CPSC 340: Machine Learning and Data Mining

Regularization

Fall 2020

Admin

- Midterm will be released Monday 19/10.
  - Take-home.
  - Kaggle competition

Last Time: Feature Selection

- Last time we discussed feature selection:
  - Choosing set of “relevant” features.

$$X = \begin{bmatrix} \quad & \quad & \quad \end{bmatrix} \qquad y = \begin{bmatrix} \quad \end{bmatrix}$$

“relevant”

- Most common approach is search and score:
  - Define “score” and “search” for features with best score.
- But it’s hard to define the “score” and it’s hard to “search”.
  - So we often use greedy methods like forward selection.
- Methods work ok on “toy” data, but are frustrating on real data.
  - Different methods may return very different results.
  - Defining whether a feature is “relevant” is complicated and ambiguous.

My advice if you want the “relevant” variables.

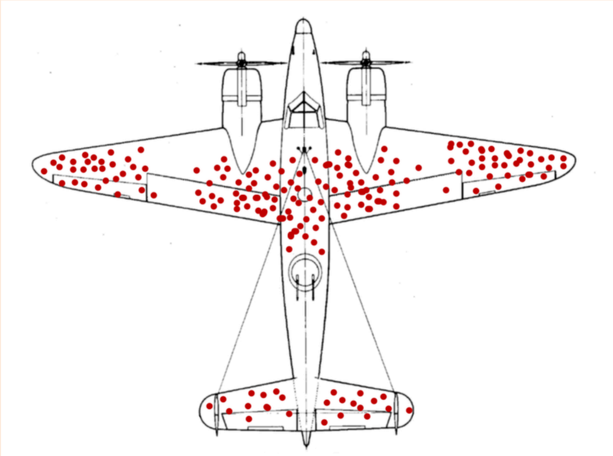
- Try the association approach.
- Try forward selection with different values of λ.
- Try out a few other feature selection methods too.

- Discuss the results with the domain expert.
  - They probably have an idea of why some variables might be relevant.

- Don’t be overconfident:
  - These methods are probably not discovering how the world truly works.
  - “The algorithm has found that these variables are helpful in predicting y_i.”
    - Then a warning that these models are not perfect at finding relevant variables.

Related: Survivorship Bias

- Plotting location of bullet holes on planes returning from WW2:



- Where are the "relevant" parts of the plane to protect?
  - "Relevant" parts are actually where there are no bullets.
  - Planes shot in other places did not come back (armor was needed).

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

Related: Survivorship Bias

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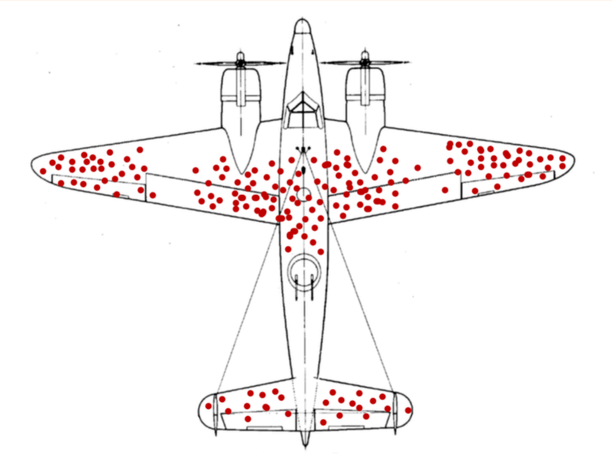

- This is an example of "survivorship bias":
  - Data is not IID because you only sample the "survivors".
  - Causes havoc for feature selection, and ML methods in general.

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

Related: Survivorship Bias

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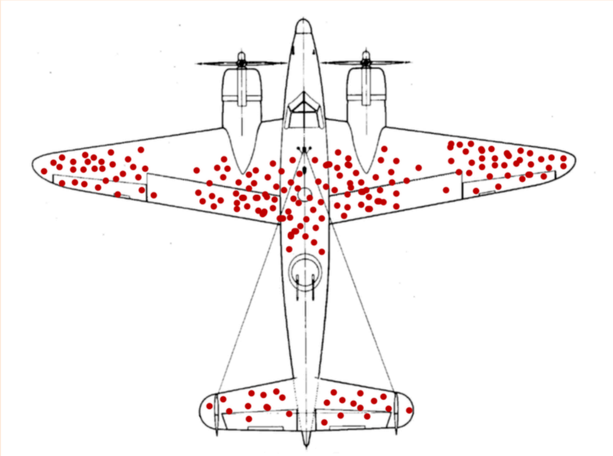

- People come to wrong conclusions due to survivor bias all the time.
  - Article on "secrets of success", focusing on traits of successful people.
  - But ignoring the number of non-super-successful with the same traits.
  - Article hypothesizing about various topics (allergies, mental illness, etc.).

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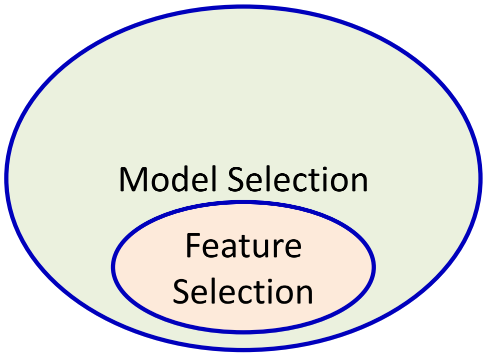
"Feature" Selection vs. "Model" Selection?

- Model selection: "which model should I use?"
  - KNN vs. decision tree, depth of decision tree, degree of polynomial basis.
- Feature selection: "which features should I use?"
  - Using feature 10 or not, using x_i^2 as part of basis.



- These two tasks are highly-related:
  - It's a different "model" if we add x_i^2 to linear regression.
  - But the x_i^2 term is just a "feature" that could be "selected" or not.
  - Usually, "feature selection" means choosing from some "original" features.
    - You could say that "feature" selection is a special case of "model" selection.

Can it help prediction to throw features away?

- Yes, because linear regression can overfit with large ‘d’.
  - Even though it’s “just” a hyper-plane.

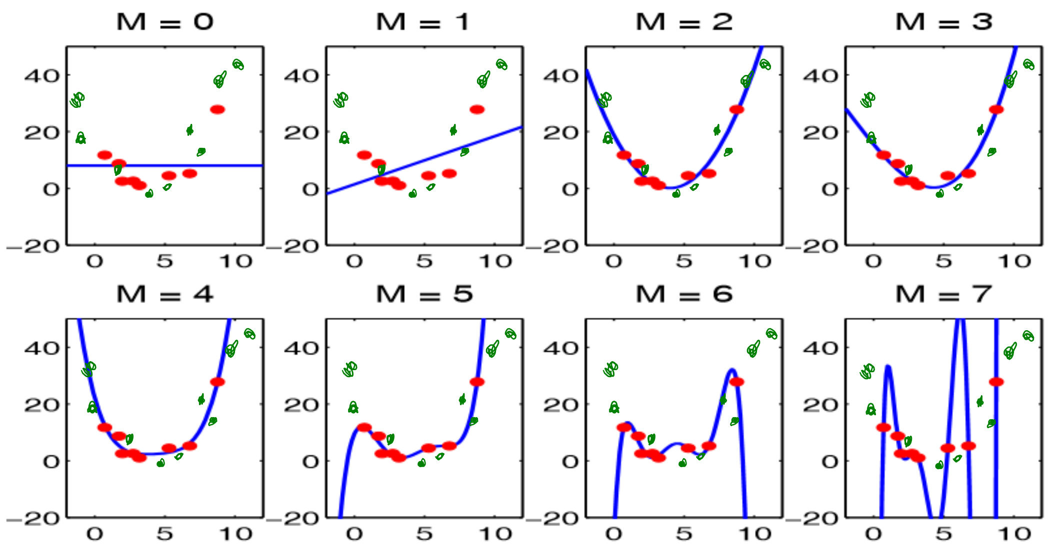
- Consider using d=n, with completely random features.
  - With high probability, you will be able to get a training error of 0.
  - But the features were random, this is completely overfitting.

- You could view “number of features” as a hyper-parameter.
  - Model gets more complex as you add more features.

(pause)

Recall: Polynomial Degree and Training vs. Testing

- We've said that complicated models tend to overfit more.



- But what if we need a complicated model?

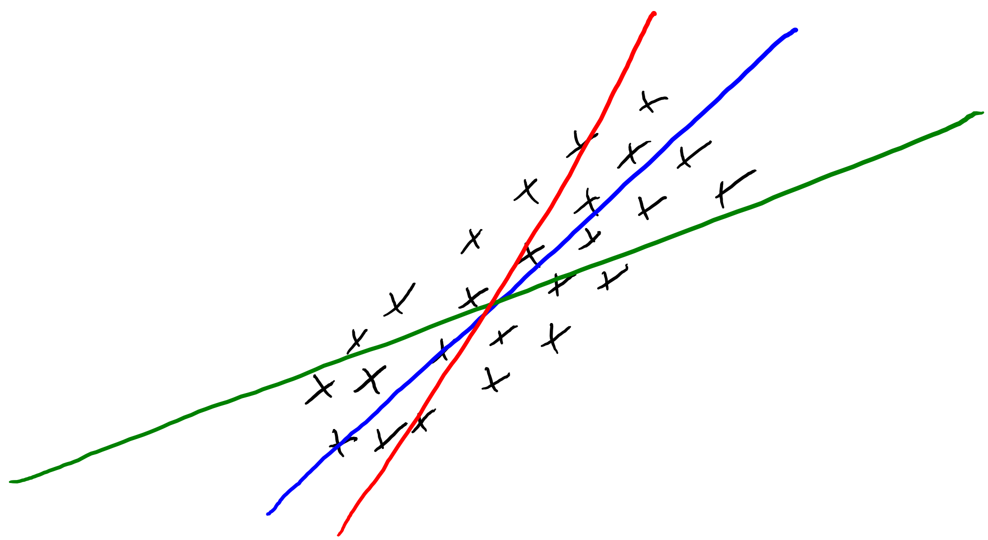
Controlling Complexity

- Usually "true" mapping from x_i to y_i is complex.
  - Might need high-degree polynomial.
  - Might need to combine many features, and don't know "relevant" ones.
- But complex models can overfit.
- So what do we do???

- Our main tools:
  - Model averaging: average over multiple models to decrease variance.
  - Regularization: add a penalty on the complexity of the model.

Would you rather?

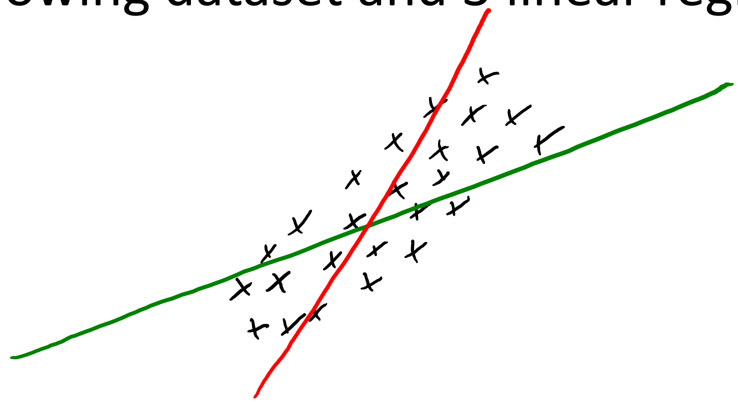
- Consider the following dataset and 3 linear regression models:



- Which line should we choose?

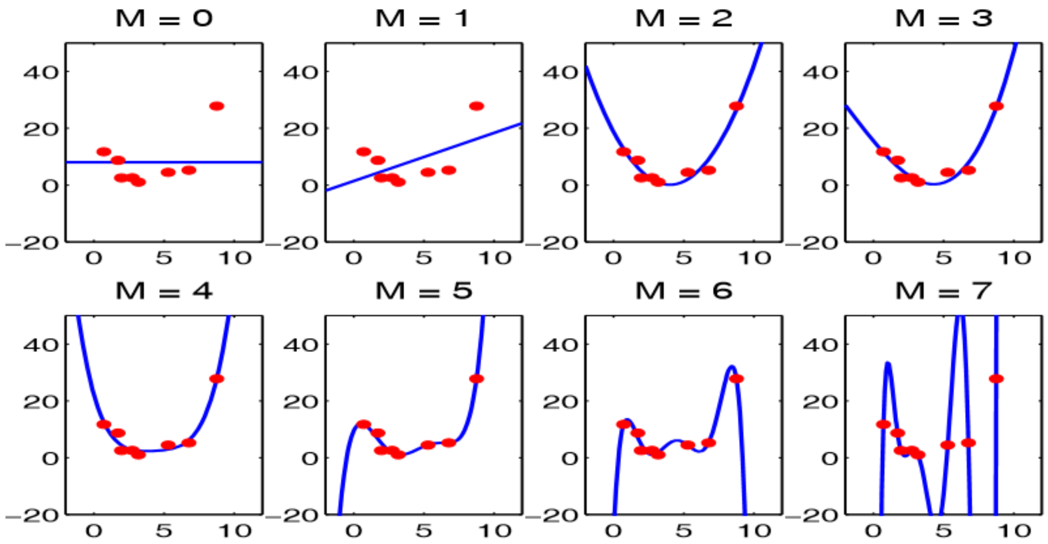
Would you rather?

- Consider the following dataset and 3 linear regression models:



- What if you are forced to choose between red and green?
  - And assume they have the same training error.
- You should pick green.
  - Since slope is smaller, small change in x_i has a smaller change in prediction y_i.
    - Green line's predictions are less sensitive to having 'w' exactly right.
  - Since green 'w' is less sensitive to data, test error might be lower.

Size of Regression Weights are Overfitting



- The regression weights w_j with degree-7 are huge in this example.
- The degree-7 polynomial would be less sensitive to the data,

  if we "regularized" the w_j so that they are small.

$\hat{y}_i = 0.0001(x_i)^7 + 0.03(x_i)^3 + 3$ vs. $\hat{y}_i = 1000(x_i)^7 - 500(x_i)^6 + 890x_i$

L2-Regularization

- Standard regularization strategy is L2-regularization:

$$f(w) = \frac{1}{2}\sum_{i=1}^{n}(w^Tx_i - y_i)^2 + \frac{\lambda}{2}\sum_{j=1}^{d} w_j^2 \quad \text{or} \quad f(w) = \frac{1}{2}\|Xw - y\|^2 + \frac{\lambda}{2}\|w\|^2$$

- Intuition: large slopes w_j tend to lead to overfitting.
- Objective balances getting low error vs. having small slopes 'w_j'.
  - "You can increase the training error if it makes 'w' much smaller."
  - Nearly-always reduces overfitting.
  - Regularization parameter λ > 0 controls "strength" of regularization.
    - Large λ puts large penalty on slopes.

L2-Regularization

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- In terms of fundamental trade-off:
  - Regularization increases training error.
  - Regularization decreases approximation error.

- How should you choose λ?
  - Theory: as 'n' grows λ should be in the range O(1) to (√n).
  - Practice: optimize validation set or cross-validation error.
    - This almost always decreases the test error.

L2-Regularization "Shrinking" Example

- Solution to a "least squares with L2-regularization" for different λ:

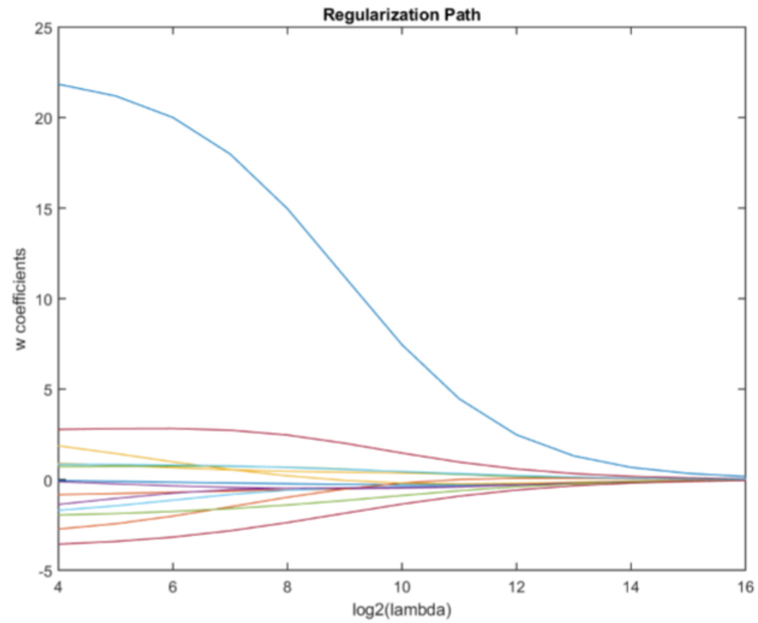
λ	w_1	w_2	w_3	w_4	w_5
0	-1.88	1.29	-2.63	1.78	-0.63
1	-1.88	1.28	-2.62	1.78	-0.64
4	-1.87	1.28	-2.59	1.77	-0.66
16	-1.84	1.27	-2.50	1.73	-0.73
64	-1.74	1.23	-2.22	1.59	-0.90
256	-1.43	1.08	-1.70	1.18	-1.05
1024	-0.87	0.73	-1.03	0.57	-0.81
4096	-0.35	0.31	-0.42	0.18	-0.36

$\|\|Xw - y\|\|^2$	$\|\|w\|\|^2$
285.64	15.68
285.64	15.62
285.64	15.43
285.71	14.76
286.47	12.77
292.60	8.60
321.29	3.33
374.27	0.56

- We get least squares with $\lambda = 0$.
  - But we can achieve similar training error with smaller $||w||$.
- $||Xw - y||$ increases with λ, and $||w||$ decreases with λ.
  - Though individual w_j can increase or decrease with lambda.
  - Because we use the L2-norm, the large ones decrease the most.

Regularization Path

- Regularization path is a plot of the optimal weights 'w_j' as 'λ' varies:



- Starts with least squares with $\lambda = 0$, and w_j converge to 0 as λ grows.

L2-regularization and the normal equations

- When using L2-regularized squared error, we can solve for ∇ f(w) = 0.
- Loss before: $f(w) = \frac{1}{2}\|Xw - y\|^2$
- Loss after: $f(w) = \frac{1}{2}\|Xw - y\|^2 + \frac{\lambda}{2}\|w\|^2$

- Gradient before: $\nabla f(w) = X^T X w - X^T y$
- Gradient after: $\nabla f(w) = X^T X w - X^T y + \lambda w$

- Linear system before: $X^T X w = X^T y$
- Linear system after: $(X^T X + \lambda I) w = X^T y$
- But unlike $X^T X$, the matrix $(X^T X + \lambda I)$ is always invertible:
  - Multiply by its inverse for unique solution: $w = (X^T X + \lambda I)^{-1}(X^T y)$

Gradient Descent for L2-Regularized Least Squares

- The L2-regularized least squares objective and gradient:

$$f(w) = \frac{1}{2}\|Xw - y\|^2 + \frac{\lambda}{2}\|w\|^2 \qquad \nabla f(w) = X^T(Xw - y) + \lambda w$$

- Gradient descent iterations for L2-regularized least squares:

$$w^{t+1} = w^t - \alpha^t \Big[\underbrace{X^T(Xw^t - y) + \lambda w^t}_{\nabla f(w^t)} \Big]$$

- Cost of gradient descent iteration is still O(nd).
  - Can show number of iterations decrease as λ increases (not obvious).

Why use L2-Regularization?

- It's a weird thing to do, but we (cs340 professors) say "always use regularization".
  - "Almost always decreases test error" should already convince you.

- But here are 6 more reasons:
  1. Solution 'w' is unique.
  2. X^TX does not need to be invertible (no collinearity issues).
  3. Less sensitive to changes in X or y.
  4. Gradient descent converges faster (bigger λ means fewer iterations).
  5. Stein's paradox: if $d \geq 3$, 'shrinking' moves us closer to 'true' w.
  6. Worst case: just set λ small and get the same performance.

(pause)

Features with Different Scales

- Consider continuous features with different scales:

Egg (#)	Milk (mL)	Fish (g)	Pasta (cups)
0	250	0	1
1	250	200	1
0	0	0	0.5
2	250	150	0

- Should we convert to some standard 'unit'?
  - It doesn't matter for decision trees or naïve Bayes.
    - They only look at one feature at a time.
  - It doesn't matter for least squares:
    - w_j*(100 mL) gives the same model as w_j*(0.1 L) with a different w_j.

Features with Different Scales

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- Should we convert to some standard 'unit'?
  - It matters for k-nearest neighbours:
    - "Distance" will be affected more by large features than small features.
  - It matters for regularized least squares:
    - Penalizing $(w_j)^2$ means different things if features 'j' are on different scales.

Standardizing Features

$X = \begin{bmatrix} & 0 & \end{bmatrix}$

average of column 'j'

- It is common to standardize continuous features:
  - For each feature:
    1. Compute mean and standard deviation:

       $$\mu_j = \frac{1}{n}\sum_{i=1}^{n} x_{ij} \qquad \sigma_j = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_{ij}-\mu_j)^2}$$

    2. Subtract mean and divide by standard deviation ("z-score")

       Replace x_{ij} with $\frac{x_{ij}-\mu_j}{\sigma_j}$

  - Now changes in 'w_j' have similar effect for any feature 'j'.
- How should we standardize test data?
  - Wrong approach: use mean and standard deviation of test data.
  - Training and test mean and standard deviation might be very different.
  - Right approach: use mean and standard deviation of training data.

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  - Now changes in 'w_j' have similar effect for any feature 'j'.
- If we're doing 10-fold cross-validation:
  - Compute μ_j and σ_j based on the 9 training folds (e.g., average over 9/10s of data).
  - Standardize the remaining ("validation") fold with this "training" μ_j and σ_j.
  - Re-standardize for different folds.

Standardizing Target

- In regression, we sometimes standardize the targets y_i.
  – Puts targets on the same standard scale as standardized features:

$$\text{Replace } y_i \text{ with } \frac{y_i - \mu_y}{\sigma_y}$$

- With standardized target, setting $w = 0$ predicts average y_i:
  – High regularization makes us predict closer to the average value.
- Again, make sure you standardize test data with the training stats.
- Other common transformations of y_i are logarithm/exponent:

$$\text{Use } \log(y_i) \text{ or } \exp(\gamma y_i)$$

  – Makes sense for geometric/exponential processes.

Regularizing the y-Intercept?

- Should we regularize the y-intercept?

- No! Why encourage it to be closer to zero? (It could be anywhere.)
  - You should be allowed to shift function up/down globally.

- Yes! It makes the solution unique and it easier to compute 'w'.

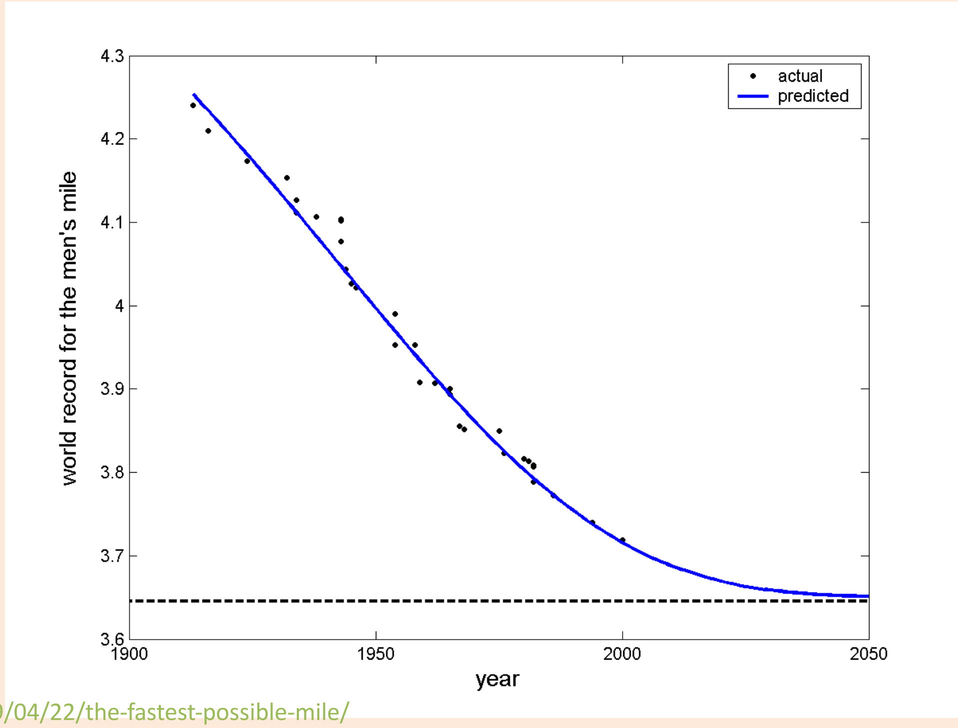
- Compromise: regularize by a smaller amount than other variables.

$$f(w, w_0) = \frac{1}{2}\|Xw + w_0 - y\|^2 + \frac{\lambda}{2}\|w\|^2 + \frac{\lambda_0}{2} w_0^2$$

(pause)

Predicting the Future

- In principle, we can use any features x_i that we think are relevant.
- This makes it tempting to use time as a feature, and predict future.



https://gravityandlevity.wordpress.com/2009/04/22/the-fastest-possible-mile/

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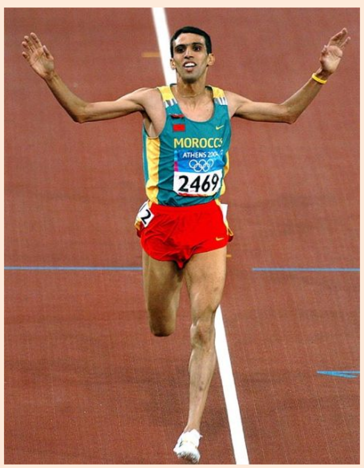
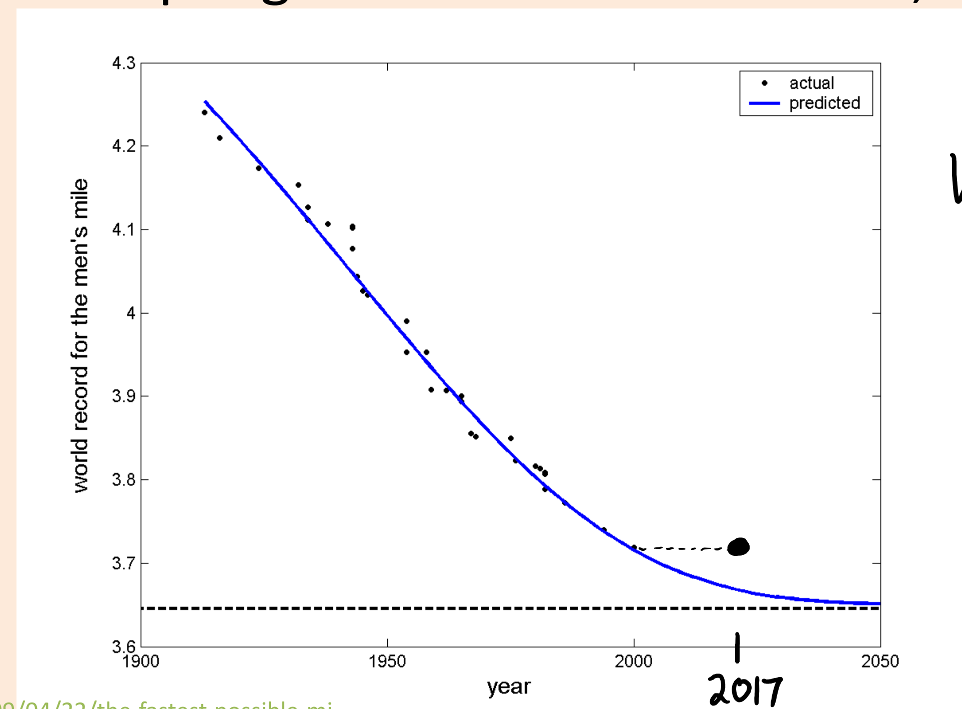
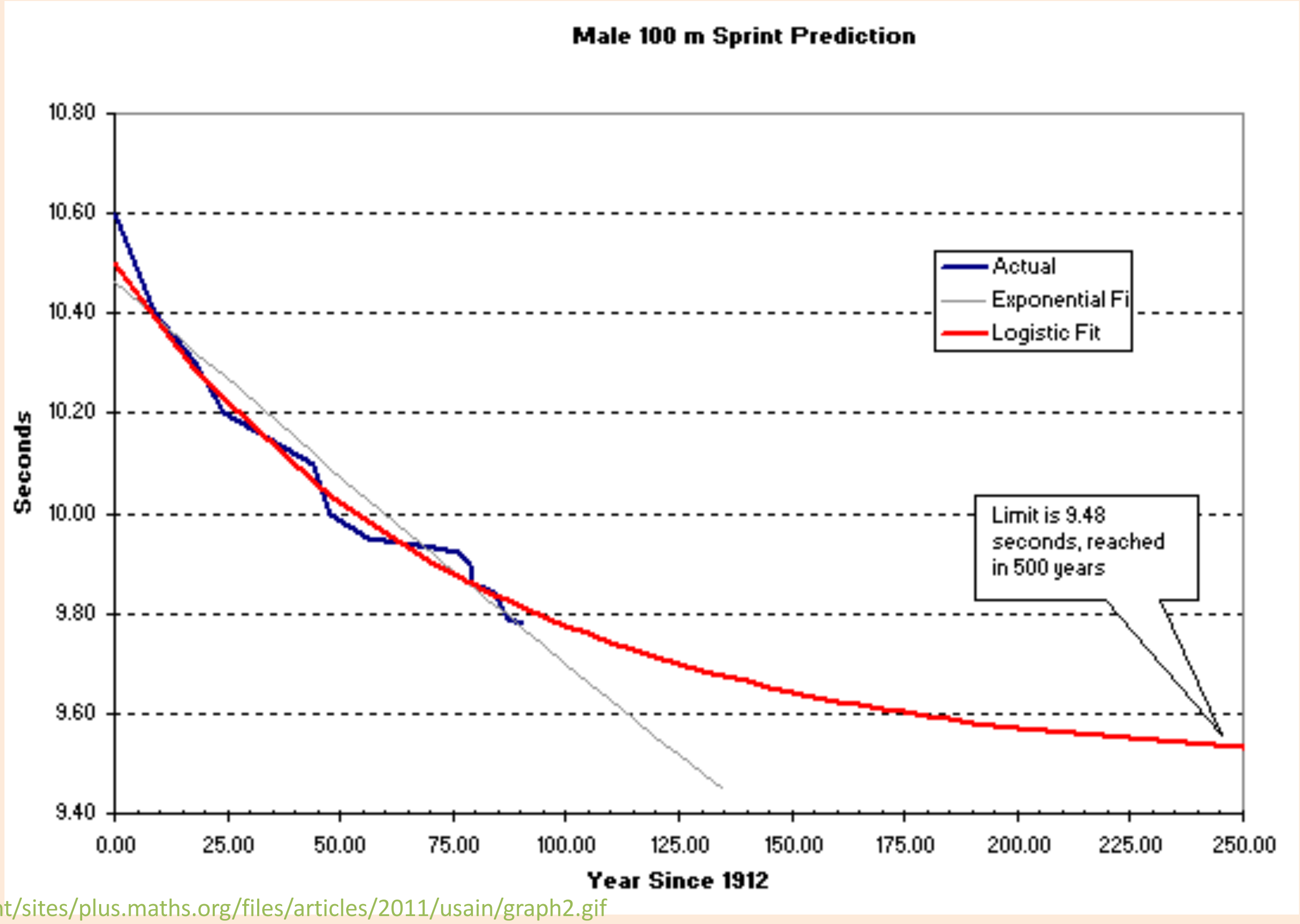




We need to be cautious about doing this.

https://gravityandlevity.wordpress.com/2009/04/22/the-fastest-possible-mi
https://overthehillsports.wordpress.com/tag/hicham-el-guerrouj/le/

Predicting 100m times 400 years in the future?



https://plus.maths.org/content/sites/plus.maths.org/files/articles/2011/usain/graph2.gif

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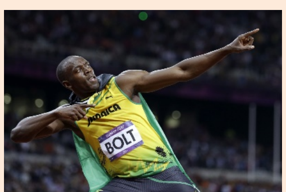

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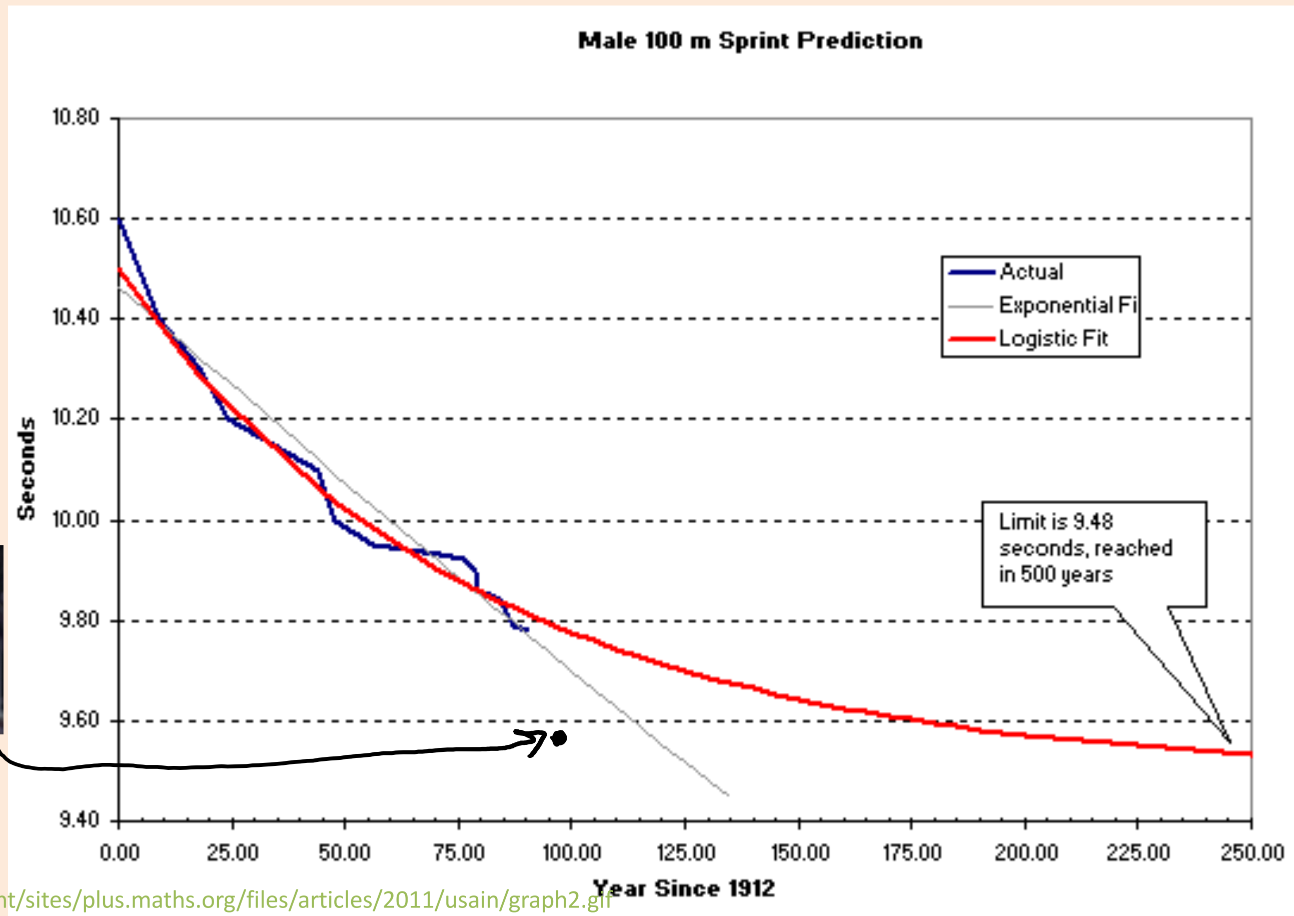


https://plus.maths.org/content/sites/plus.maths.org/files/articles/2011/usain/graph2.gif
http://www.washingtonpost.com/blogs/london-2012-olympics/wp/2012/08/08/report-usain-bolt-invited-to-tryout-for-manchester-united/

Interpolation vs Extrapolation

- Interpolation is task of predicting "between the data points".
  - Regression models are good at this if you have enough data and function is continuous.
- Extrapolation is task of prediction outside the range of the data points.
  - Without assumptions, regression models can be embarrassingly-bad at this.

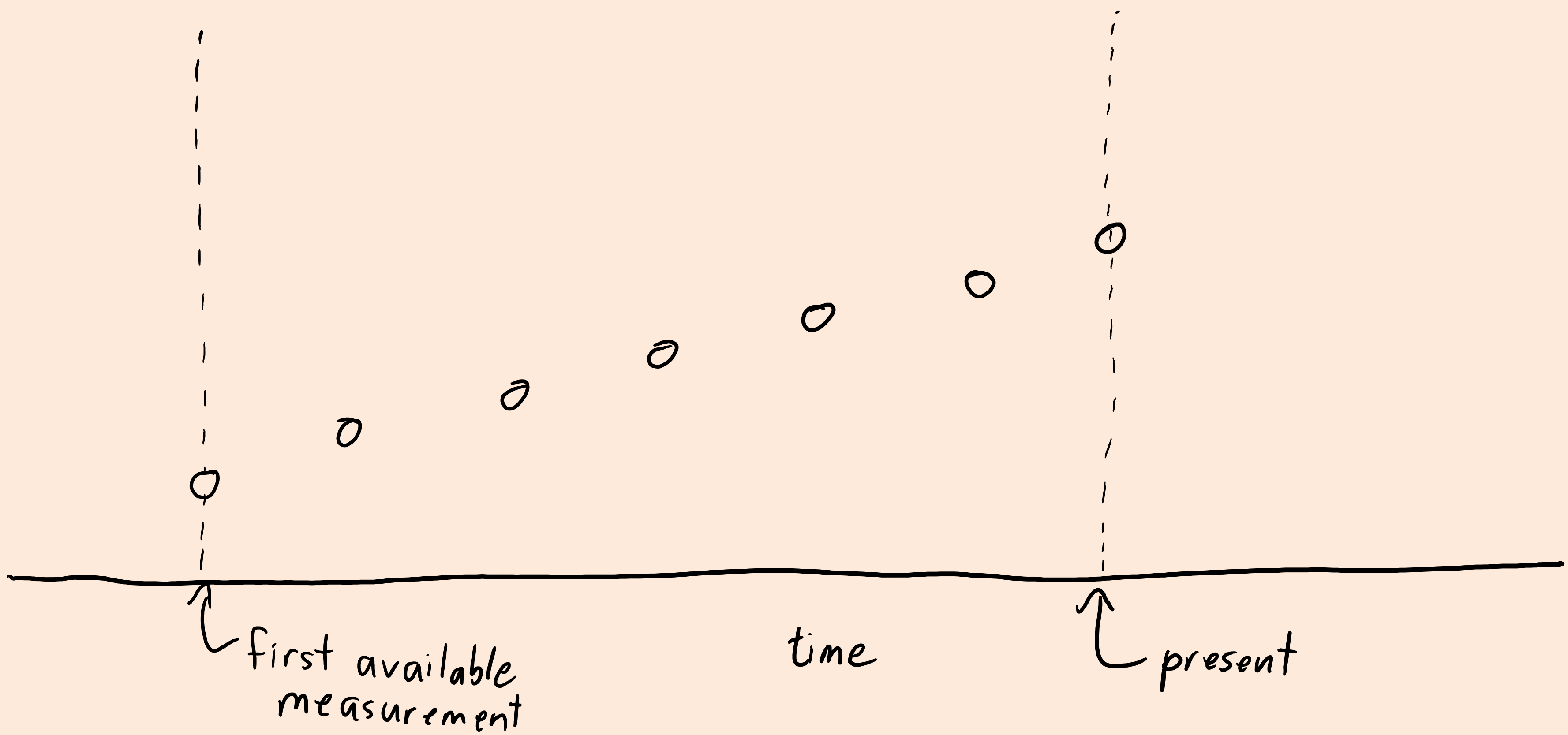
- If you run the 100m regression models backwards in time:
  - They predict that humans used to be really really slow!

- If you run the 100m regression models forwards in time:
  - They might eventually predict arbitrarily-small 100m times.
  - The linear model actually predicts negative times in the future.
    - These time traveling races in 2060 should be pretty exciting!

- Some discussion here:
  - http://callingbullshit.org/case_studies/case_study_gender_gap_running.html

https://www.smbc-comics.com/comic/rise-of-the-machines

No Free Lunch, Consistency, and the Future



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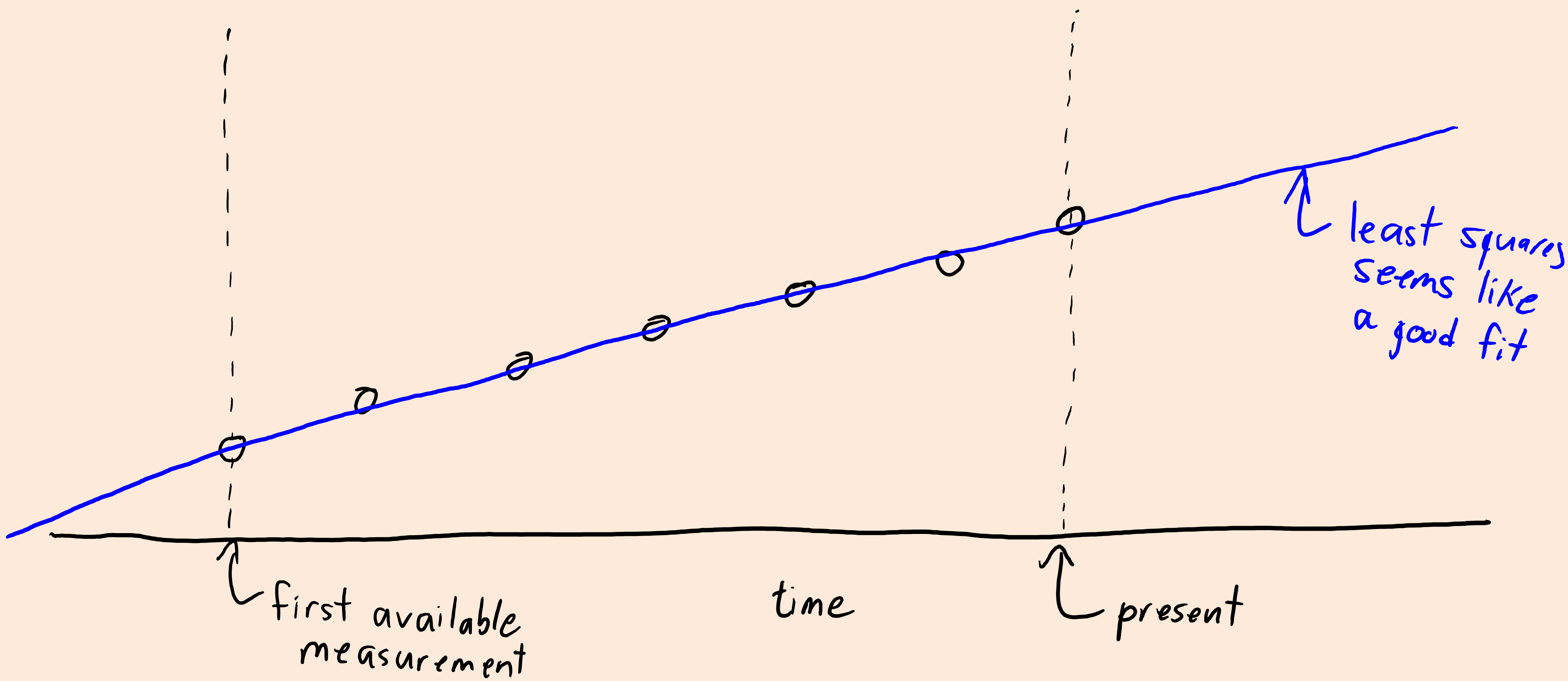

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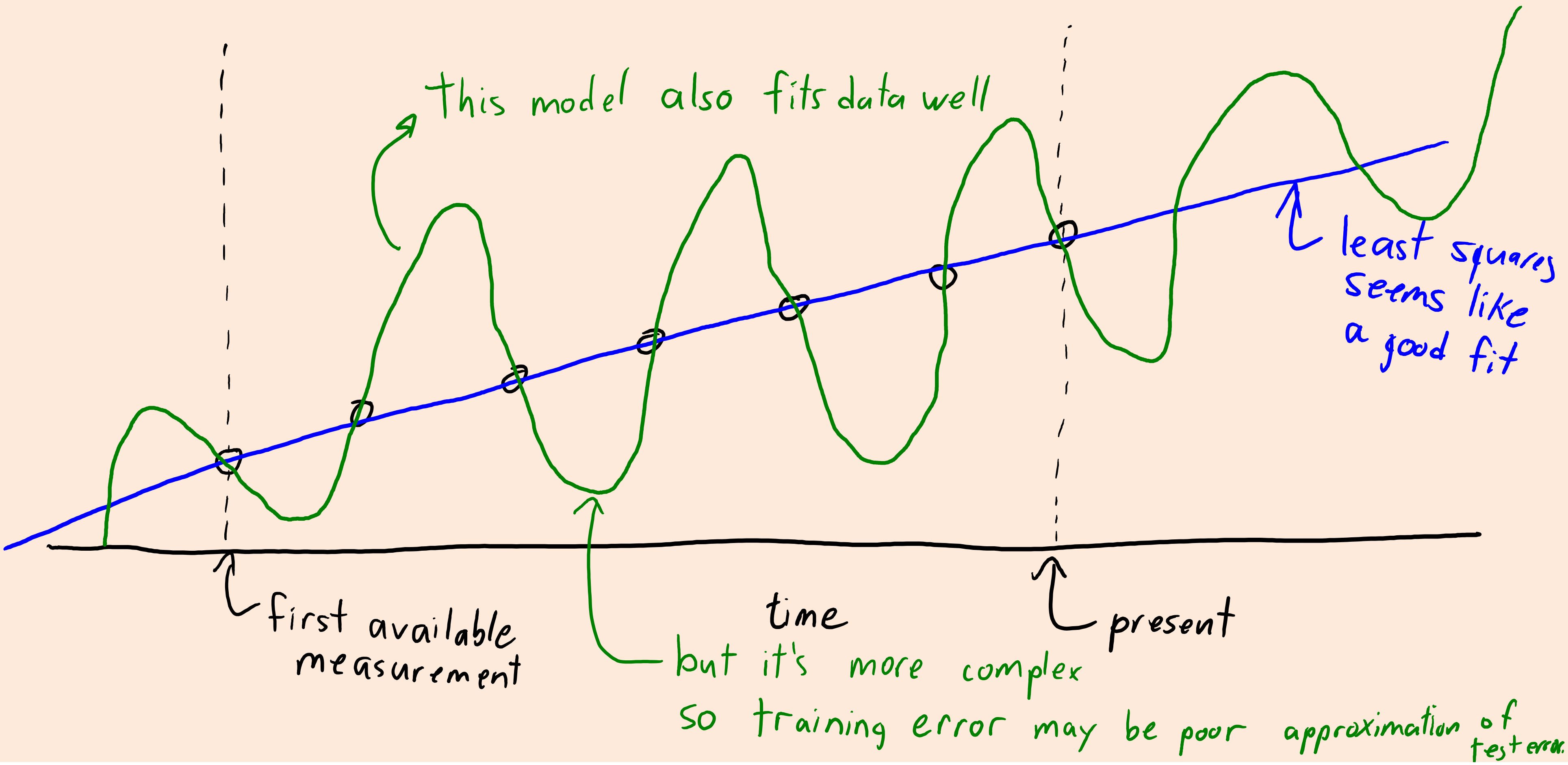
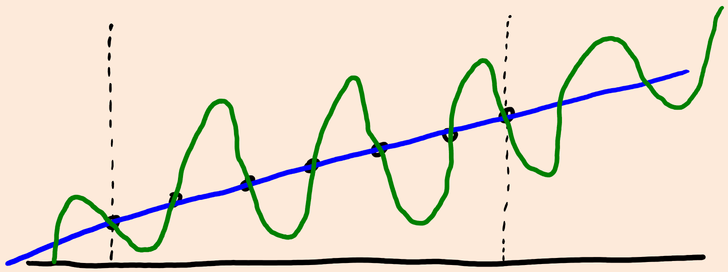


Ockham's Razor vs. No Free Lunch

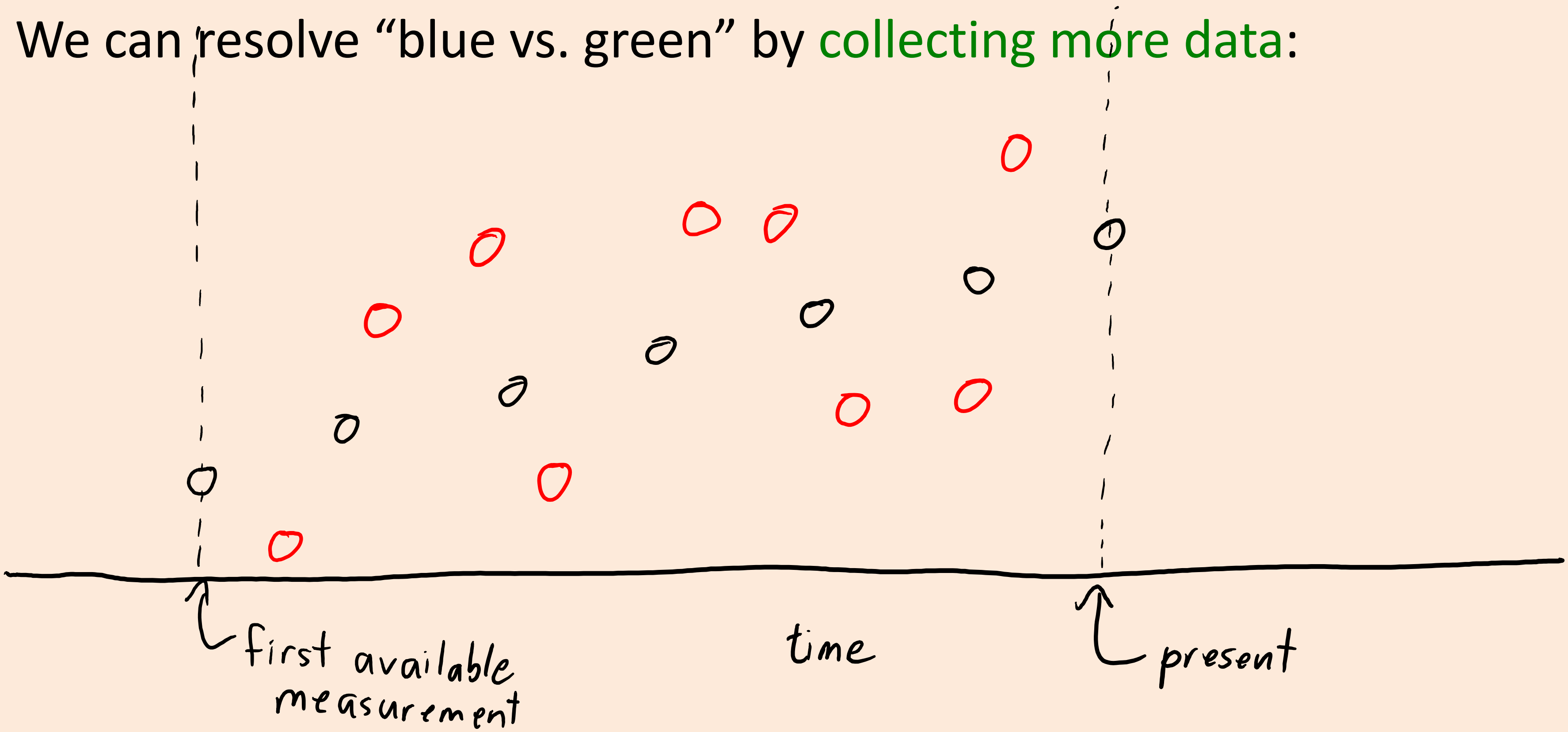
- Ockham's razor is a problem-solving principle:
  - "Among competing hypotheses, the one with the fewest assumptions should be selected."
  - Suggests we should select linear model.



- Fundamental trade-off:
  - If same training error, pick model less likely to overfit.
  - Formal version of Occam's problem-solving principle.
  - Also suggests we should select linear model.
- No free lunch theorem:
  - There *exists possible datasets* where you should select the green model.

No Free Lunch, Consistency, and the Future

- We can resolve "blue vs. green" by collecting more data:



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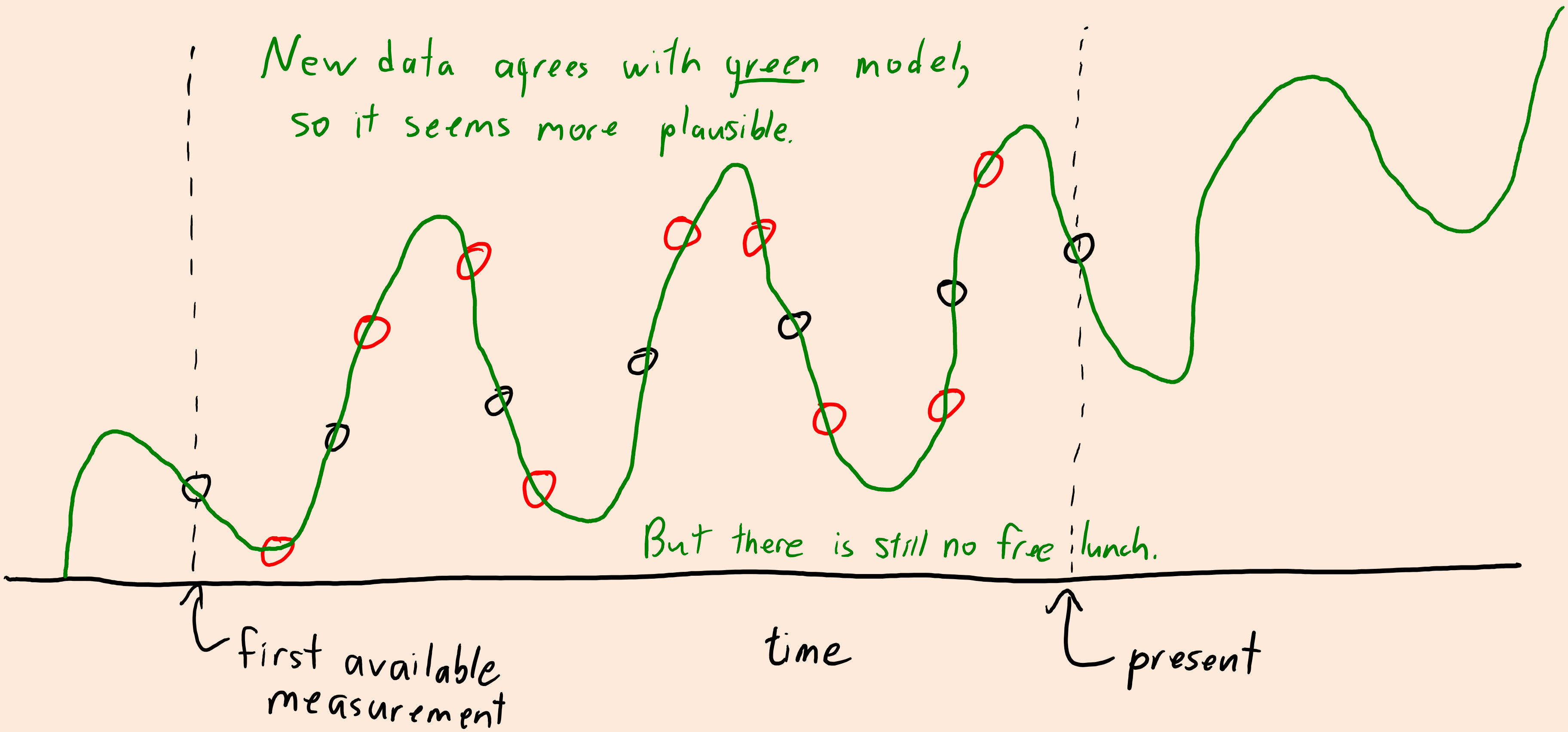

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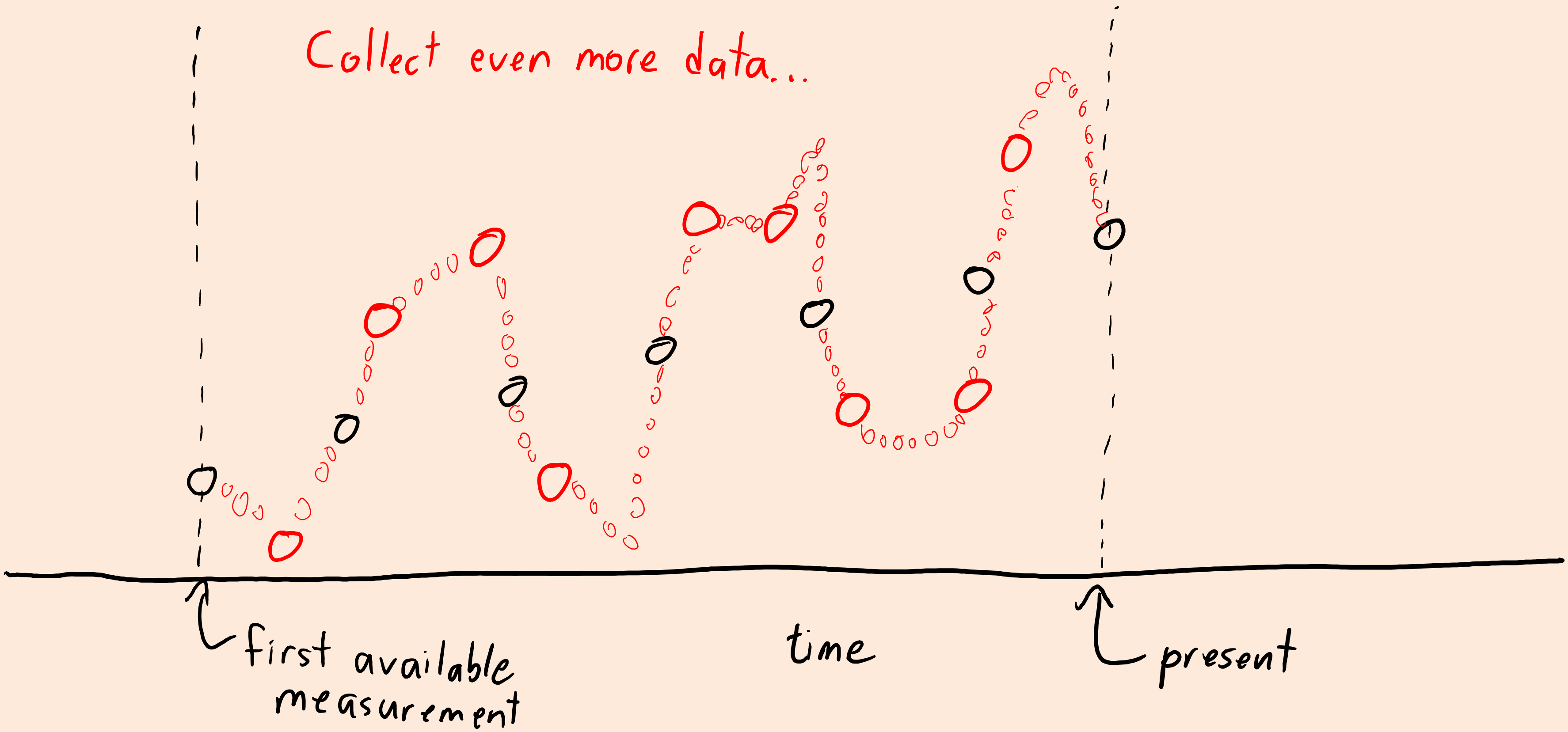

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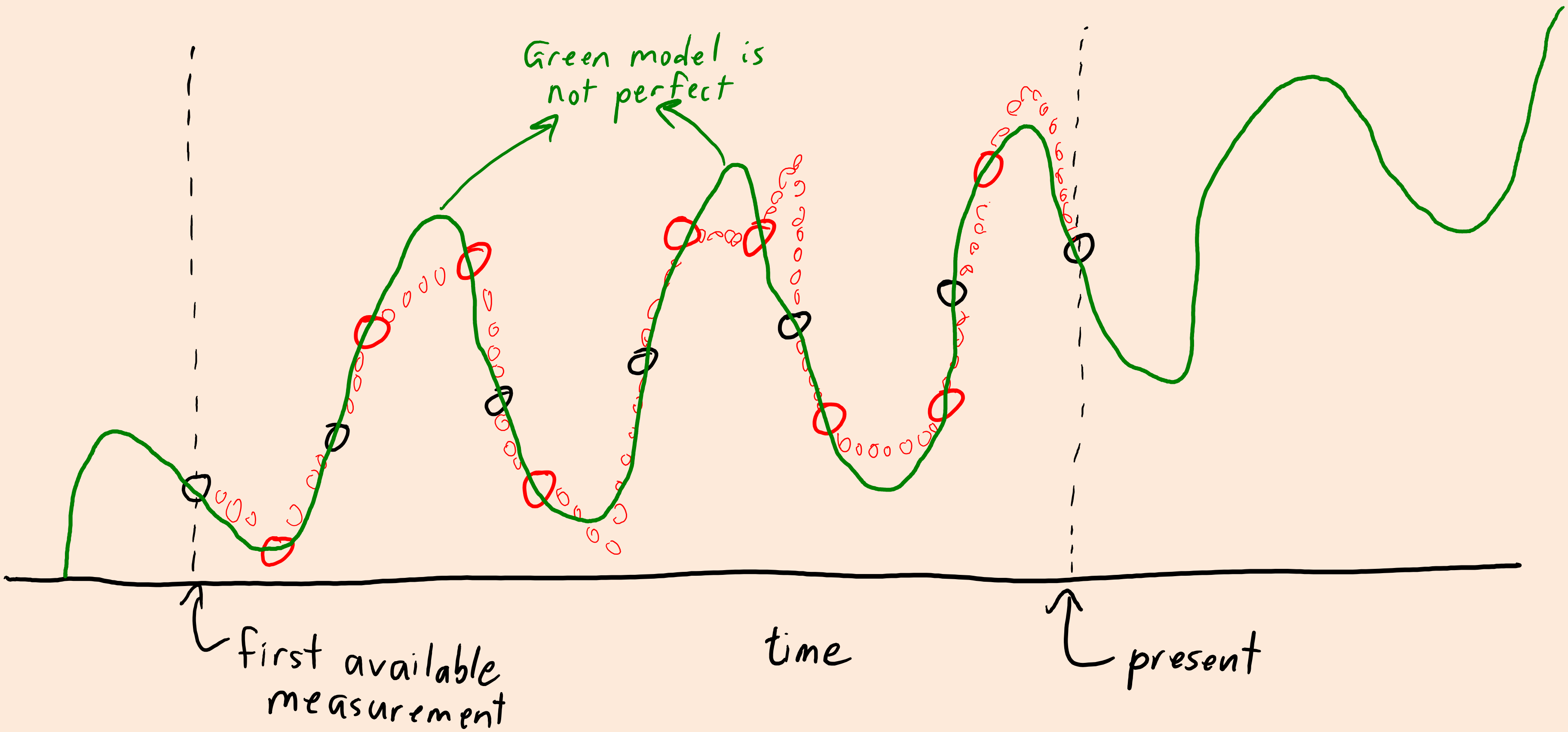

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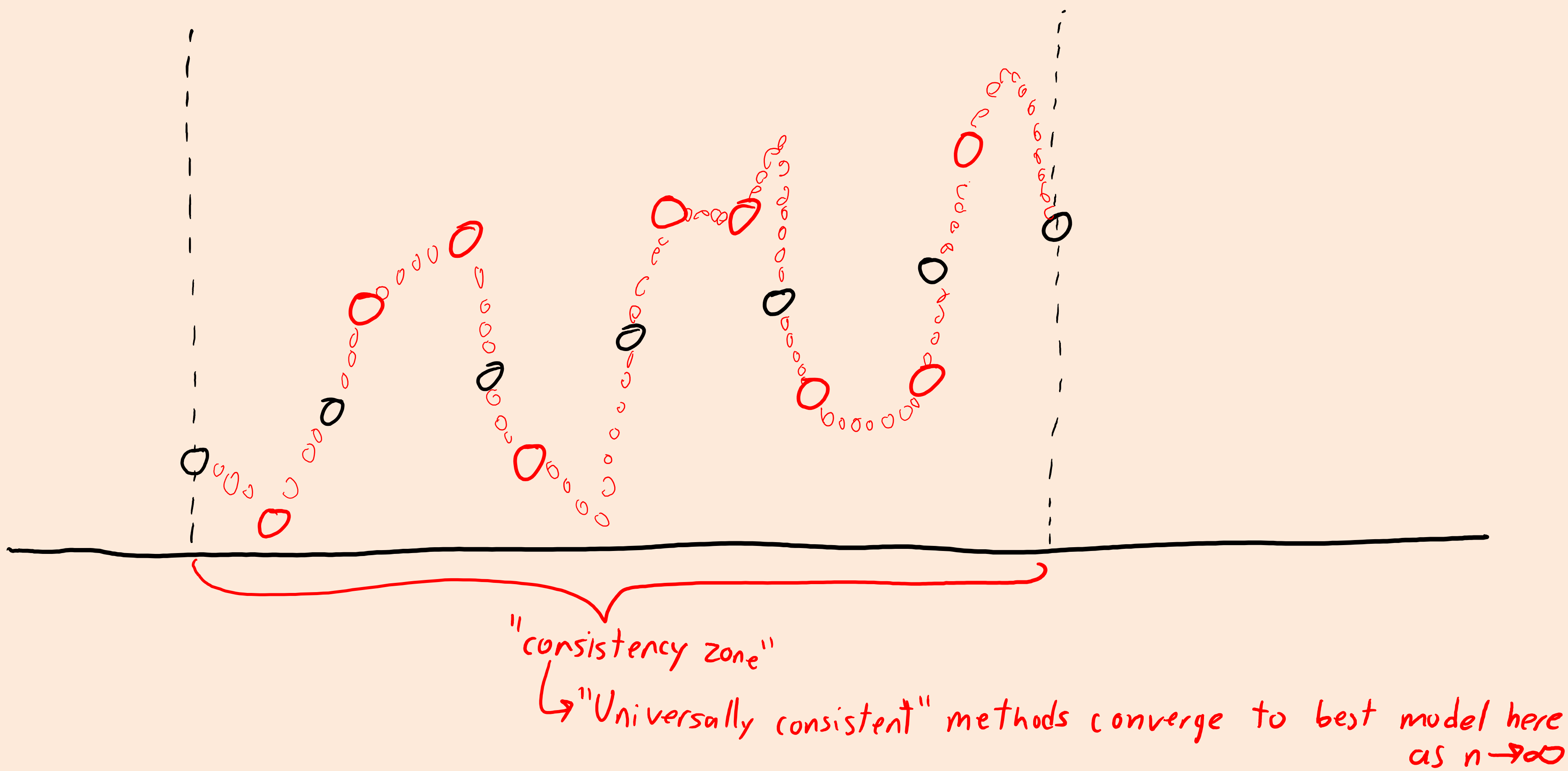

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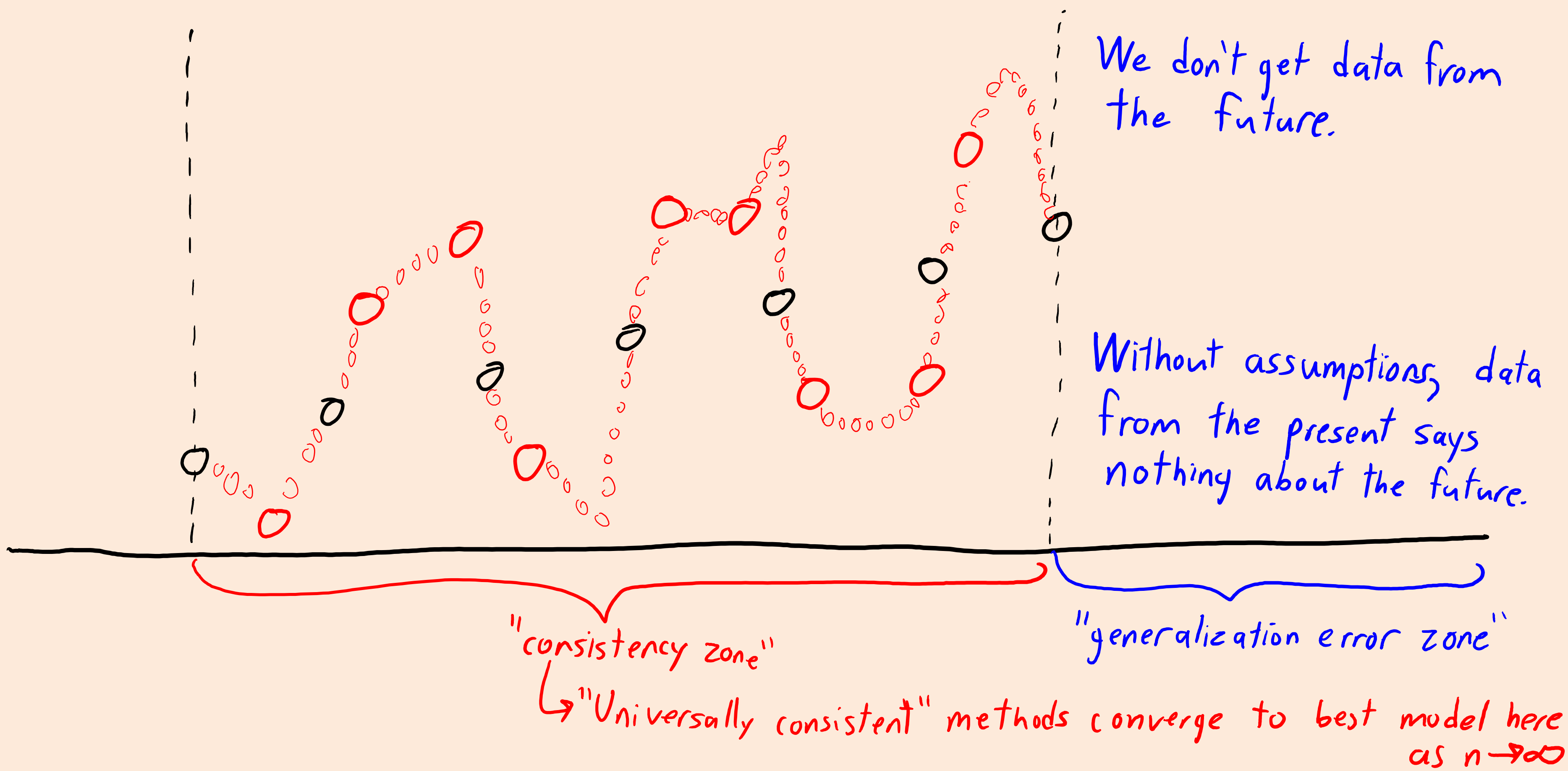

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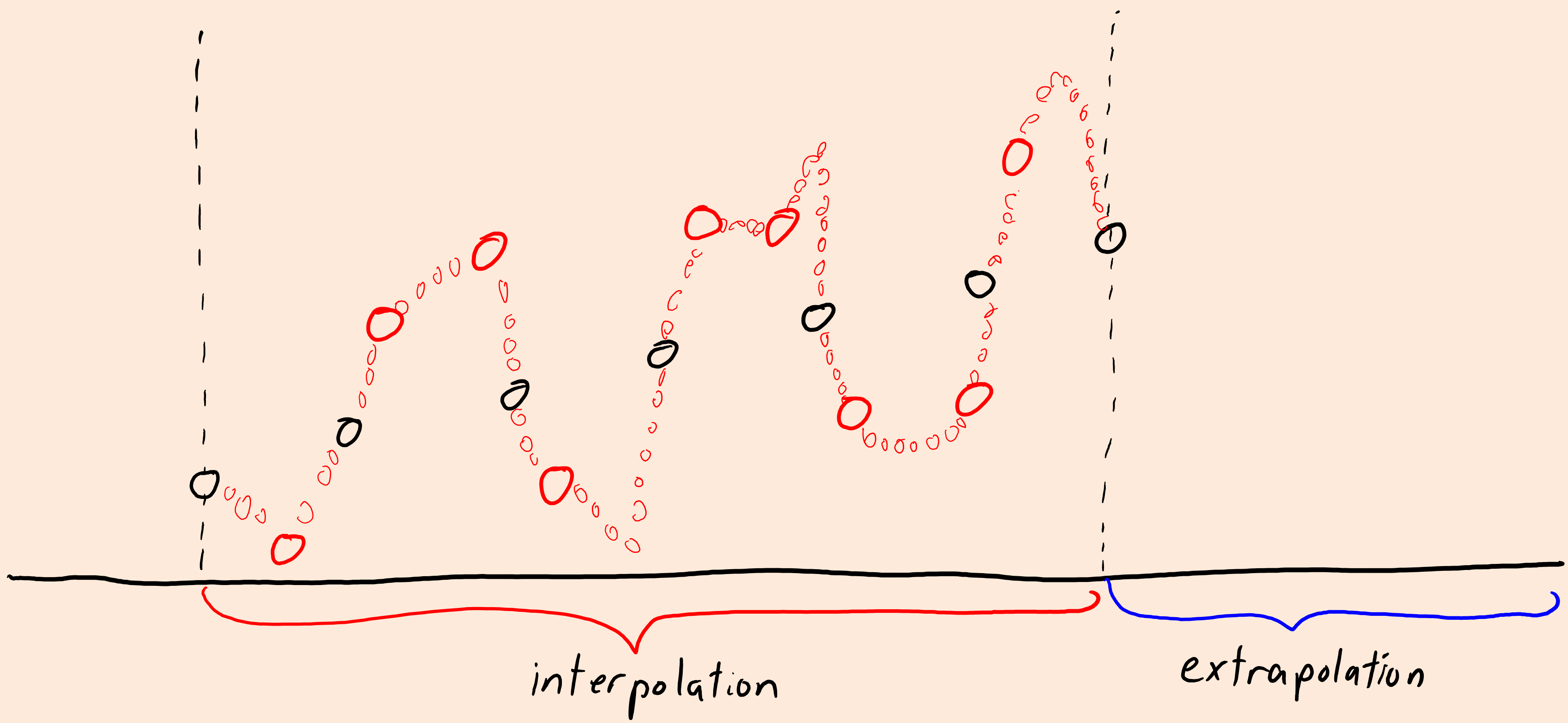
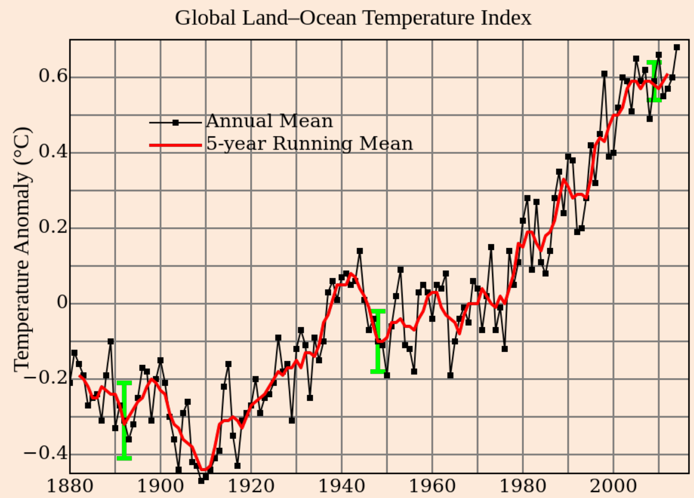


Discussion: Climate Models

- Has Earth warmed up over last 100 years? (Consistency zone)
  - Data clearly says “yes”.

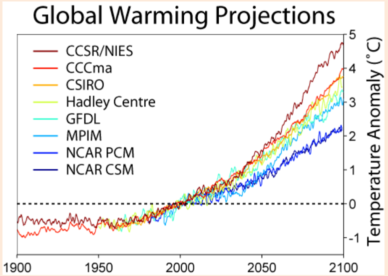


- Will Earth continue to warm over next 100 years? (generalization error)
  - We should be more skeptical about models that predict future events.

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

Discussion: Climate Models

- So should we all become global warming skeptics?
- If we average over models that overfit in *independent* ways, we expect the test error to be lower, so this gives more confidence:

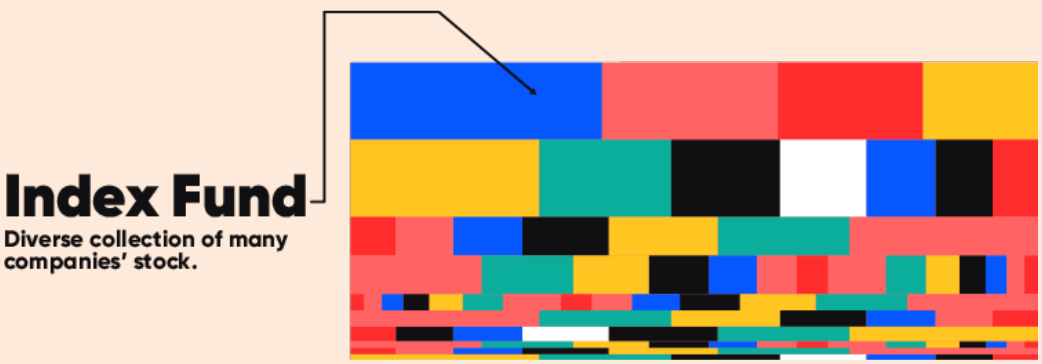


  - We should be skeptical of individual models, but agreeing predictions made by models with different data/assumptions are more likely be true.
- All the near-future predictions agree, so they are likely to be accurate.
  - And it's probably reasonable to assume fairly continuous change (no big "jumps").
- Variance is higher further into future, so predictions are less reliable.
  - Relying more on assumptions and less on data.

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

Index Funds: Ensemble Extrapolation for Investing

- Want to do extrapolation when investing money.
  - What will this be worth in the future?
- Index funds can be viewed as an ensemble method for investing.
  - For example, buy stock in top 500 companies proportional to value.
  - Tries to follow average price increase/decrease.



  - This simple investing strategy outperforms most fund managers.

http://fibydesign.com/005-introduction-to-index-investing-stocks-index-funds-vtsax/

Summary

- Regularization:
  - Adding a penalty on model complexity.
- L2-regularization: penalty on L2-norm of regression weights 'w'.
  - Almost always improves test error.
- Standardizing features:
  - For some models it makes sense to have features on the same scale.
- Interpolation vs. Extrapolation:
  - Machine learning with large 'n' is good at predicting "between the data".
  - Without assumptions, can be arbitrarily bad "away from the data".

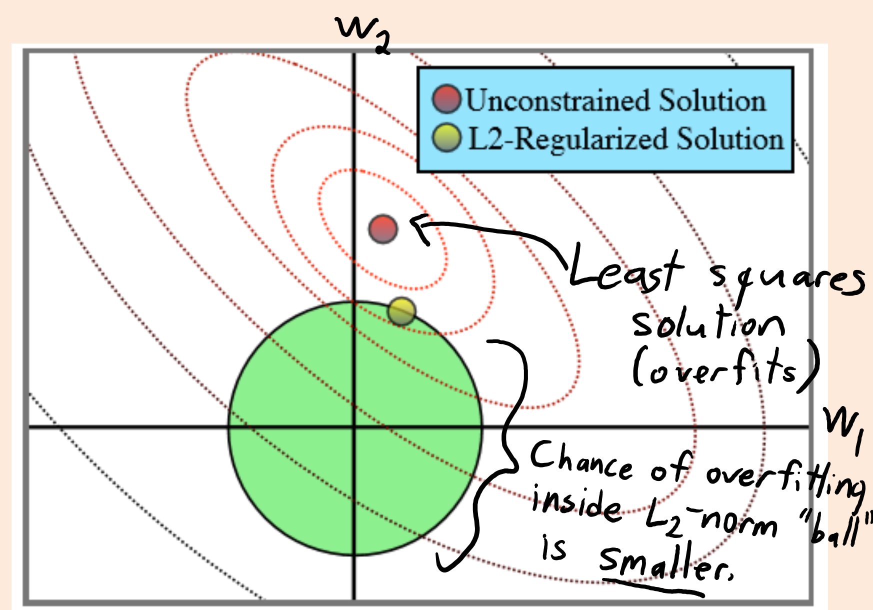
- Next time: learning with an exponential number of irrelevant features.

L2-Regularization

- Standard regularization strategy is L2-regularization:

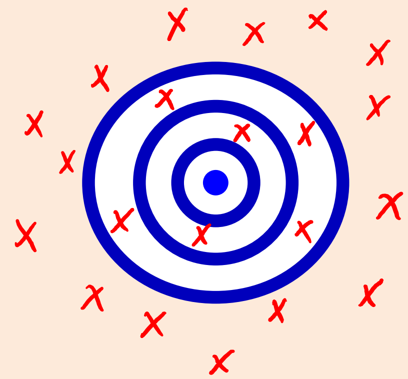
$$f(w) = \frac{1}{2}\sum_{i=1}^{n}(w^Tx_i - y_i)^2 + \frac{\lambda}{2}\sum_{j=1}^{d} w_j^2 \quad \text{or} \quad f(w) = \frac{1}{2}\|Xw - y\|^2 + \frac{\lambda}{2}\|w\|^2$$

- Equivalent to minimizing squared error but keeping L2-norm small.



Regularization/Shrinking Paradox

- We throw darts at a target:
  - Assume we don't always hit the exact center.
  - Assume the darts follow a symmetric pattern around center.



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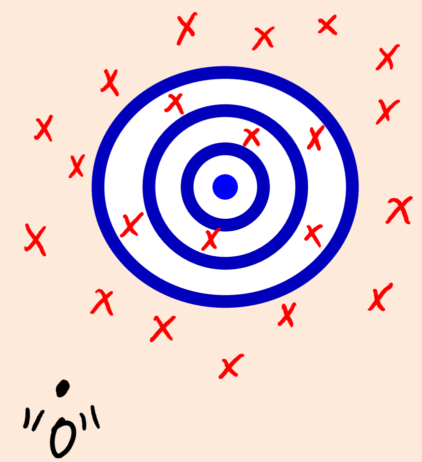
  1. Choose some arbitrary location '0'.
  2. Measure distances from darts to '0'.



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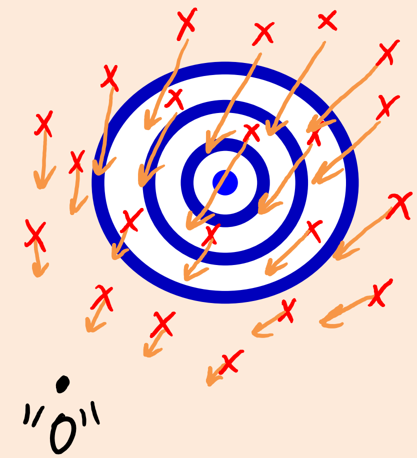
  3. Move misses towards '0', by *small* amount proportional to distance from 0.
- If small enough, darts will be closer to center on average.



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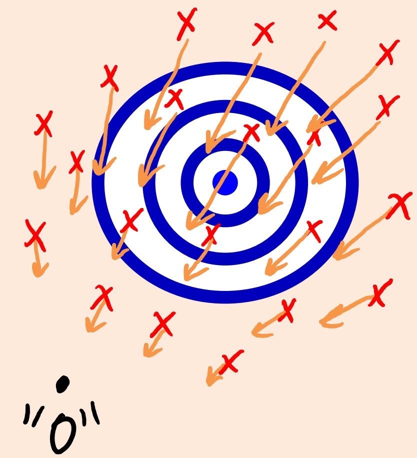

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Visualization of the related higher-dimensional paradox that the mean of data coming from a Gaussian is not the best estimate of the mean of the Gaussian in 3-dimensions or higher: https://www.naftaliharris.com/blog/steinviz