CPSC 340:
Machine Learning and Data Mining

Regularization

Fall 2018

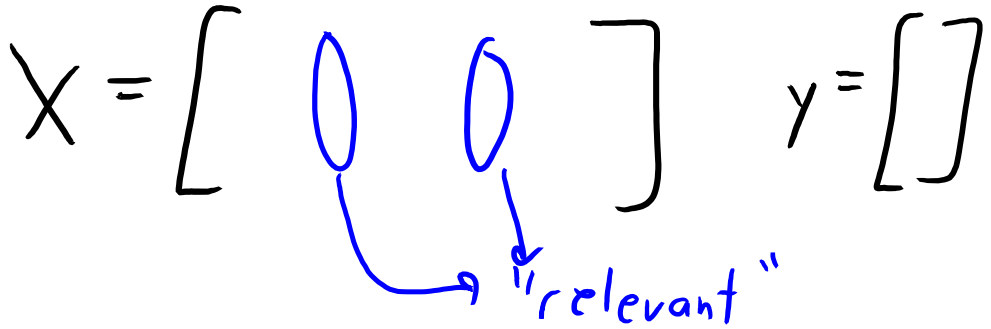
Admin

- Midterm is Thursday.
  - October 18th at 6:30pm.
  - Last names starting with A-L: BUCH A102.
  - Last names starting with M-Z: BUCH 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: Feature Selection

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



- 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.

“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 quadratic as part of polynomial basis.

- These two tasks are highly-related:
  - It’s a differnet “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?

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

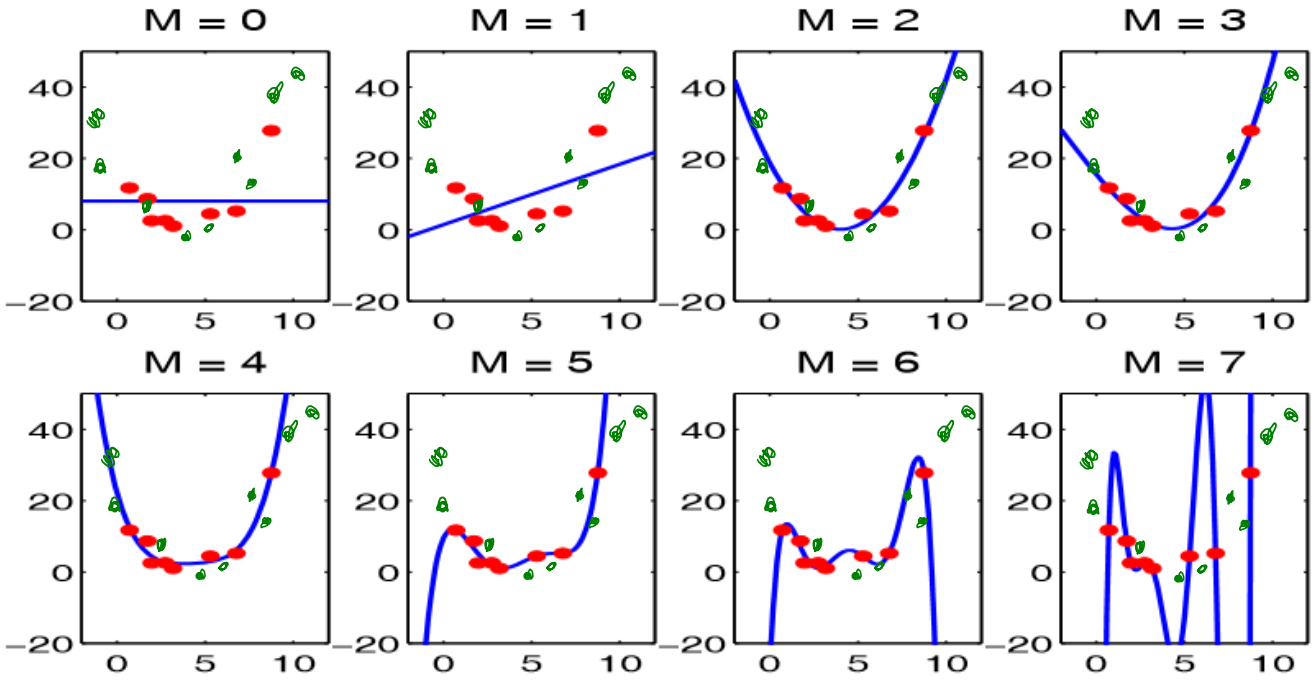
- Consider using d=n, with completely random features.
  - With high probability, you will be able to get a training error of 0.
  - But the features were random, this is completely overfitting.

- 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?

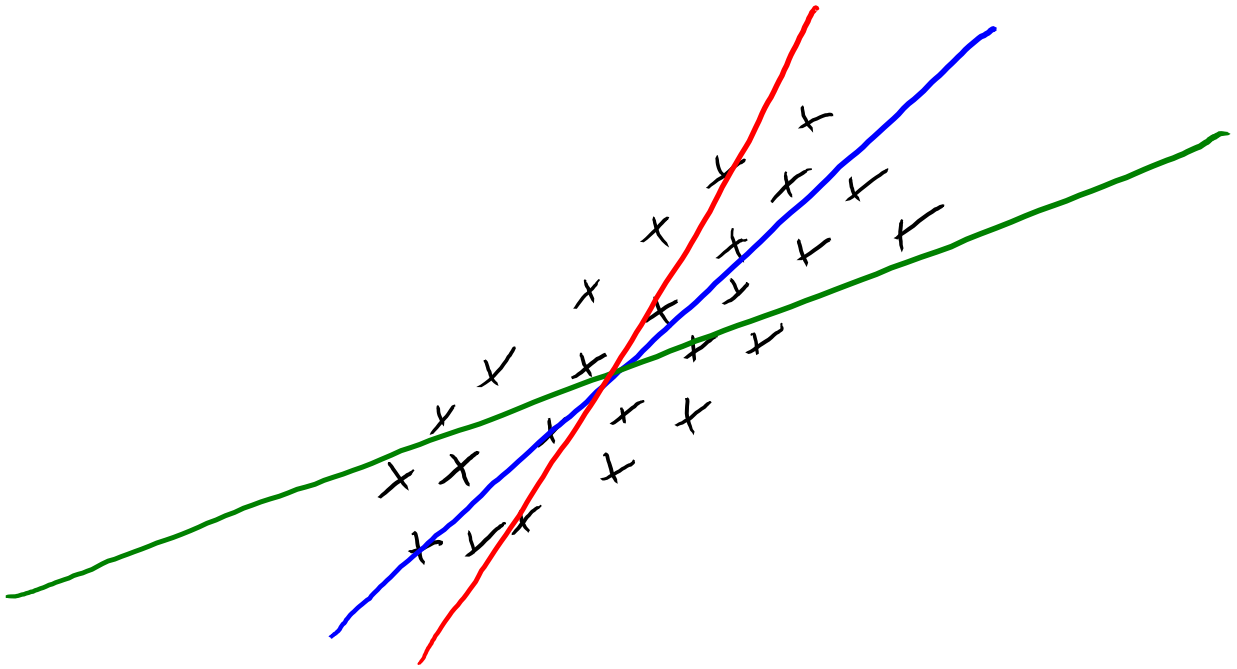
Controlling Complexity

- 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?

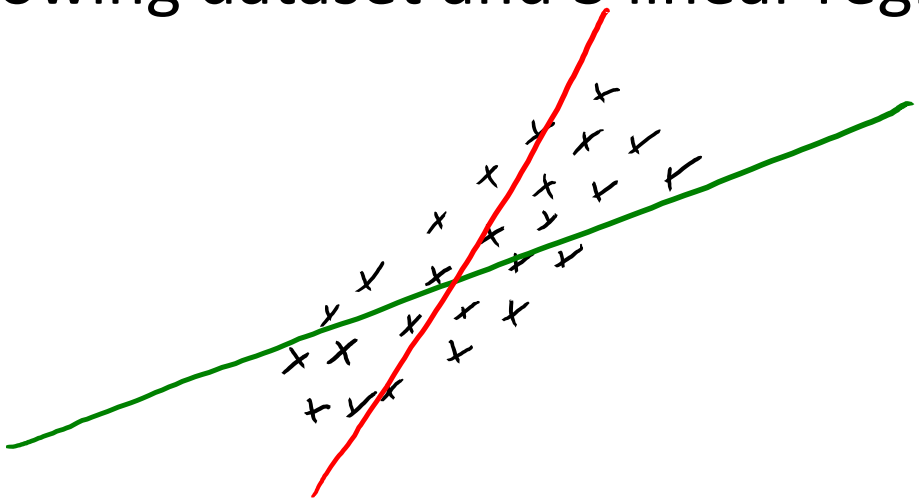
- Consider the following dataset and 3 linear regression models:



- Which line should we choose?

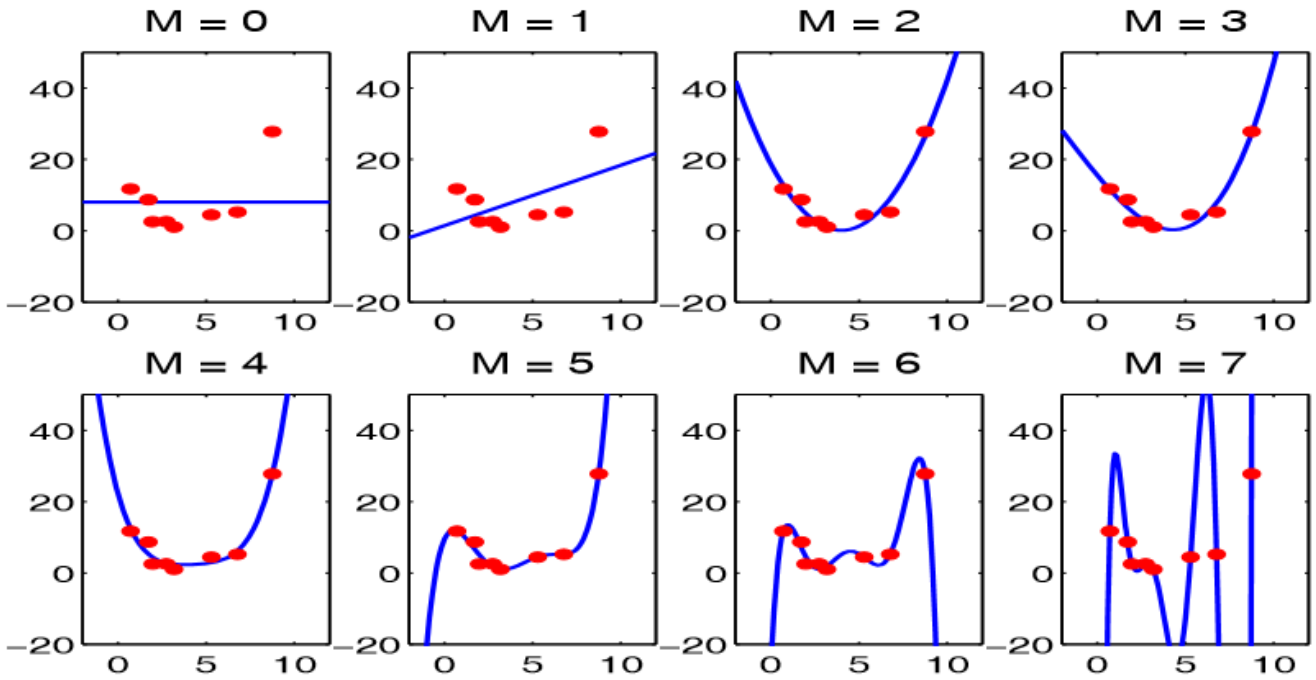
Would you rather?

- Consider the following dataset and 3 linear regression models:



- What if you are forced to choose between red and green?
  - They have the same training error.
- You should pick green.
  - The slope is smaller, so 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:

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

- 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 $\lambda > 0$ controls "strength" of regularization.
    - Large λ puts large penalty on slopes.

L2-Regularization

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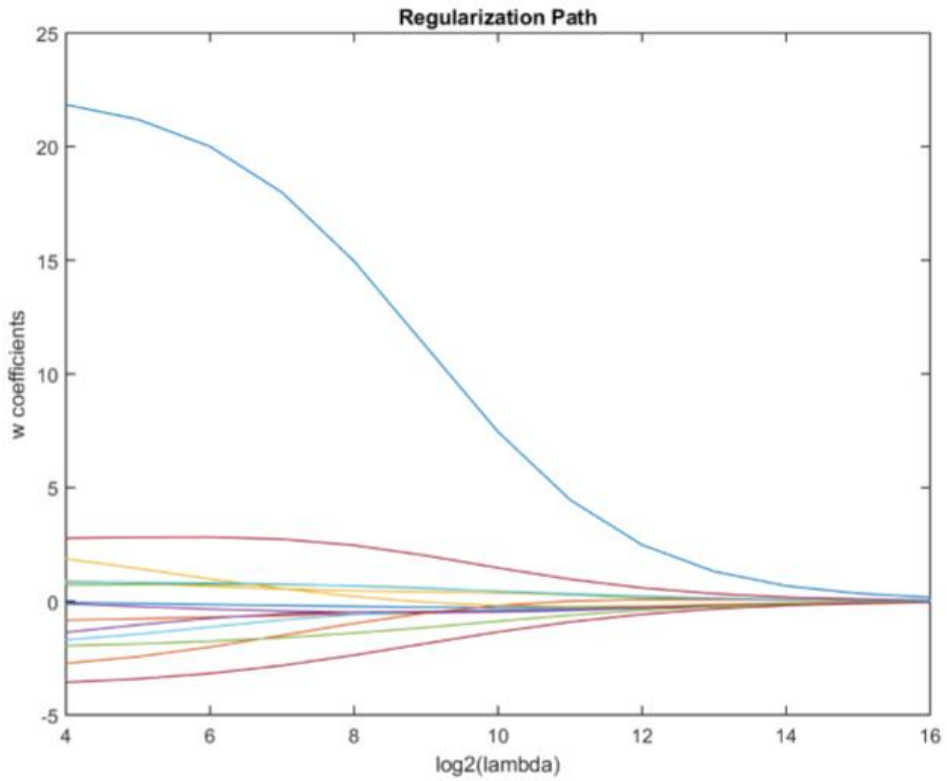
- In terms of fundamental trade-off:
  - Regularization increases training error.
  - Regularization decreases approximation error.

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

Regularization Path

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



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

L2-regularization and the normal equations

- When using L2-regularization we can just set ∇ f(w) to 0 and solve.
- Loss before: $f(w) = ||Xw - y||_2^2$
- Loss after: $f(w) = ||Xw - y||_2^2 + \lambda||w||_2^2$

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

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

Gradient Descent for L2-Regularizaed 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:

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

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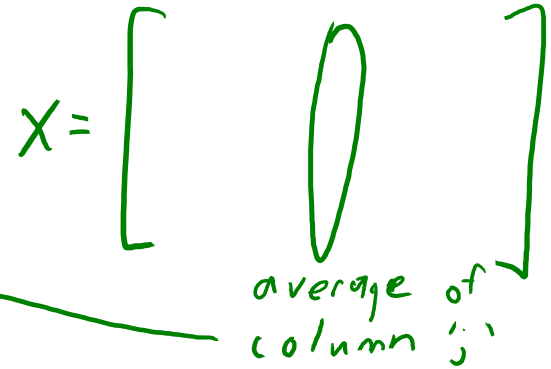
- Should we convert to some standard 'unit'?
  - It matters for k-nearest neighbours:
    - "Distance" will be affected more by large features than small features.
  - It matters for regularized least squares:
    - Penalizing $(w_j)^2$ means different things if features 'j' are on different scales.

Standardizing Features



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

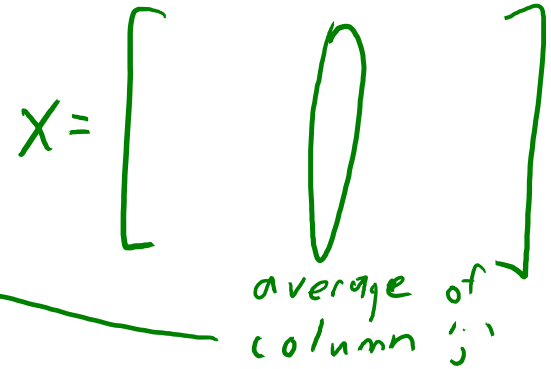
$$\mu_j = \frac{1}{n}\sum_{i=1}^{n} x_{ij} \qquad \sigma_j = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_{ij} - \mu_j)^2}$$

    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.

Standardizing Features



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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?

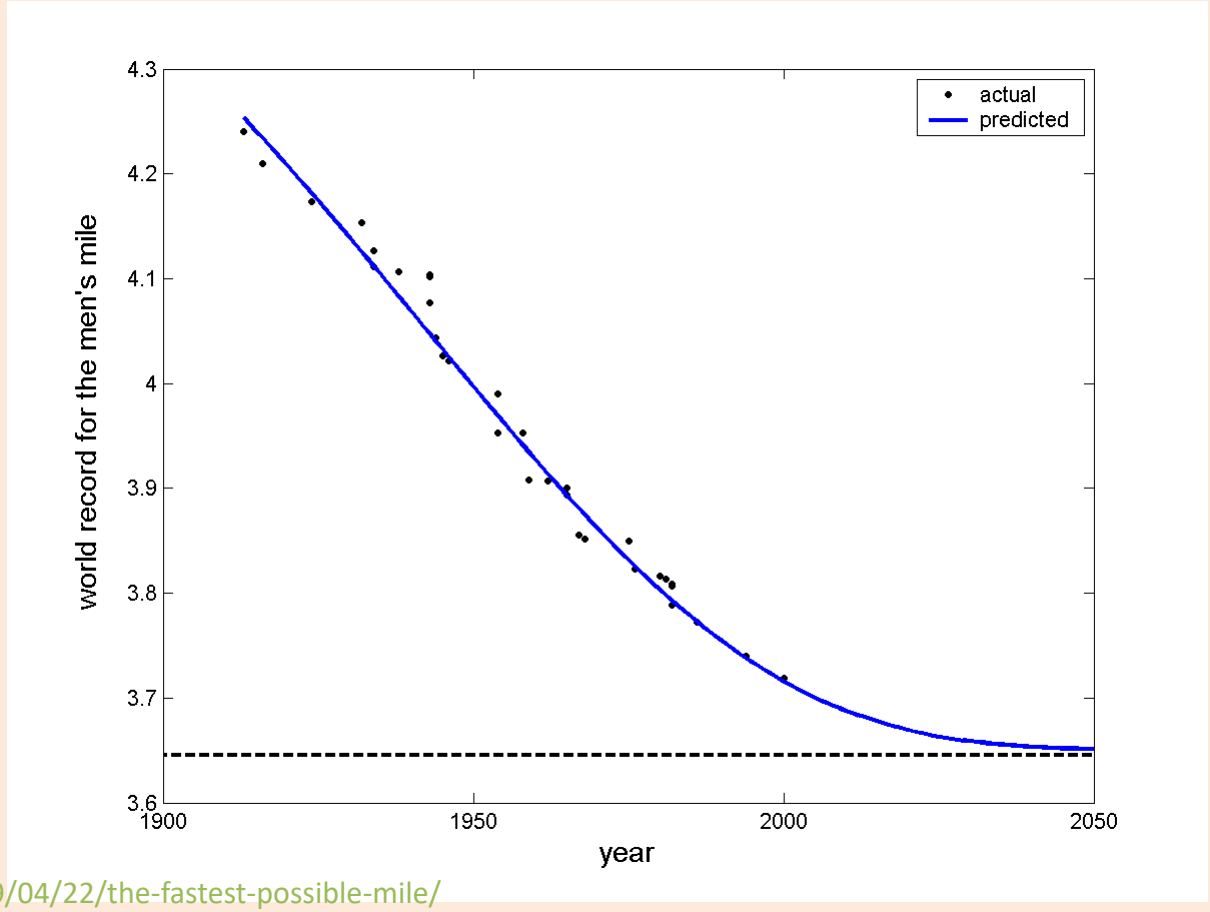
- Should we regularize the y-intercept?
- No! Why encourage it to be closer to zero (it could be anywhere)?
  - You should be allowed to shift function up/down globally.
- Yes! It makes the solution unique and it easier to compute 'w'.
- Compromise: regularize by a smaller amount than other variables.

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

(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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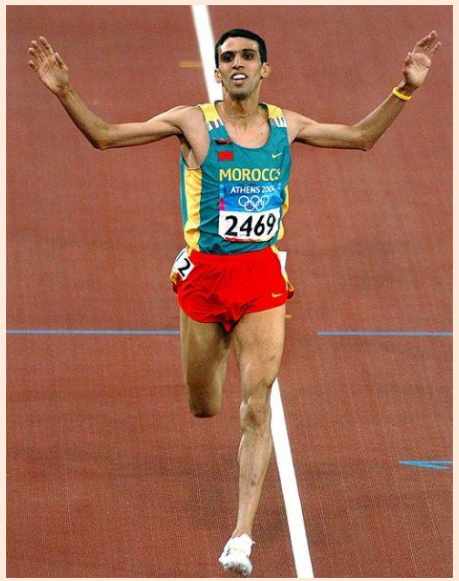
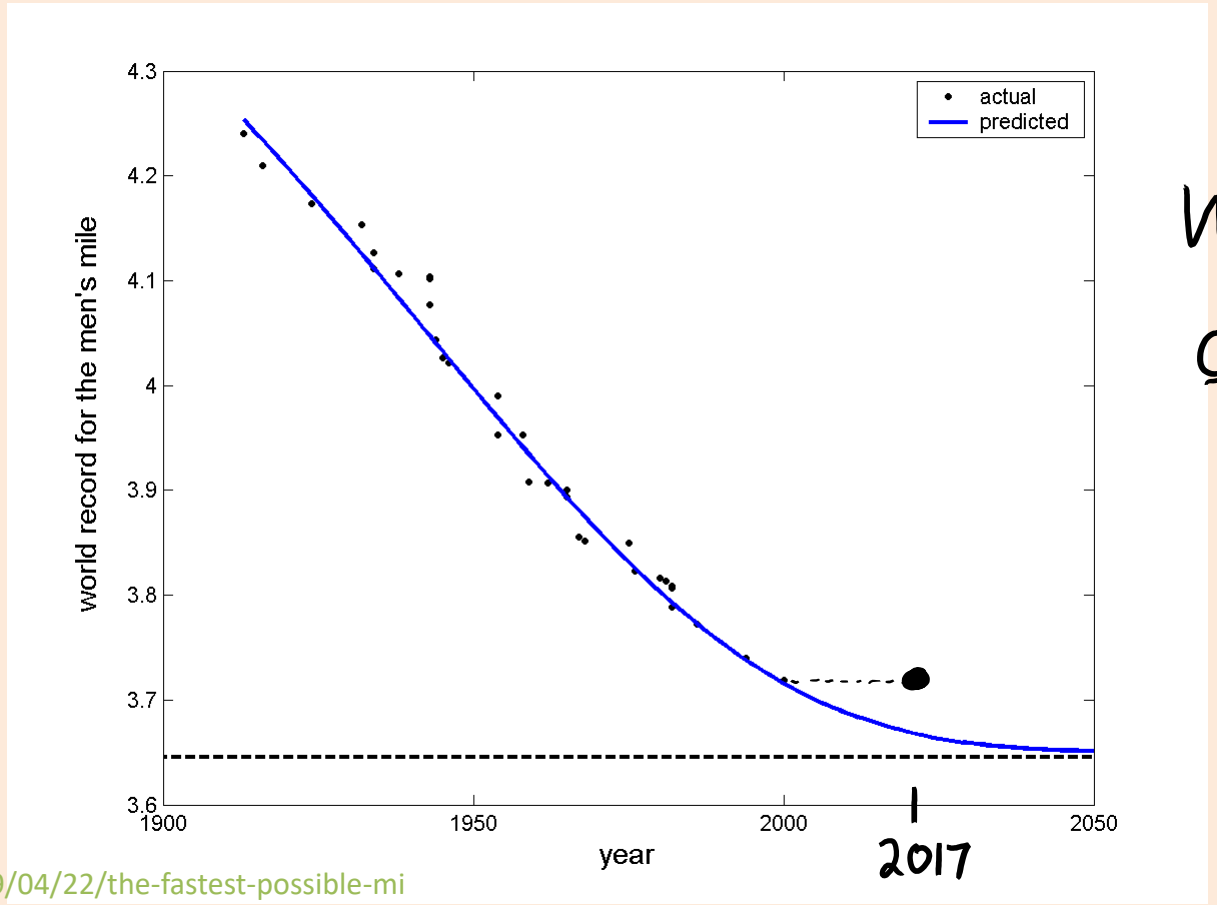
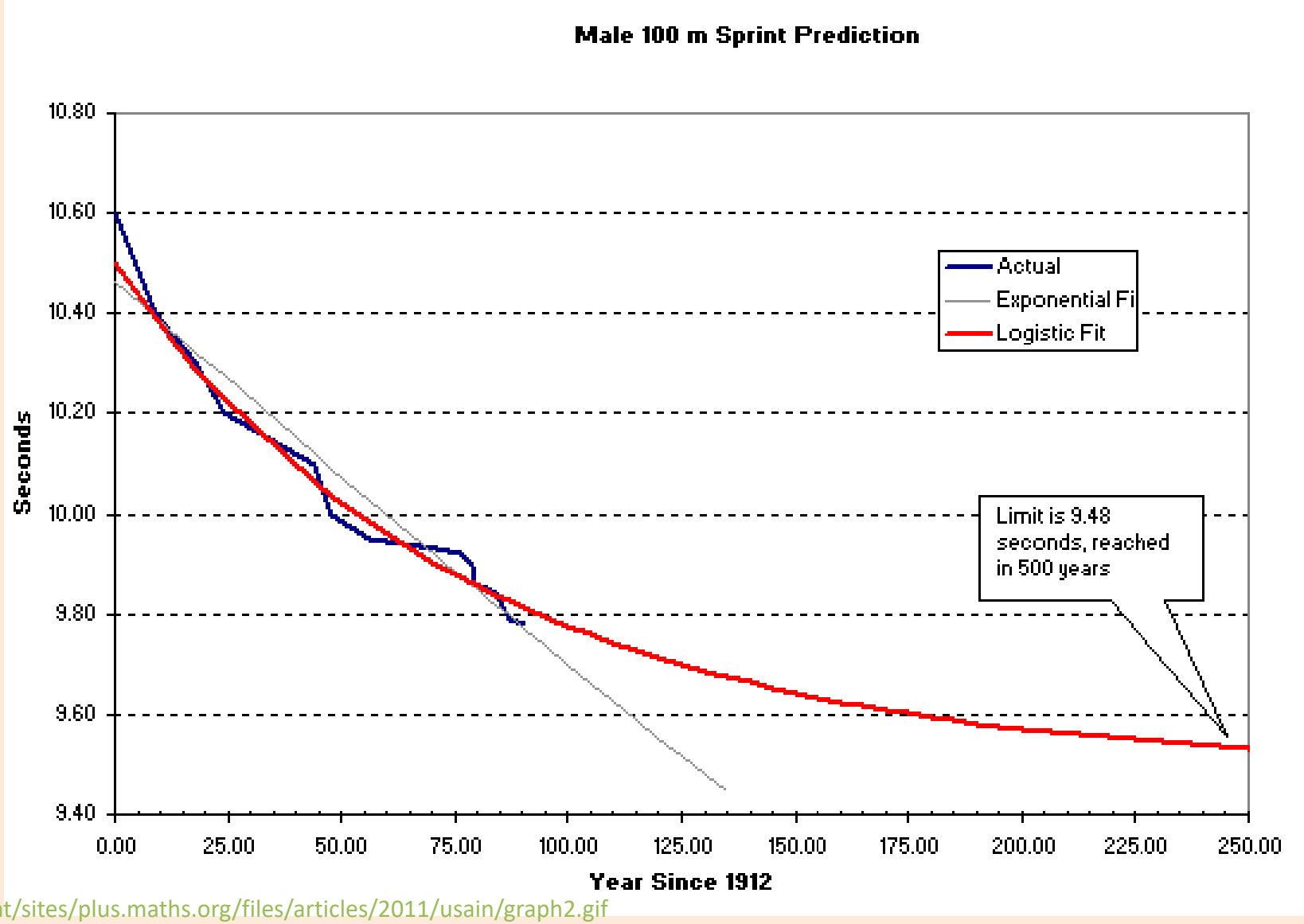




We need to be cautious about doing this.

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?



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Predicting 100m times 400 years in the future?

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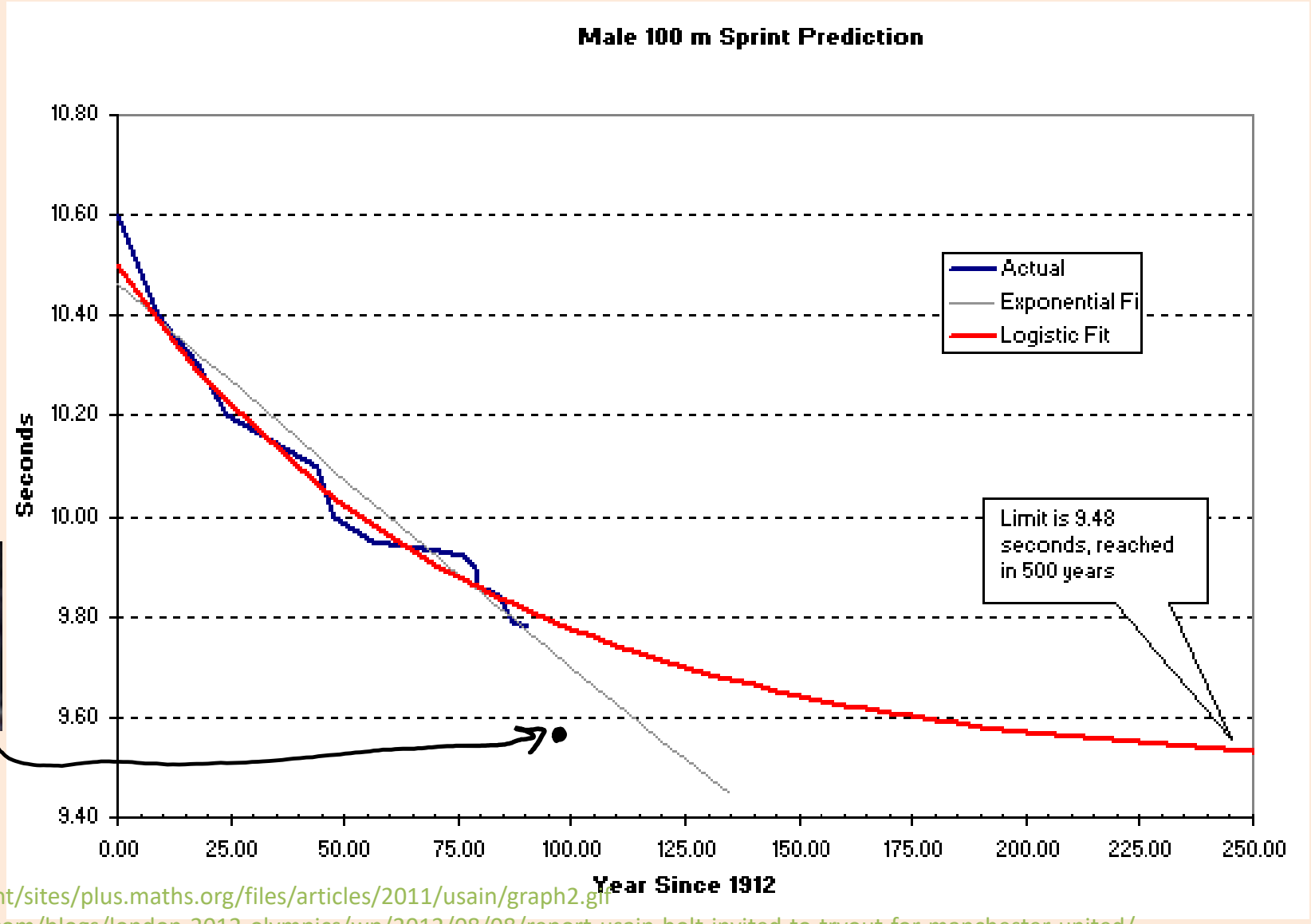

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http://www.washingtonpost.com/blogs/london-2012-olympics/wp/2012/08/08/report-usain-bolt-invited-to-tryout-for-manchester-united/

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 smooth.
- Extrapolation is task of prediction outside the range of the data points.
  - Without assumptions, regression models can be embarrassingly-bad at this.

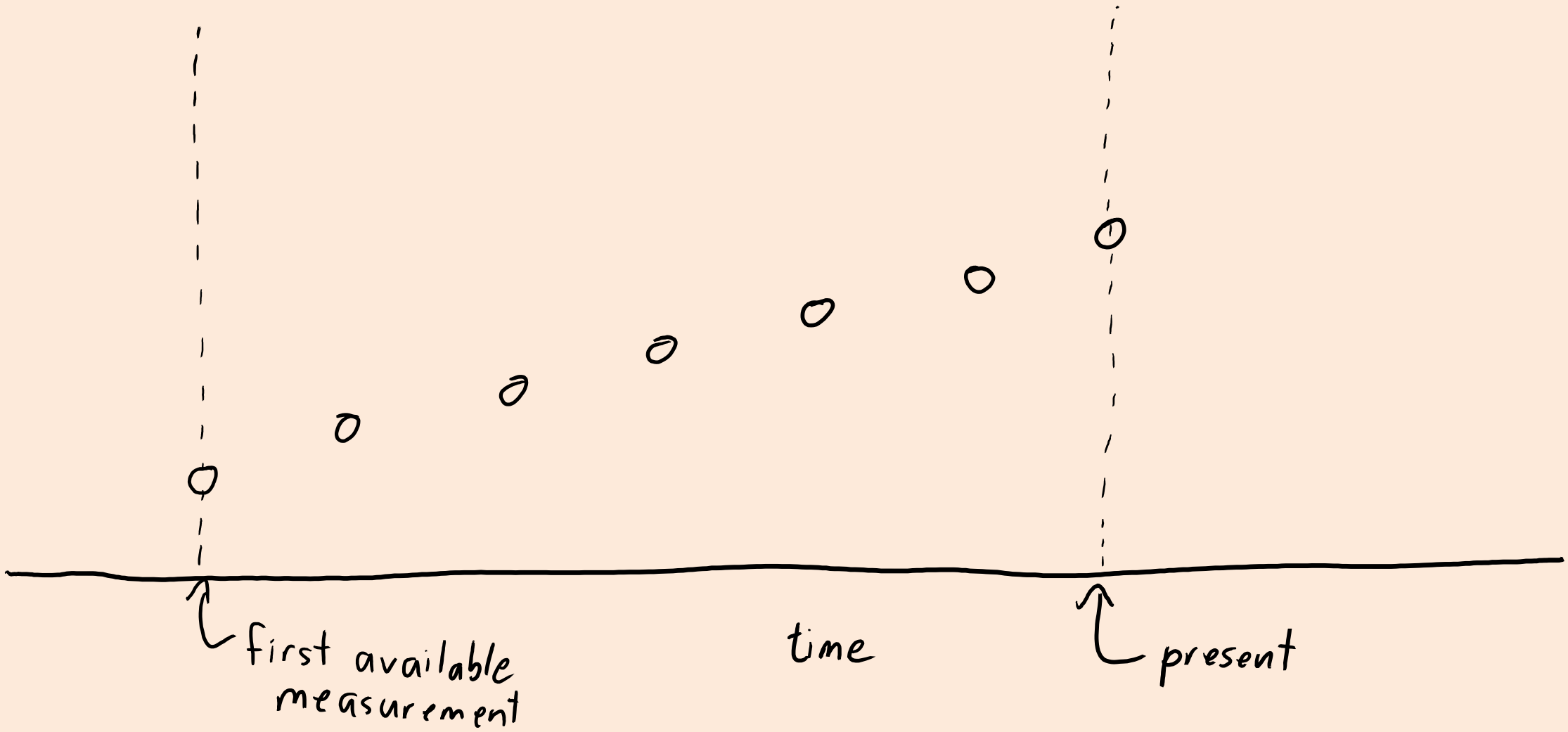
- If you run the 100m regression models backwards in time:
  - They predict that humans used to be really really slow!

- 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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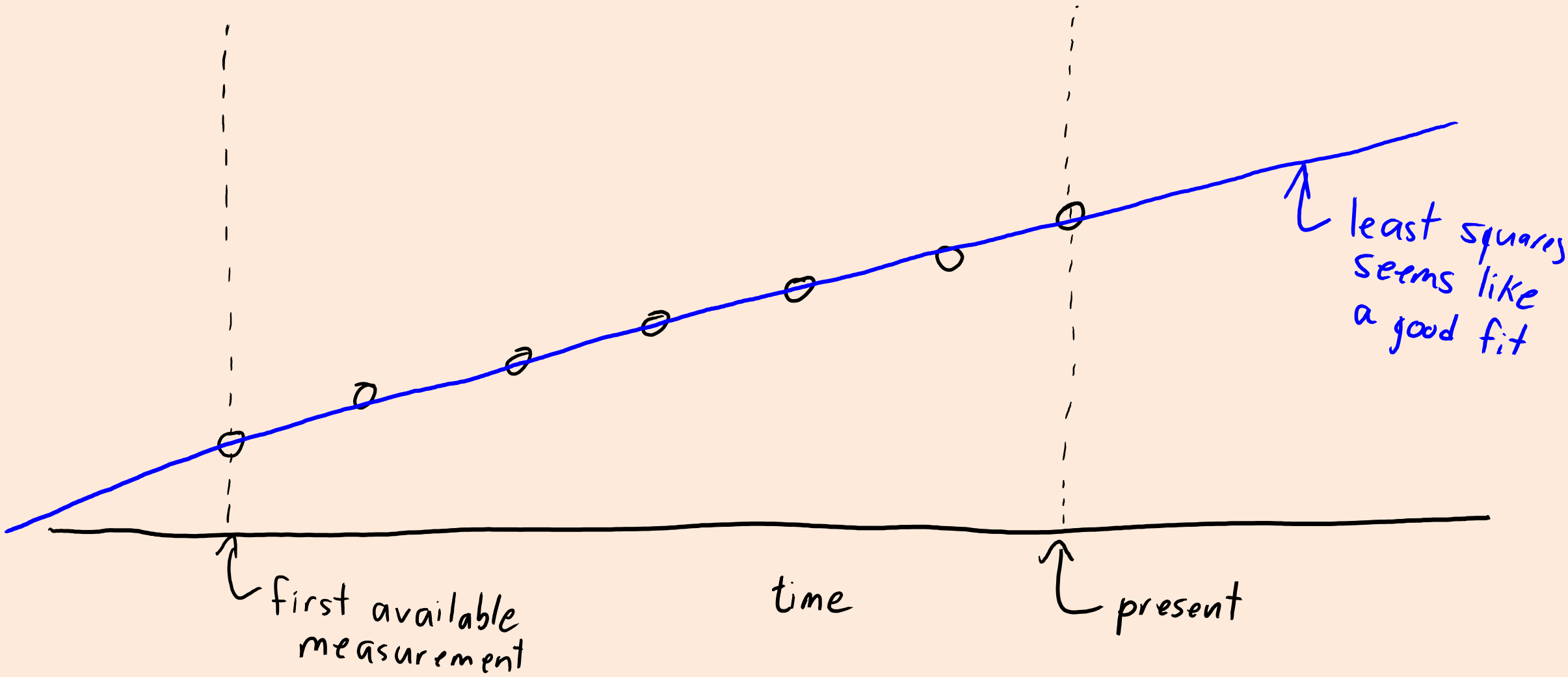

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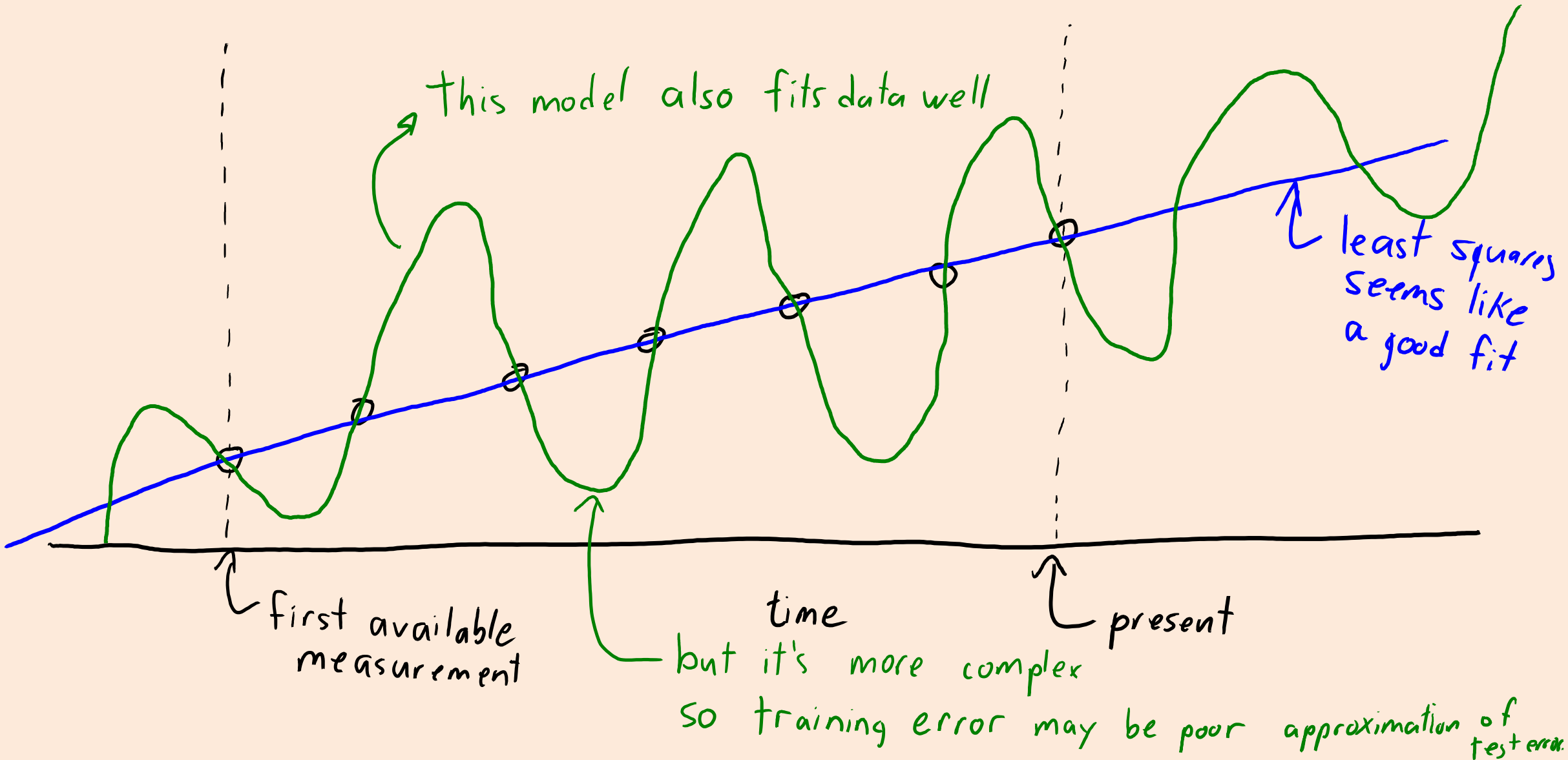
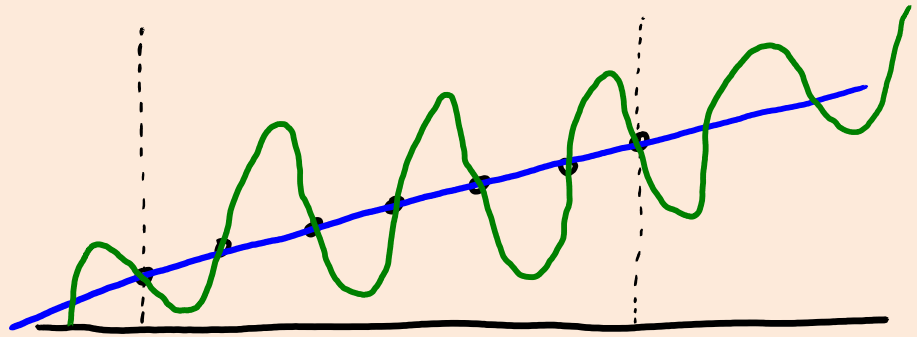


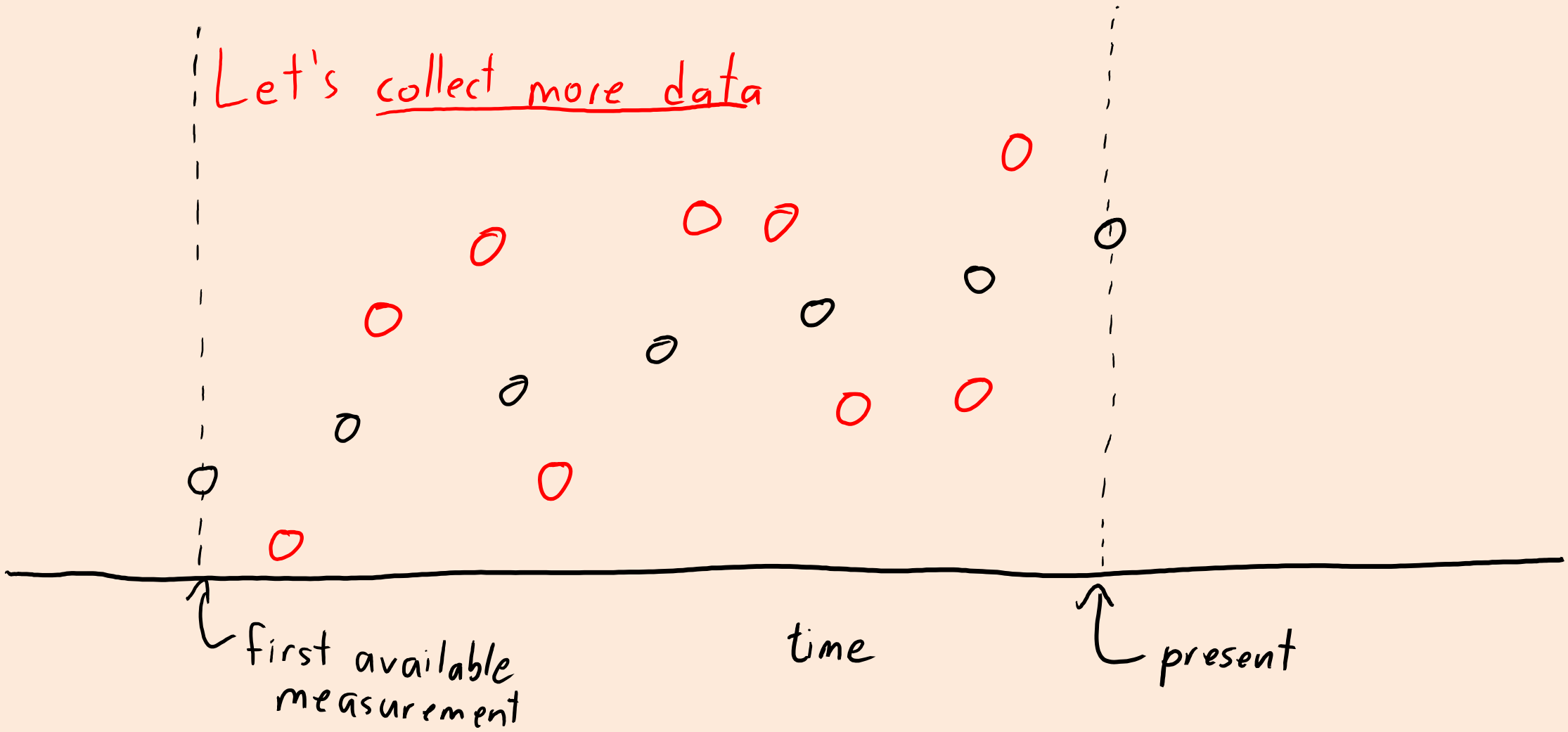
Ockham's Razor vs. No Free Lunch

- 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



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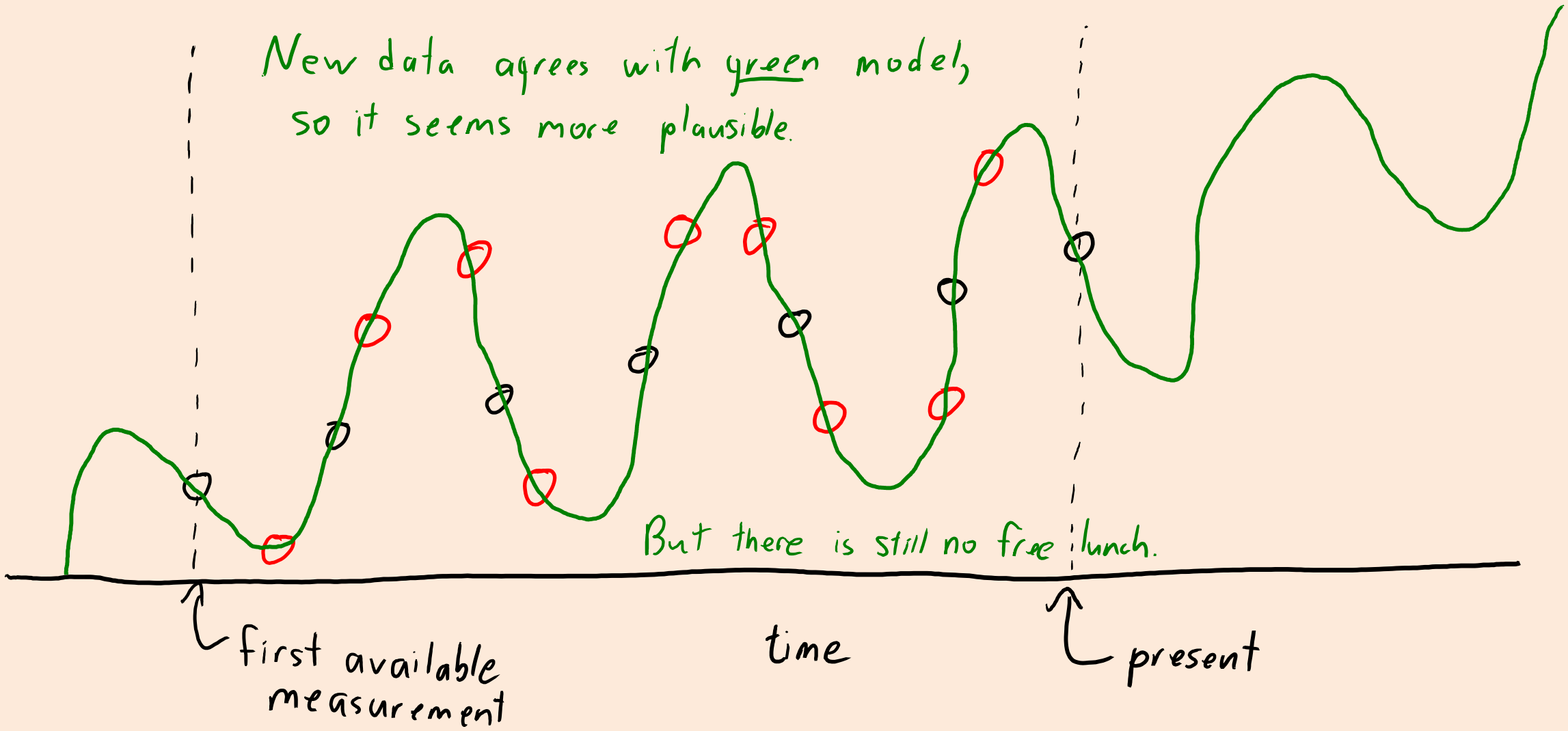

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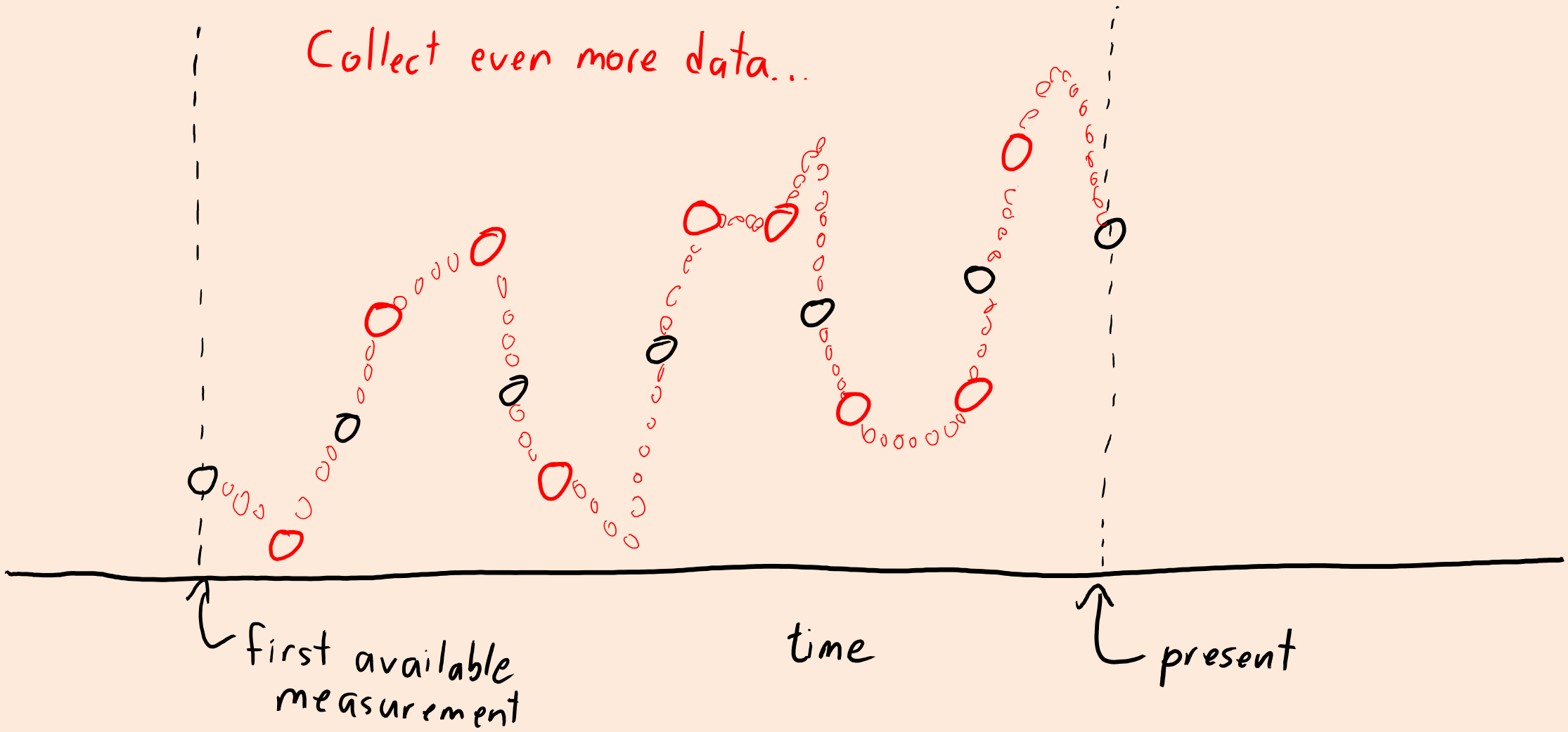

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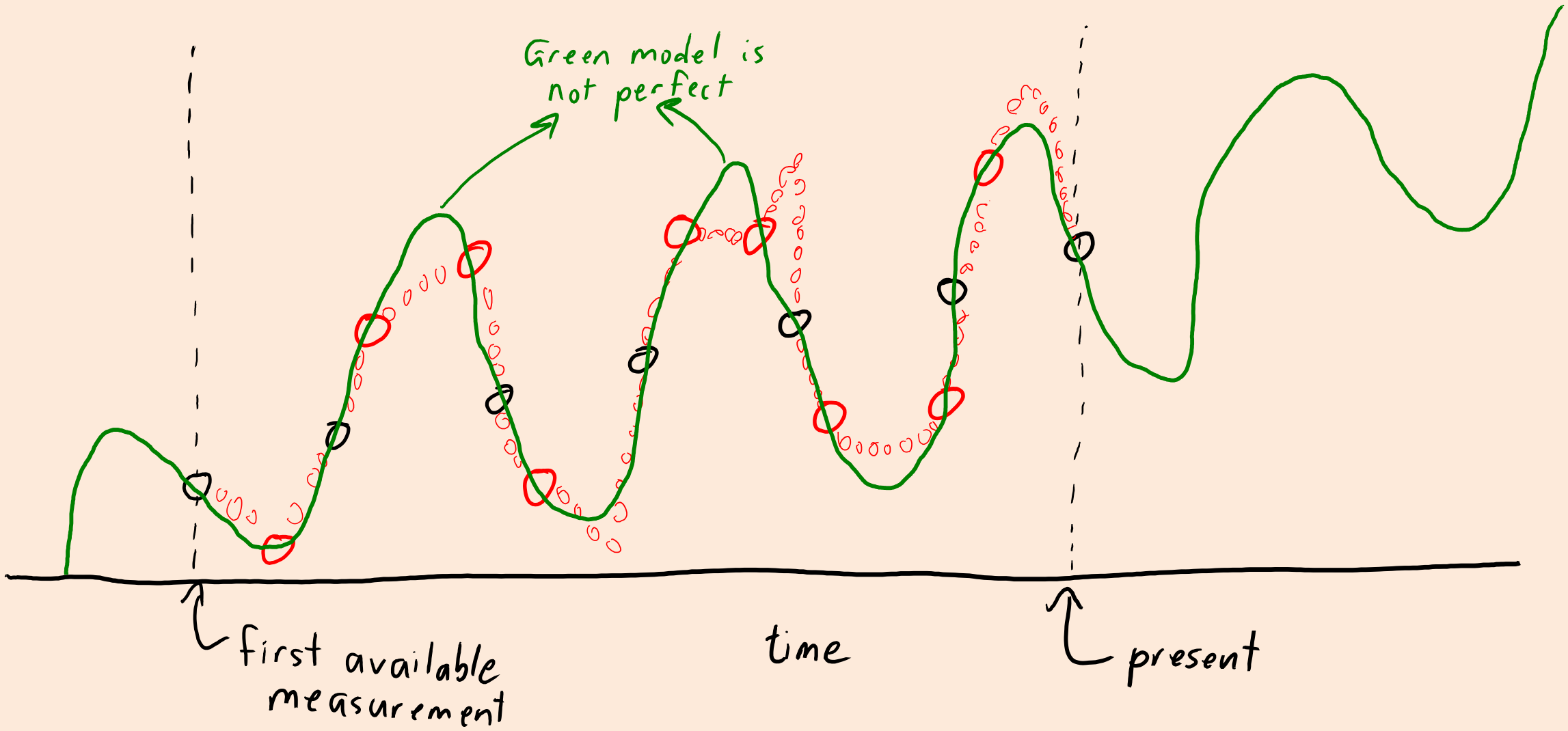

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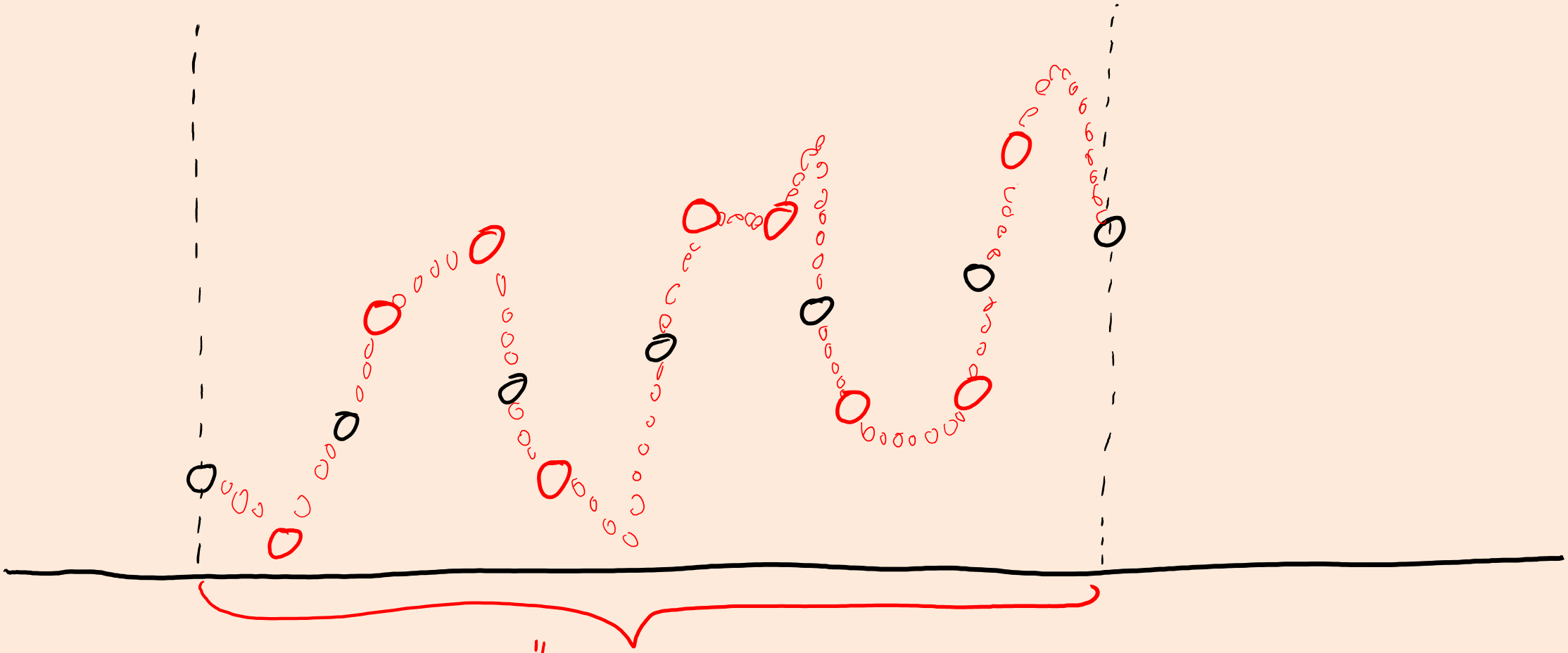

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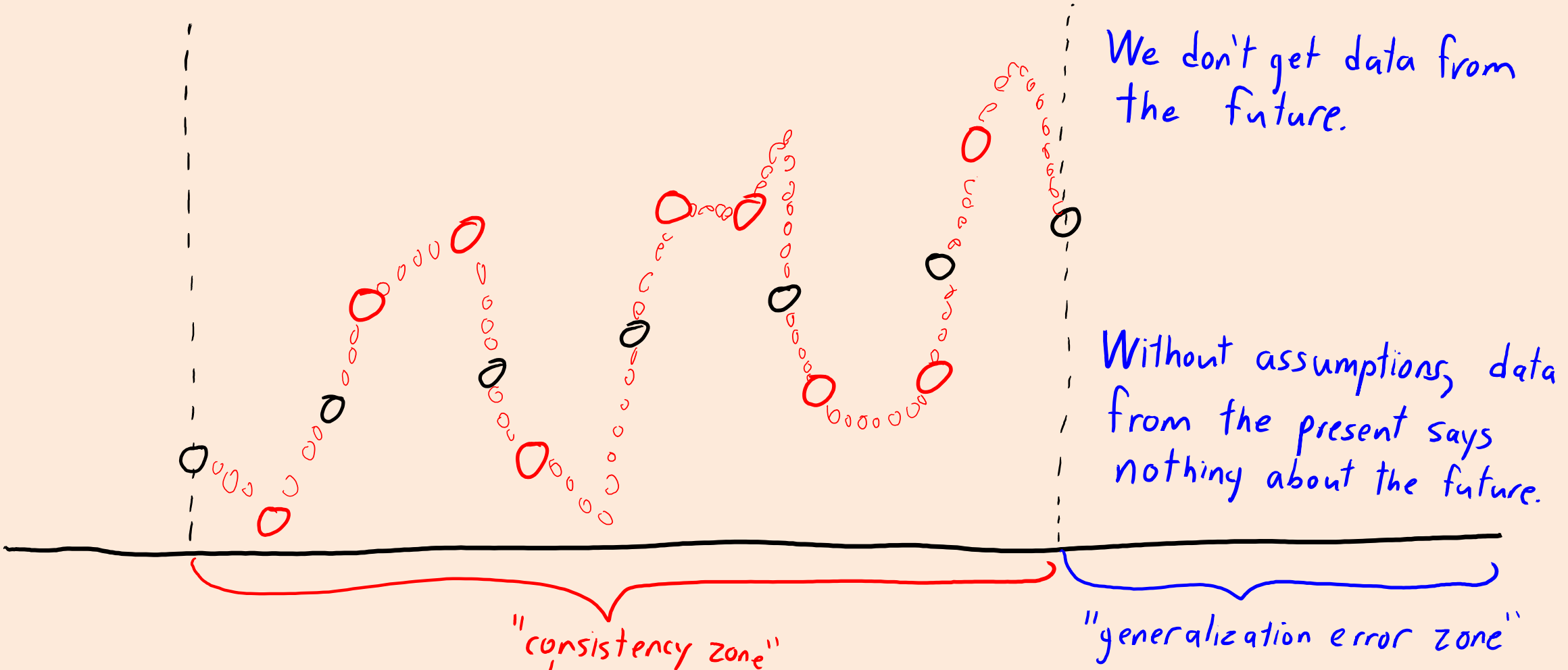

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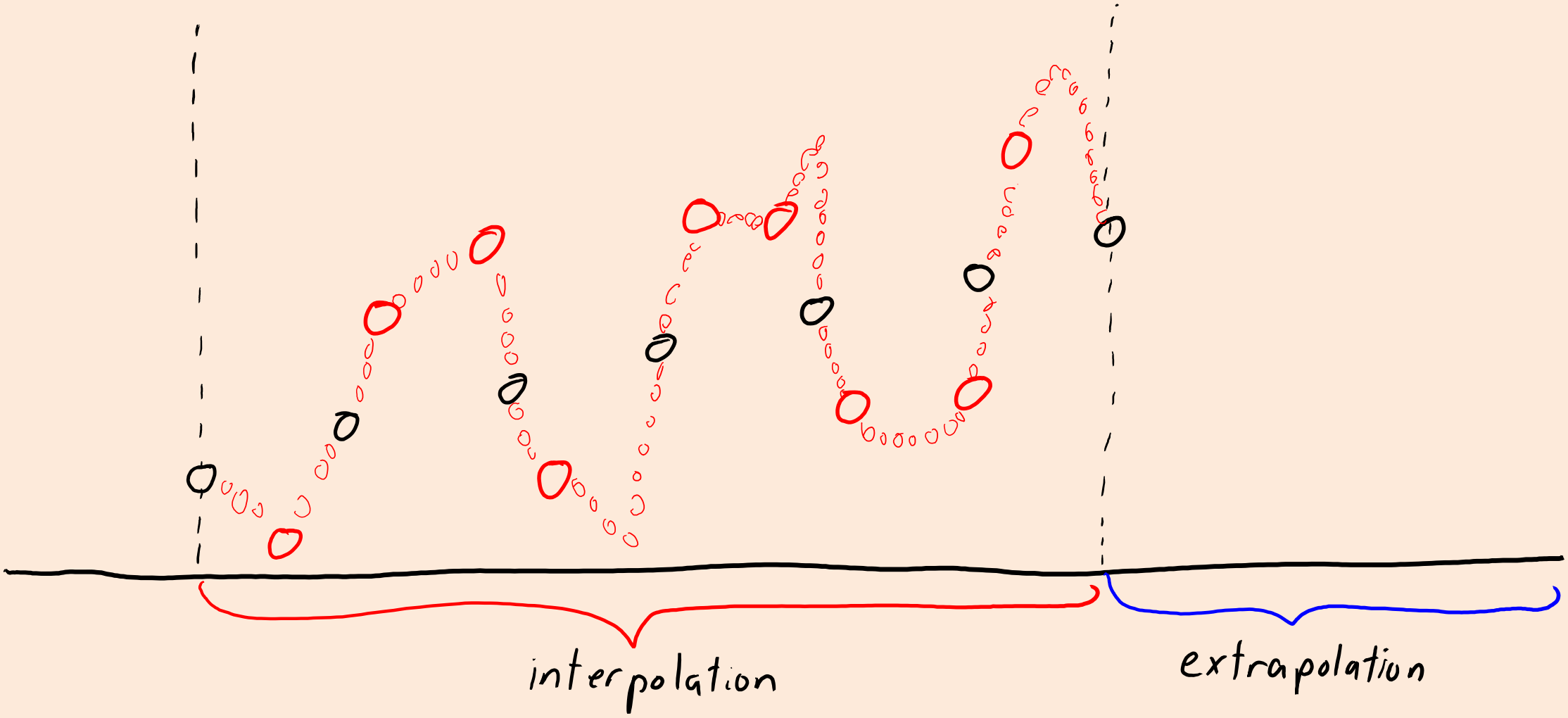
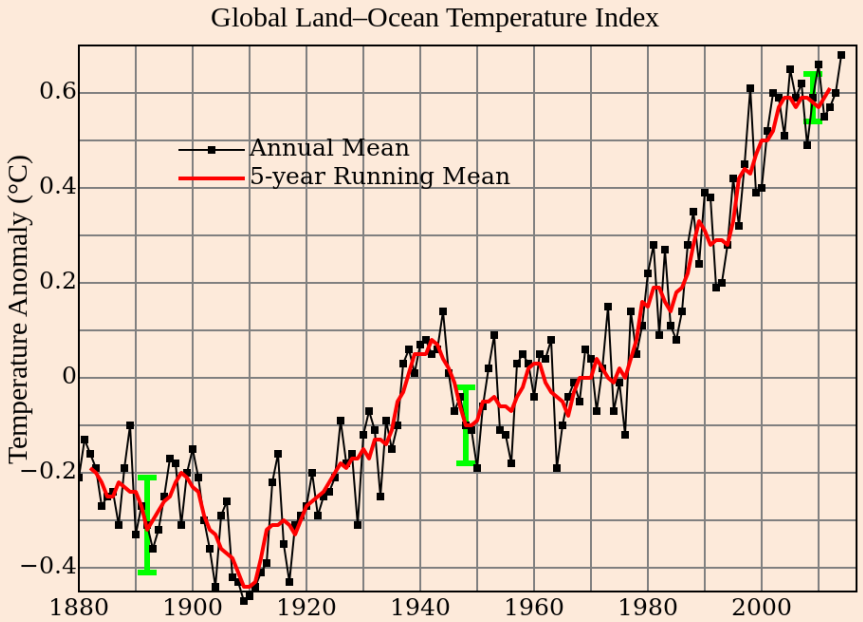


Discussion: Climate Models

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

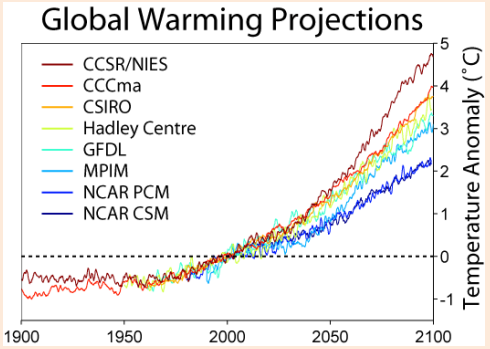


- Will Earth continue to warm over next 100 years? (generalization error)
  - We should be more skeptical about models that predict future events.

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 temperature changes are likely to change continuously.
- 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

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”.

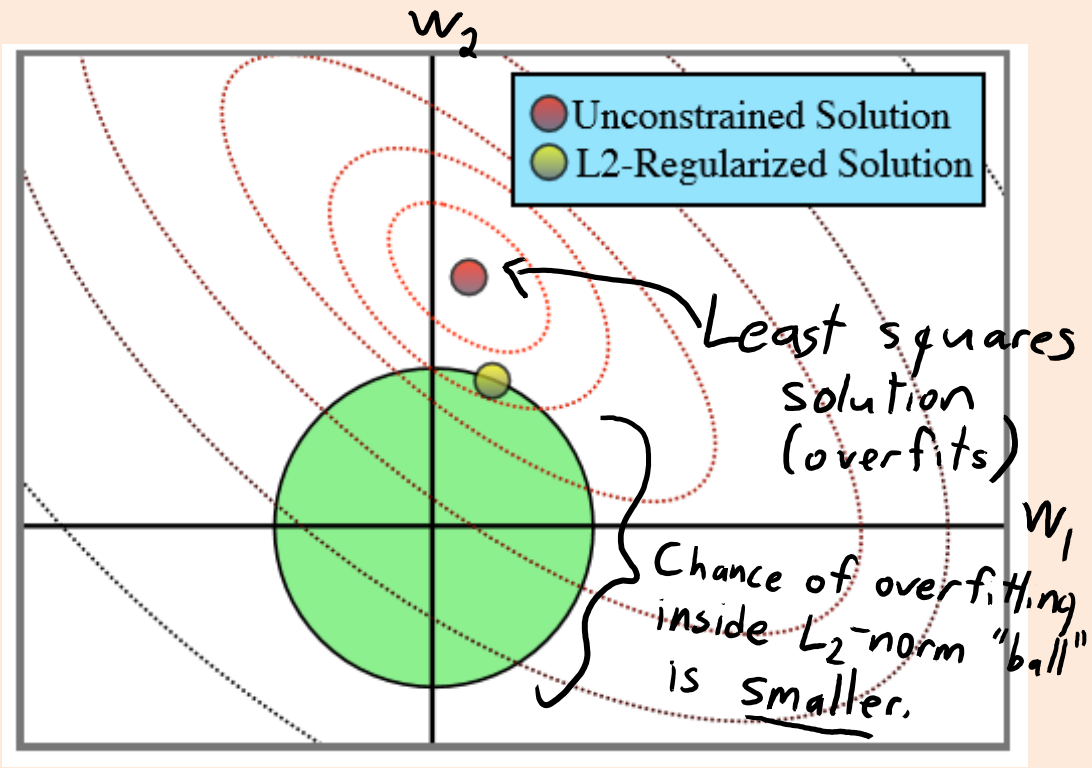
- Next time: learning with an exponential number of irrelevant features.

L2-Regularization

- Standard regularization strategy is L2-regularization:

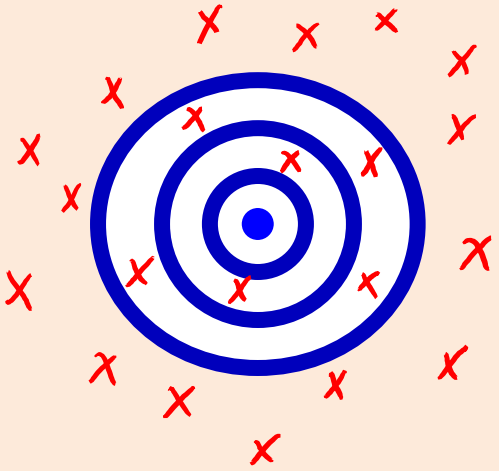
$$f(w) = \frac{1}{2}\sum_{i=1}^{n}(w^T x_i - y_i)^2 + \frac{\lambda}{2}\sum_{j=1}^{d} w_j^2 \quad \text{or} \quad f(w) = \frac{1}{2}\|Xw - y\|^2 + \frac{\lambda}{2}\|w\|^2$$

- 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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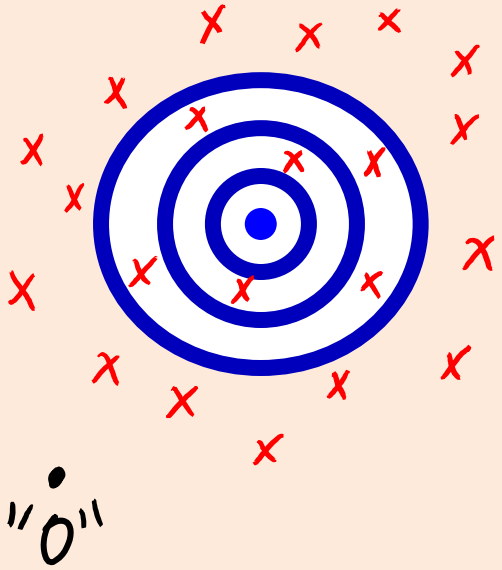

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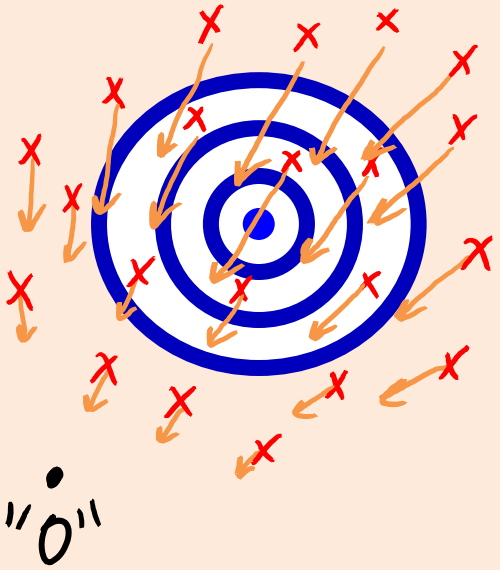
- If small enough, darts will be closer to center on average.



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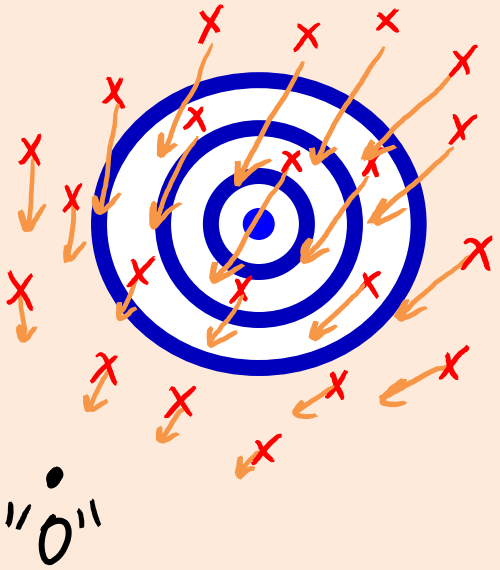

Visualization of the related higher-dimensional paradox that the mean of data coming from a Gaussian is not the best estimate of the mean of the Gaussian in 3-dimensions or higher: https://www.naftaliharris.com/blog/steinviz