CPSC 340:
Machine Learning and Data Mining

Feature Selection

Bonus Slides

Bayesian Information Criterion (BIC)

- A disadvantage of these methods:
  - Still prefers a larger ‘p’ as ‘n’ grows.

- Solution: make λ depend on ‘n’.
- For example, the Bayesian information criterion (BIC) uses:

$$\lambda = \frac{1}{2}\log(n)$$

- BIC penalizes a bit more than AIC for large ‘n’.
  - As ‘n’ goes to ∞, recovers “true” model (“consistent” for model selection).
- In practice, we usually just try a bunch of different λ values.
  - Picking λ is like picking ‘k’ in k-means.

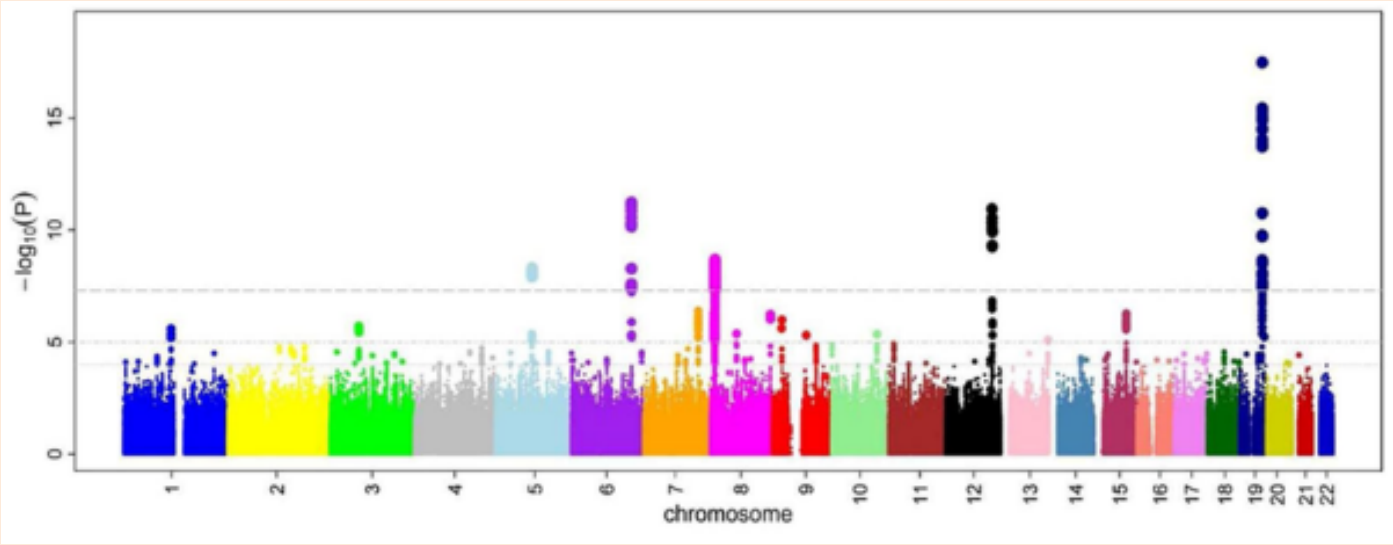
Discussion of other Scores for Model Selection

- There are many other scores:
  - Elbow method (corresponds to specific choice of λ).
    - You could also use BIC for choosing 'k' in k-means.
  - Methods based on validation error.
    - "Take smallest 'p' within one standard error of minimum cross-validation error".
  - Minimum description length.
  - Risk inflation criterion.
  - False discovery rate.
  - Marginal likelihood (CPSC 540).

- These can adapted to use the L1-norm and other errors.

Genome-Wide Association Studies

- Genome-wide association studies:
  - Measure if there exists a dependency between each individual “single-nucleotide 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).

https://en.wikipedia.org/wiki/Genome-wide_association_study

Backward Selection and RFE

- Forward selection often works better than naïve methods.
- A related method is backward selection:
  - Start with all features, compute score after removing each feature, remove the one that improves the score the most.
- 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.

Is “Relevance” Clearly Defined?

- Consider a supervised classification task:

gender	mom	dad
F	1	0
M	0	1
F	0	0
F	1	1

SNP
1
0
0
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.

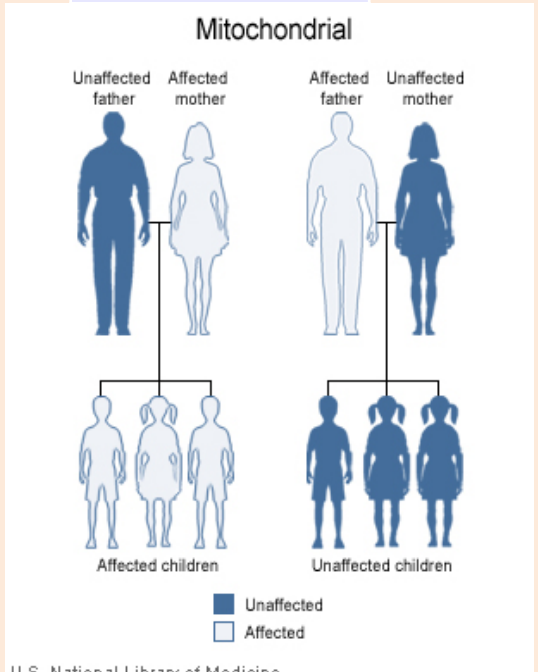
Is “Relevance” Clearly Defined?

- Consider a supervised classification task:

gender	mom	dad
F	1	0
M	0	1
F	0	0
F	1	1

SNP
1
0
0
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.



https://en.wikipedia.org/wiki/Human_mitochondrial_genetics

Is “Relevance” Clearly Defined?

- What if “mom” feature is repeated?

gender	mom	dad	mom2
F	1	0	1
M	0	1	0
F	0	0	0
F	1	1	1

SNP
1
0
0
1

- Are “mom” and “mom2” relevant?
  - Should we pick them both?
  - Should we pick one because it predicts the other?

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

- If features can be predicted from features, can’t know which to pick.
  - Collinearity is a special case of “dependence” (which may be non-linear).

Is “Relevance” Clearly Defined?

- What if we add (maternal) “grandma”?

gender	mom	dad	grandma
F	1	0	1
M	0	1	0
F	0	0	0
F	1	1	1

SNP
1
0
0
1

- Is “grandma” relevant?
  - You can predict SNP very accurately from “grandma” alone.
  - But “grandma” is irrelevant if I know “mom”.
- A feature is only “relevant” in the context of available features.
  - Adding/removing features can make features relevant/irrelevant.

Is “Relevance” Clearly Defined?

- What if we don’t know “mom”?

gender	grandma	dad
F	1	0
M	0	1
F	0	0
F	1	1

SNP
1
0
0
1

- Now is “grandma” is relevant?
  - Without “mom” variable, using “grandma” is the best you can do.

- A feature is only “relevant” in the context of available features.
  - Adding/removing features can make features relevant/irrelevant.

Is “Relevance” Clearly Defined?

- What if we don’t know “mom” or “grandma”?

gender	dad
F	0
M	1
F	0
F	1

SNP
1
0
0
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.
- A “relevant” feature may have a tiny effect.

Is “Relevance” Clearly Defined?

- What if we don’t know “mom” or “grandma”?

gender	dad
F	0
M	1
F	0
F	1

SNP
1
0
0
1

- Now there are no relevant variables, right?
  - What if “mom” likes “dad” because he has the same SNP as her?

- Confounding factors can make “irrelevant” variables “relevant”.

Is “Relevance” Clearly Defined?

- What if we add “sibling”?

gender	dad	sibling
F	0	1
M	1	0
F	0	0
F	1	1

SNP
1
0
0
1

- Sibling is “relevant” for predicting SNP, but it’s not the cause.

- “Relevance” for prediction does not imply a causal relationship.
  - Causality can even be reversed…

Is “Relevance” Clearly Defined?

- What if don’t have “mom” but we have “baby”?

gender	dad	baby
F	0	1
M	1	1
F	0	0
F	1	1

SNP
1
0
0
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.
- “Relevance” may depend on values of certain features.
  - “Context-specific” relevance.

Is “Relevance” Clearly Defined?

- Warnings about feature selection:
  - If features can be predicted from features, you can’t know which to pick.
  - A feature is only “relevant” in the context of available features.
  - A “relevant” feature may have a tiny effect.
  - Confounding factors can make “irrelevant” variables the most “relevant”.
  - “Relevance” for prediction does not imply a causal relationship.
  - “Relevance” may depend on values of certain features.

Is this hopeless?

- We often want to do feature selection we so have to try!
- Different methods are affected by problems in different ways.
- 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 (all “grandma” information is captured by “mom”).
    - Should take “grandma” only if “mom” missing.
- These “problems” have application-specific answers:
  - Tiny effects.
  - Context-specific relevance (is “gender” relevant if given “baby”?).
- See bonus slides for discussion causality and confounding issues.
  - Unless you control data collection, standard feature selection methods cannot address those issues.

Rough Guide to Feature Selection

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.	Ignores (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/ L0-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")

Feature Selection in Tree-Based Methods

- Decision trees naturally do feature selection while learning:
  - The features used for the splits are the ones that are “selected”.

- There are a variety of ways evaluate features in random forests:
  - Compute proportion of trees that use feature ‘j’.
  - Compute average infogain increase when using feature ‘j’.
  - Permute all values of feature ‘j’, and see how “out of bag” error increases.
- You could use any of above to select features from random forest.

Mallow's Cp

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

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

least squares weights if we used all features.

- Minimizing this score is equivalent to L0-regularization:

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

with $\lambda = \frac{\|X\hat{w} - y\|^2}{n}$

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

Adjusted R^2

- Older than AIC and BIC and Mallow's Cp is adjusted R^2:

$$f(w) = 1 - (1 - R^2)\frac{n-1}{n-\|w\|_0-1} \quad \text{where} \quad R^2 = 1 - \frac{\|Xw - y\|^2}{\|X\hat{w} - y\|^2}$$

- Maximizing this score is equivalent to L0-regularization:

$$= \frac{1}{2}\|Xw - y\|^2 + \lambda \|w\|_0$$

$$\text{with} \quad \lambda = \frac{\|X\hat{w} - y\|^2}{2(n-1)}$$

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

ANOVA

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

$$f(w) = \frac{\|Xw - \bar{y}\|^2}{\|y - \bar{y}\|^2}$$

↑ mean of y_i values repeated 'n' times

- This is based on the decomposition of "total squared error" as:

$$\underbrace{\|y - \bar{y}\|^2}_{\text{"total" error}} = \underbrace{\|Xw - \bar{y}\|^2}_{\text{"explained" error}} + \underbrace{\|Xw - y\|^2}_{\text{"residual" (usual) error.}}$$

- 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 L0-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:

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

- The first term comes from assuming $y_i = w^T x_i + \varepsilon$, 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 aren't doing least squares, replace first term by "log-likelihood".
- If you treat variance as a parameter, then after some manipulation:

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

- However, this is again equivalent to just changing λ.

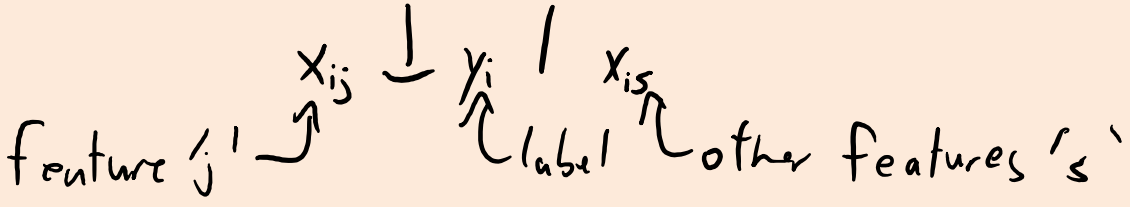
Complexity Penalties for Other Models

- 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 "L0-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 I know features in 's' does feature 'j' tell me anything about label?"

  - 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 $x_{ij} \perp y_i$

If still dependant test $x_{ij} \perp y_i \mid x_{is}$ where 's' has one feature

If still dependent test $x_{ij} \perp y_i \mid x_{is}$ where 's' now has two features

Often choose features to minimize dependence.

⋮

If still dependant when 's' includes all other features, declare 'j' relevant.

- "Association approach" is the greedy method where you only do the first test (subsequent tests remove a lot of false positives).

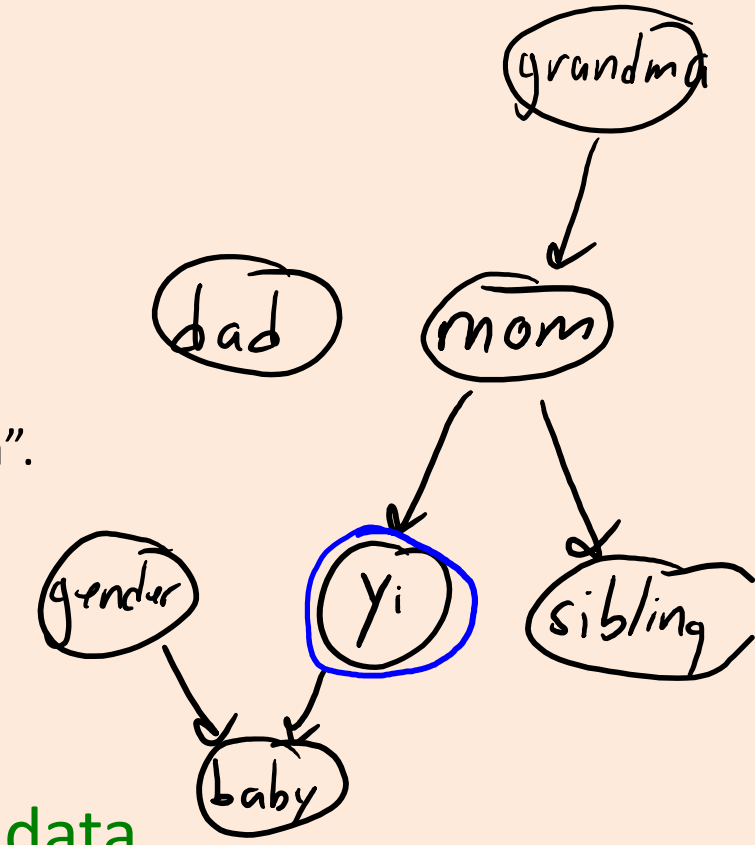
Hypothesis-Based Feature Selection

- 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.
    - Randomization means they aren't taking the pill due to confounding factors.
    - Differences between people who did and did not take pill should be caused by pill.
  - Include a "control" as a value to prevent placebo effect as confounding.

- See also Simpson's Paradox:
  - https://www.youtube.com/watch?v=ebEkn-BiW5k

Structure Learning: Unsupervised Feature Selection

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

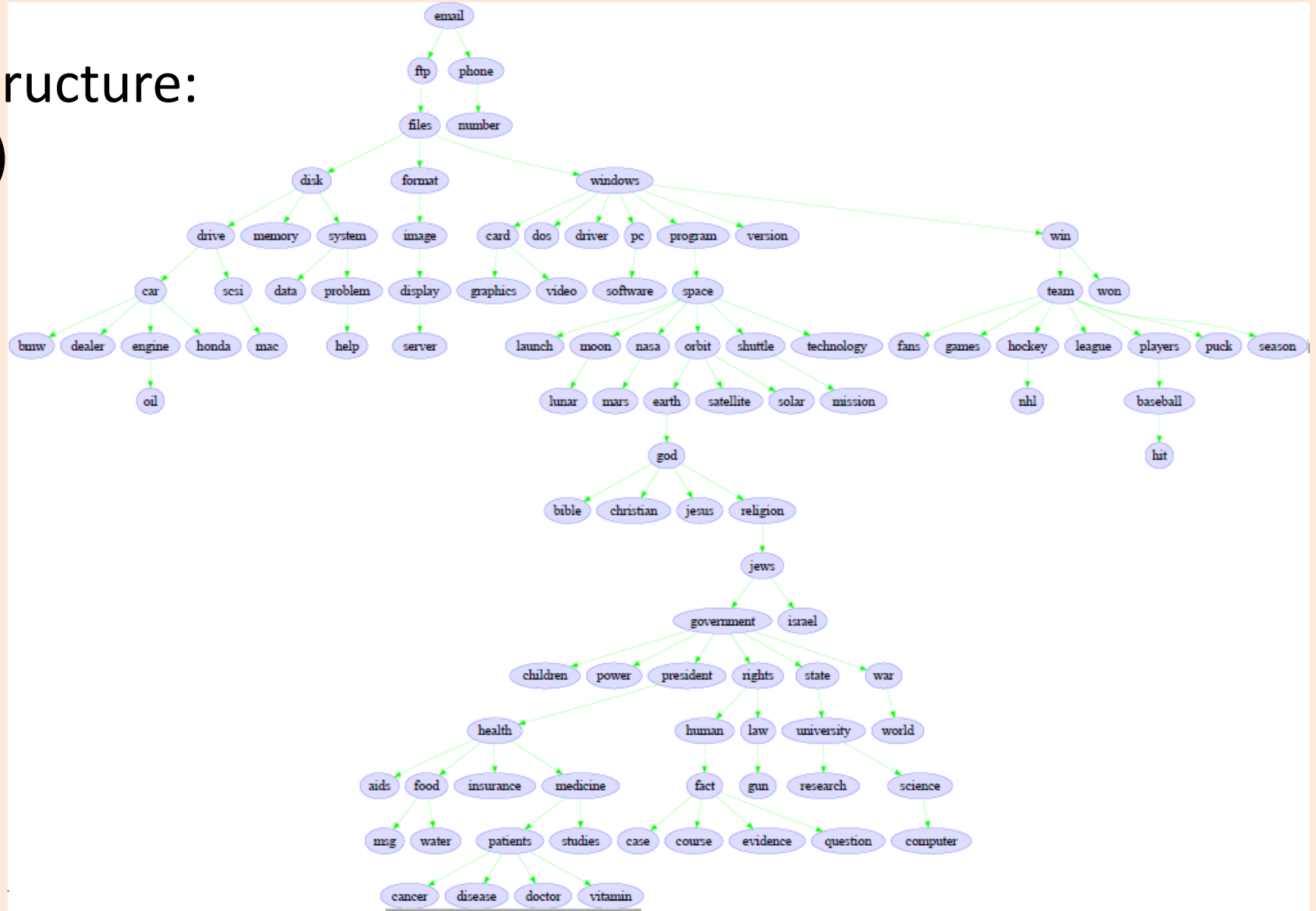
car	drive	files	hockey	mac	league	pc	win
0	0	1	0	1	0	1	0
0	0	0	1	0	1	0	1
1	1	0	0	0	0	0	0
0	1	1	0	1	0	0	0
0	0	1	0	0	0	1	1

- Which words are related to each other?

- Problem of structure learning: unsupervised feature selection.

Structure Learning: Unsupervised Feature Selection

- Optimal tree structure: (ignore arrows)



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 n^2 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

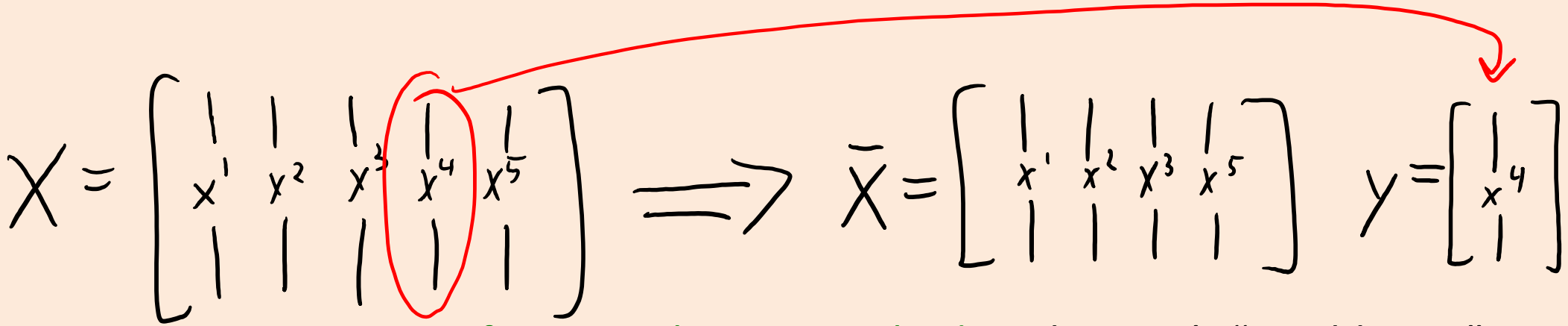
- Consider modeling the "Vancouver rain" dataset.

	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	
Month 4	1	1	1	1	0	0	1	1	1	
Month 5	0	0	0	0	1	1	0	0	0	
Month 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.

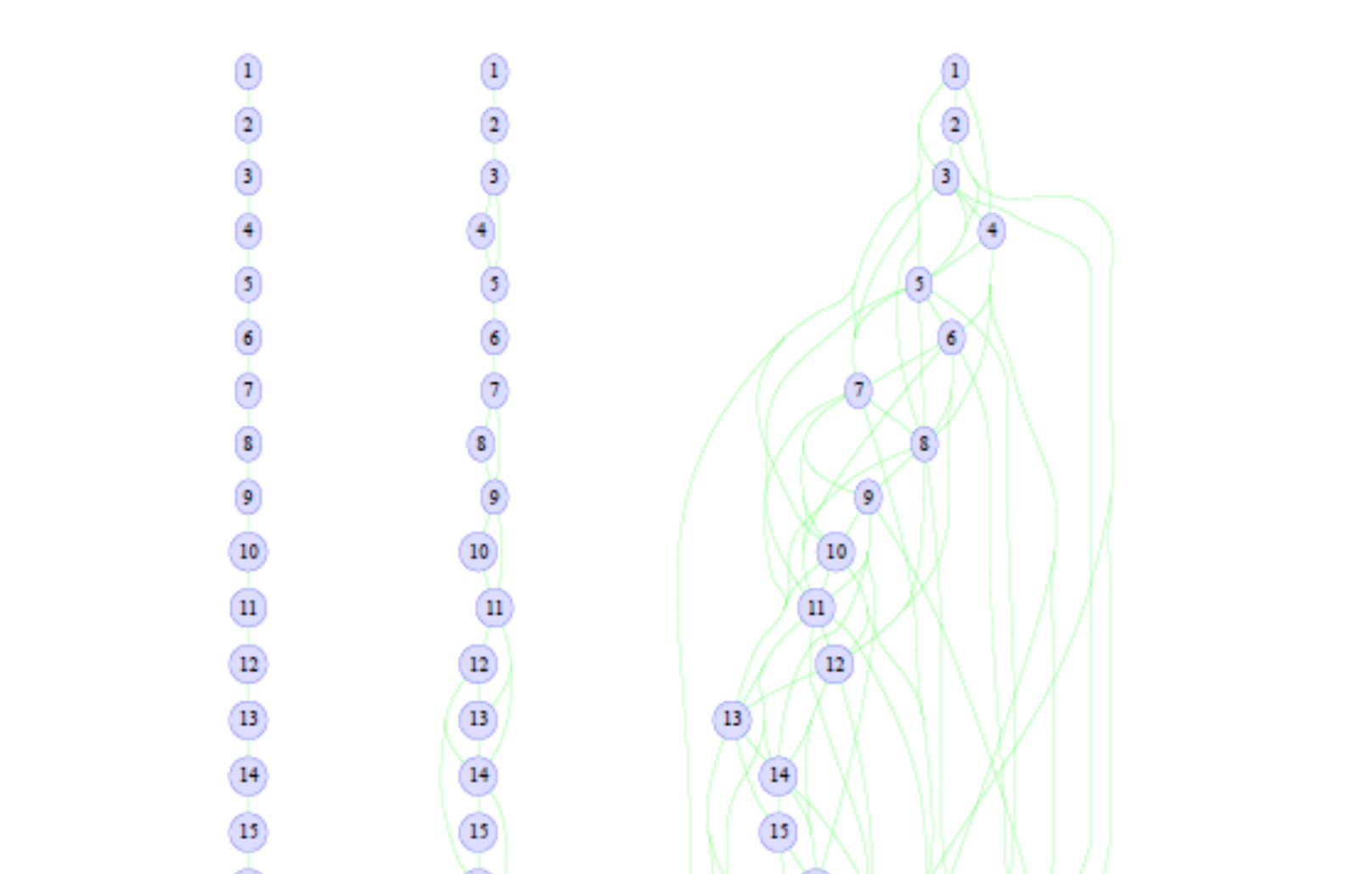


  - Now we can use any feature selection method to choose j’s “neighbours”.
    - Forward selection, L1-regularization, ensemble methods, etc.

- Can capture conditional independence:
  - Might connect “sick” to “tacos”, and “tacos” to “Tuesdays” (w/o sick-tacos).

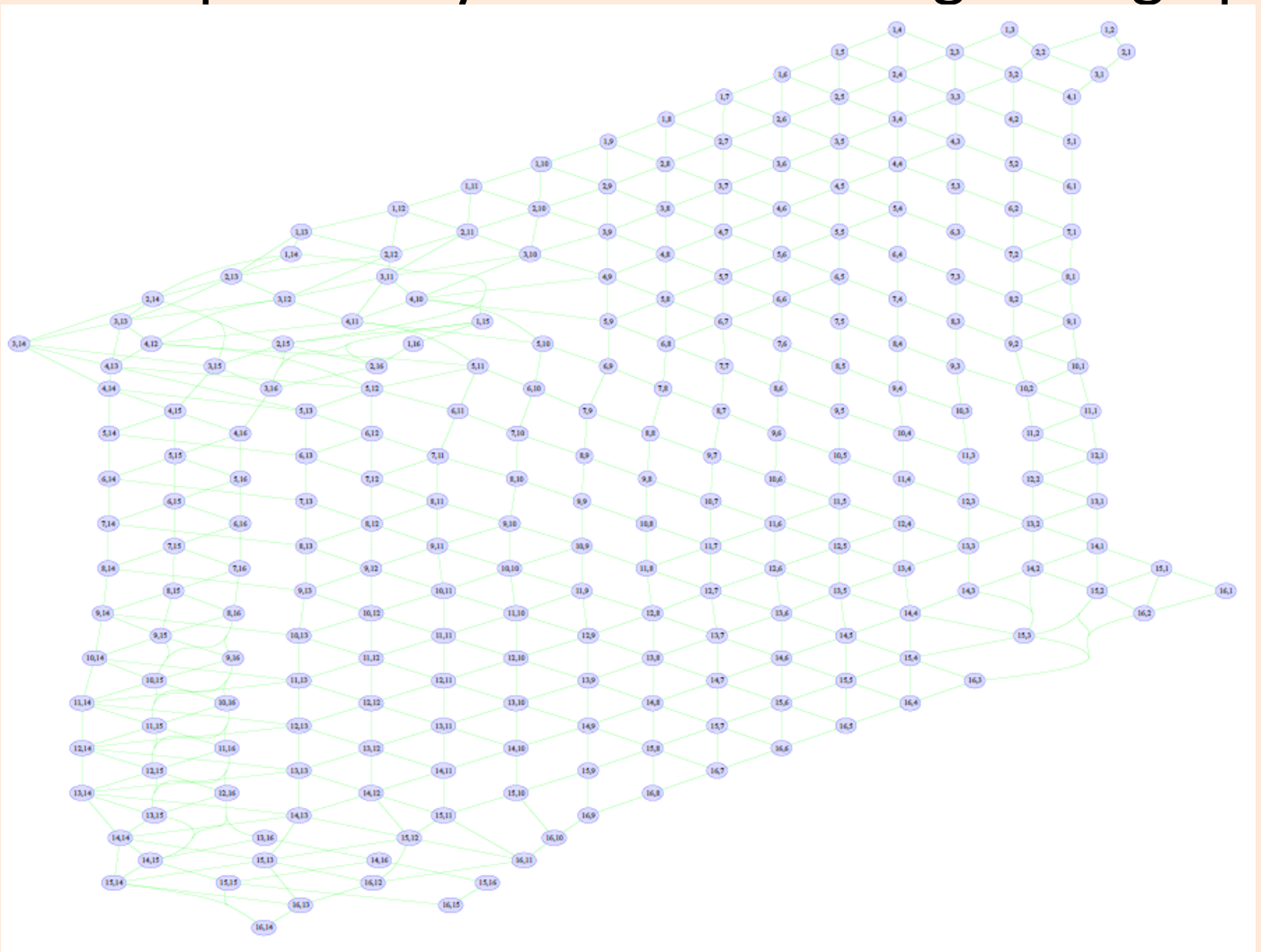
Dependency Networks

- 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.