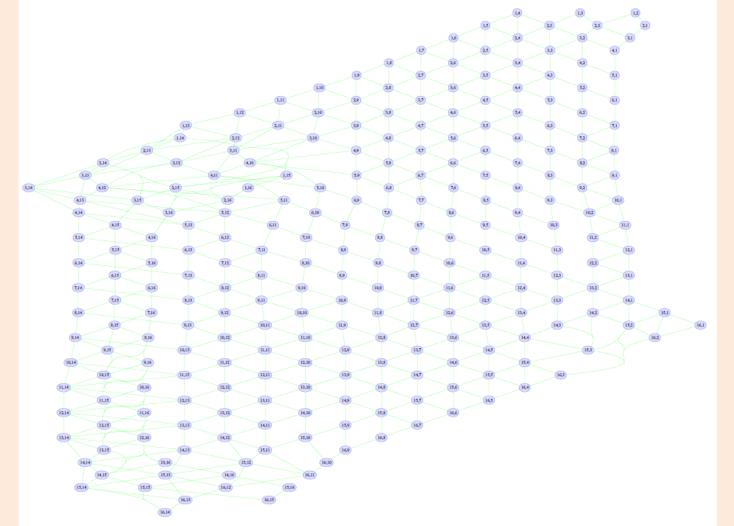
Dependency Networks

• Dependency network fit to Vancouver rain data (different λ values):



Dependency Networks

• Variation on dependency networks on digit image pixels:



Another popular structure learning method is the "PC" algorithm.