CPSC 340:
Machine Learning and Data Mining

Regularization

Spring 2022 (2021W2)

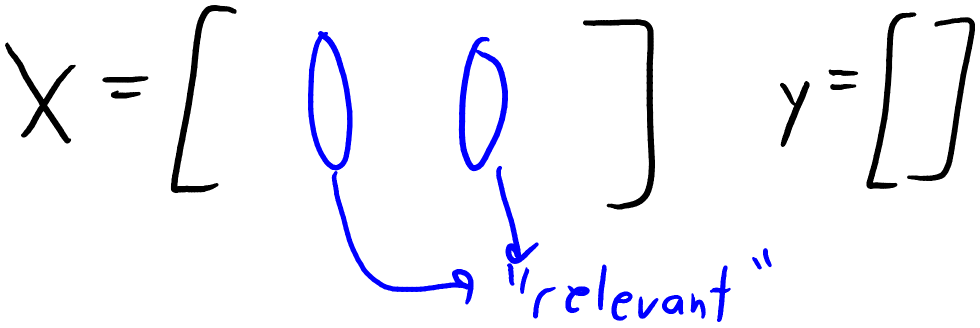
Admin

- Midterm is Thursday, 6-7:30pm.
  - On Canvas, take it anywhere
  - 85 minutes inside that 90-minute block.
  - Open book (/ notes / slides / anything on the internet / …)
  - No communication with anyone (whether they're in the class or not).
  - Auditors, do not take the midterm.

- There will be …. :
  - Multiple choice questions (choose one that satisfies the question) that might be conceptual or more technical/specific.
  - Multiple answer questions (choose all that satisfy the question)
  - Essay-like questions involving math.

Last Time: Feature Selection

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



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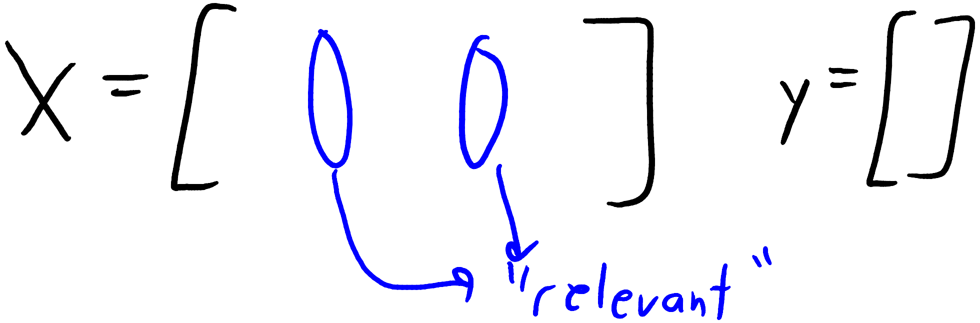

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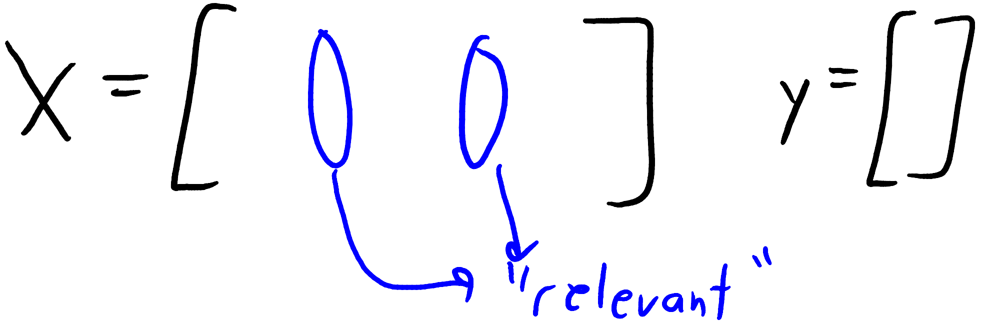

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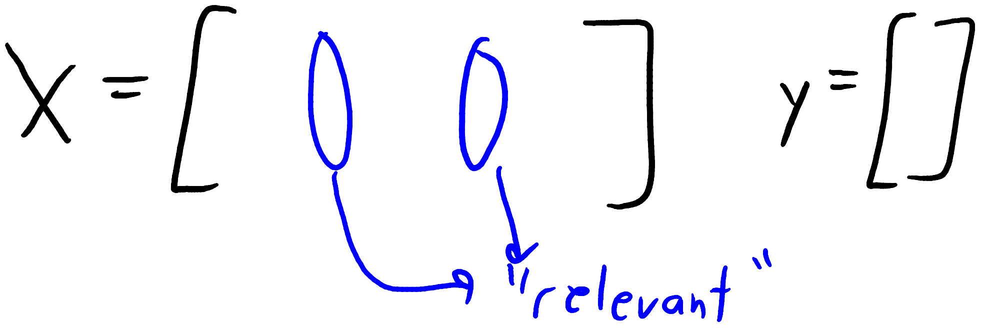

- Most common approach is search and score:
  - Define “score” and “search” for features with best score.
- But it’s hard to define the “score” and it’s hard to “search”.
  - So we often use greedy methods like forward selection.
- Methods work okay on “toy” data, but are frustrating on real data.
  - 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.
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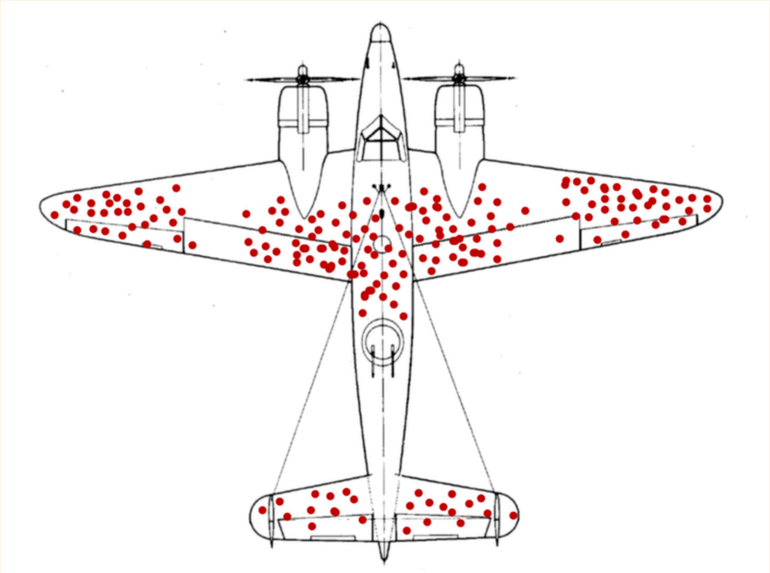
- Don’t be overconfident:
  - These methods are probably not discovering how the world truly works.
  - “The algorithm has found that these variables are helpful in predicting y_i.”
    - Then a warning that these models are not perfect at finding relevant variables.

bonus!

Related: Survivorship Bias

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



- Where are the “relevant” parts of the plane to protect?

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

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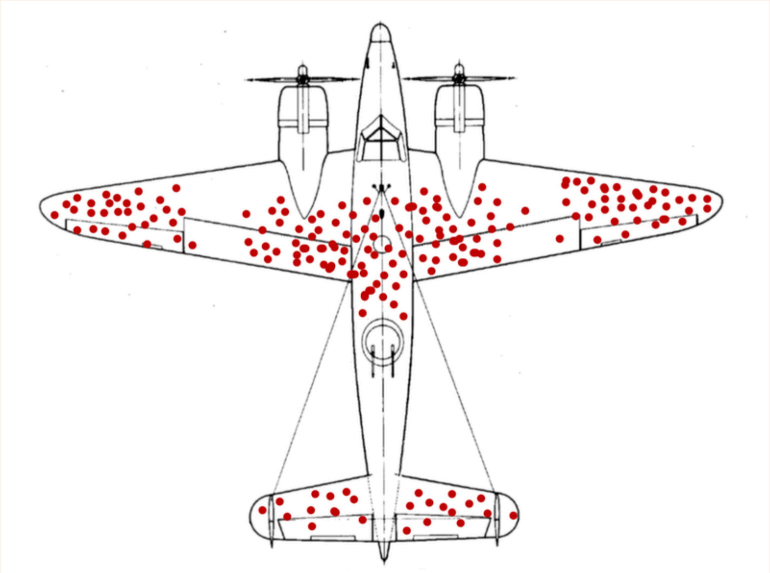

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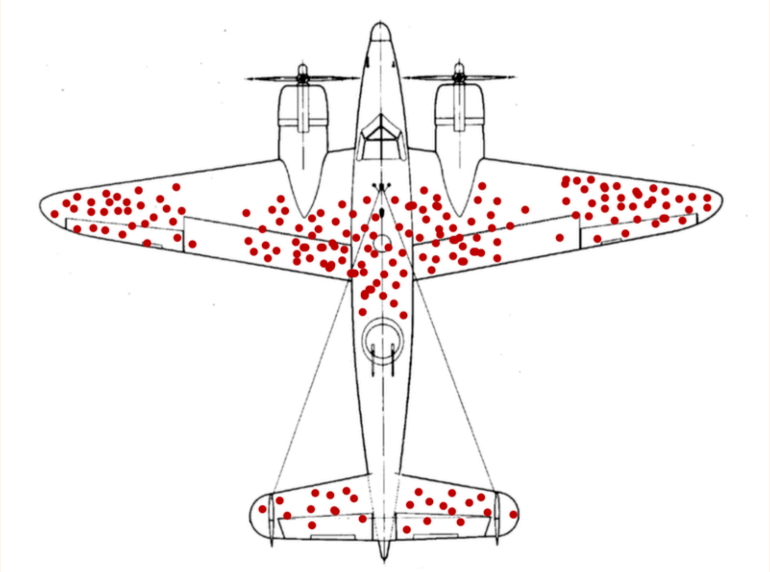

- Where are the "relevant" parts of the plane to protect?
  - "Relevant" parts are actually where there are no bullets.
  - Planes shot in other places did not come back (armor was needed).

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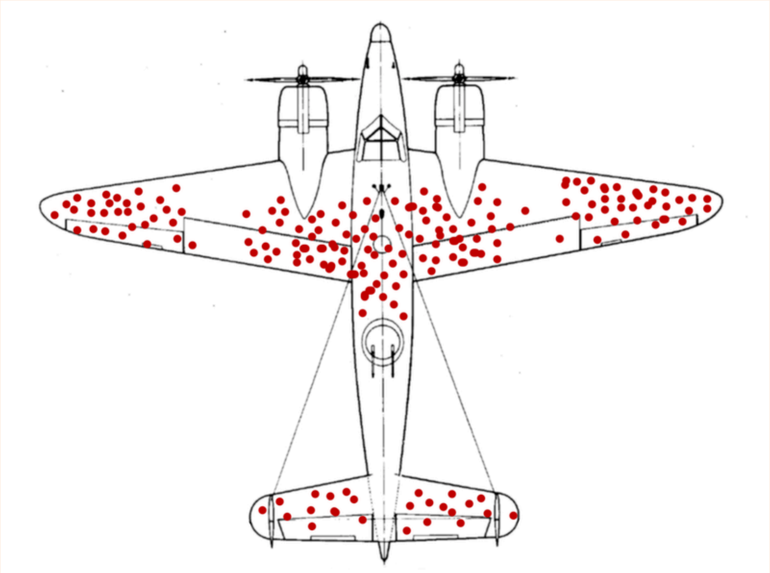

- This is an example of "survivorship bias":
  - Data is not IID because you only sample the "survivors".
  - Causes havoc for feature selection, and ML methods in general.

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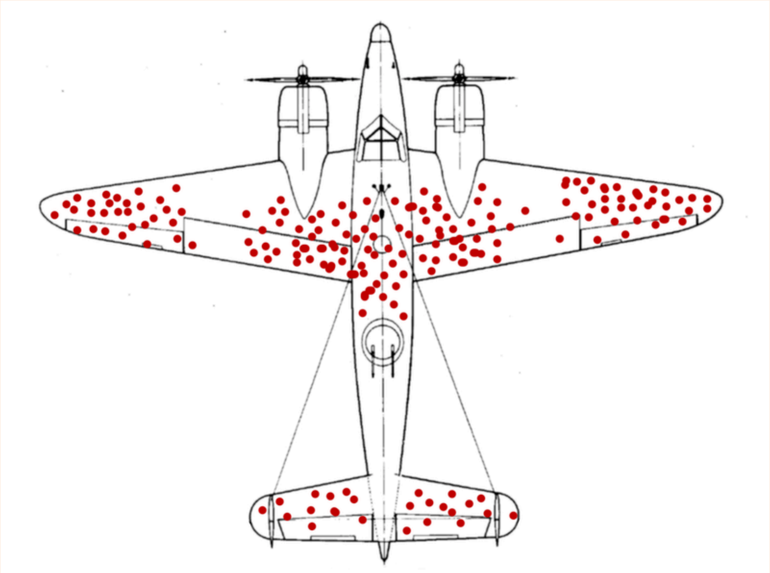

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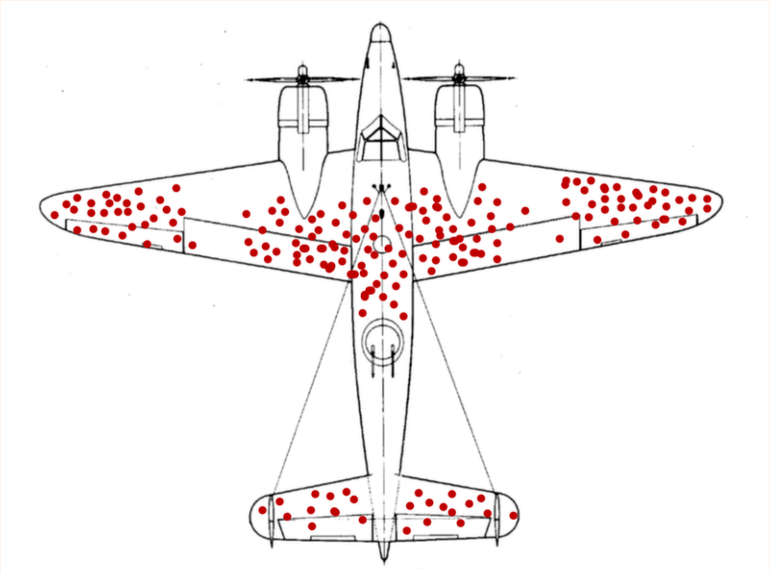

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  - Article on "secrets of success", focusing on traits of successful people.
    - But ignoring the number of non-super-successful people with the same traits.
  - Article hypothesizing about various topics (allergies, mental illness, etc.).

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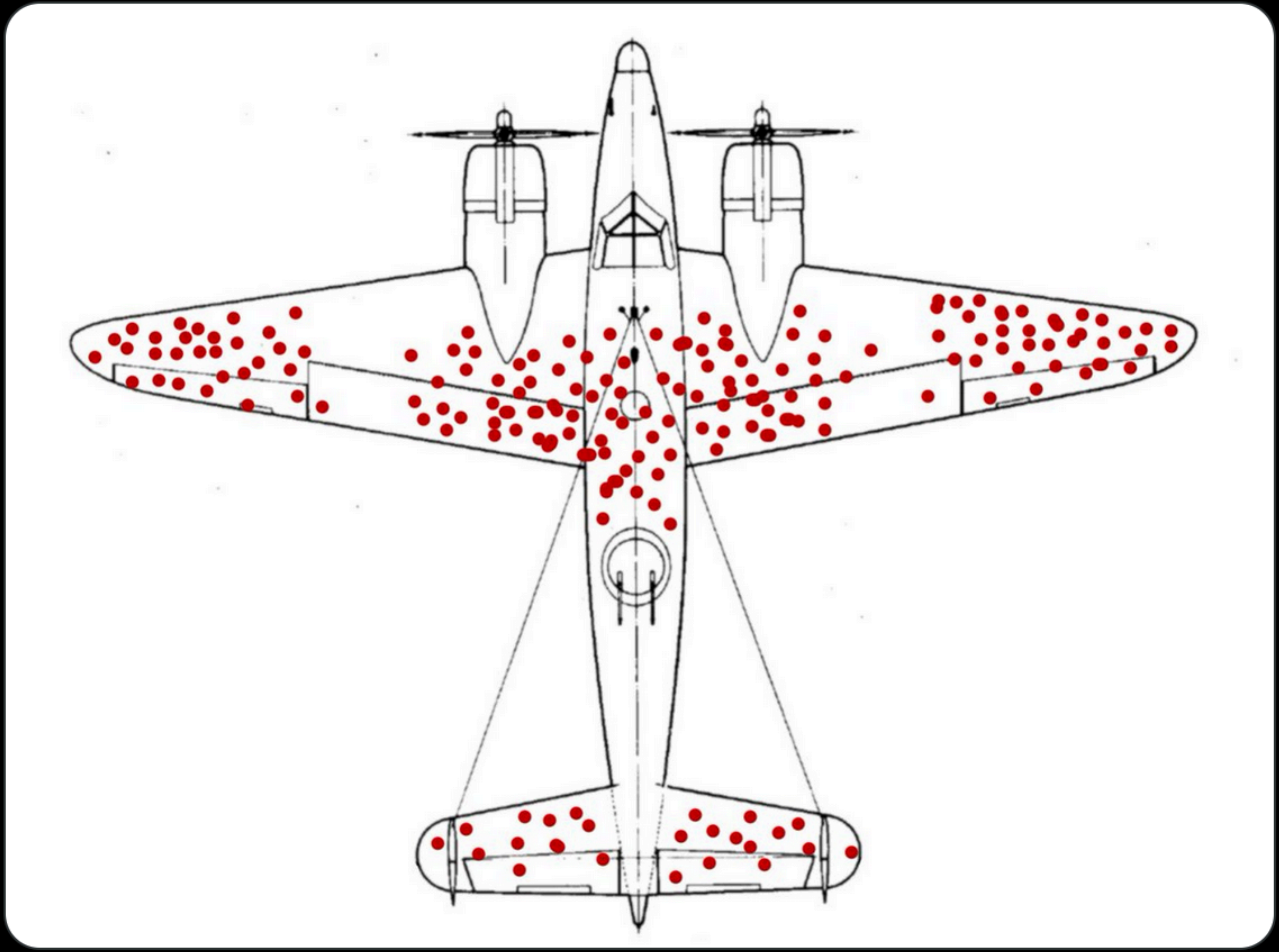
bonus!

Jake VanderPlas
@jakevdp

weird how every time you see this image on twitter it has a ton of retweets



8:15 AM · Dec 8, 2020 · Twitter Web App

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  - It’s a different “model” if we add x_i^2 to linear regression.
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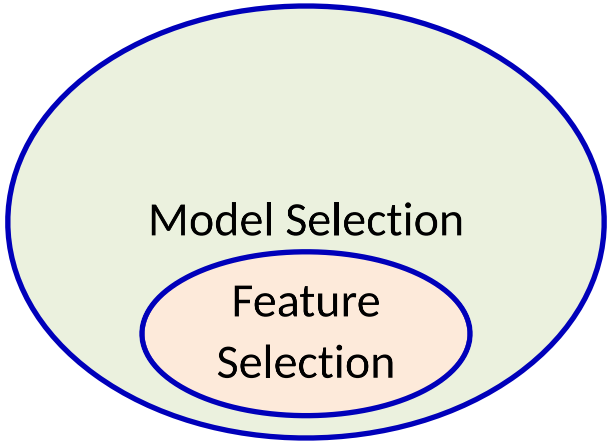

- These two tasks are highly-related:
  - It's a different "model" if we add x_i^2 to linear regression.
  - But the x_i^2 term is just a "feature" that could be "selected" or not.
  - Usually, "feature selection" means choosing from some "original" features.
    - You could say that "feature" selection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

Feature selection as a case of model selection

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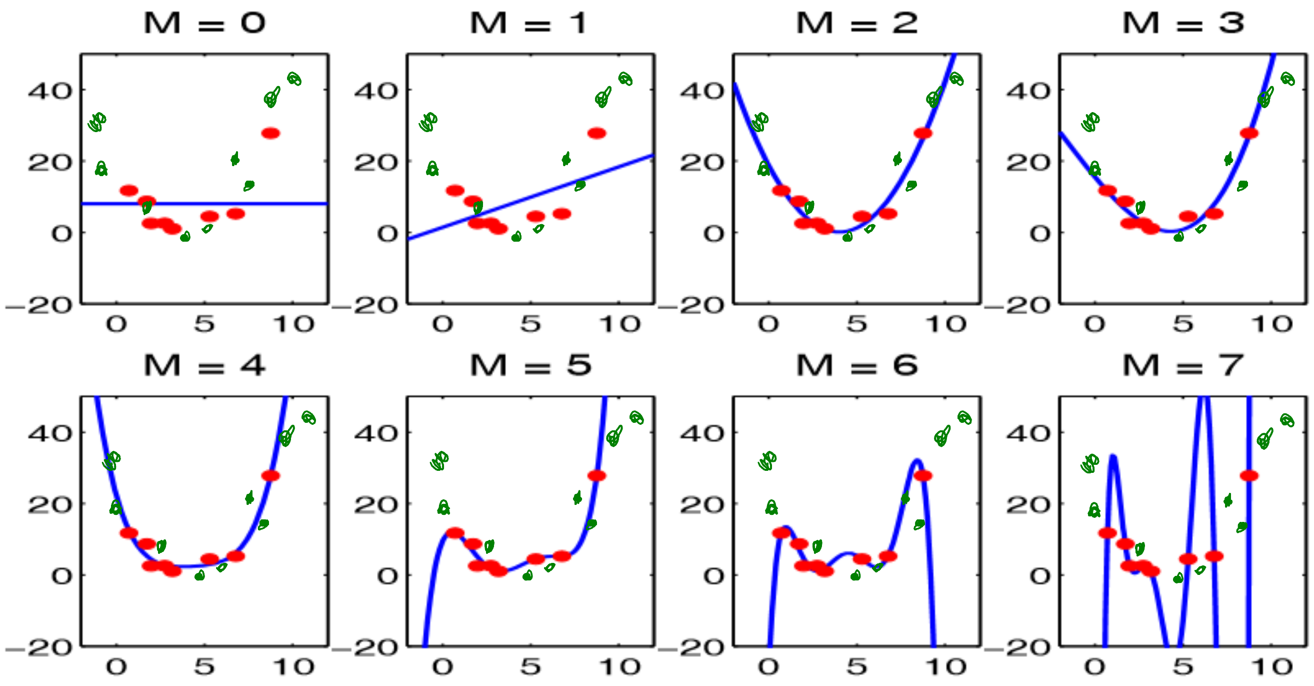
- Consider using d=n, with completely random features.
  - With high probability, you will be able to get a training error of 0.
  - But the features were random, this is completely overfitting.
- You could view “number of features” as a hyper-parameter.
  - Model gets more complex as you add more features.

(pause)

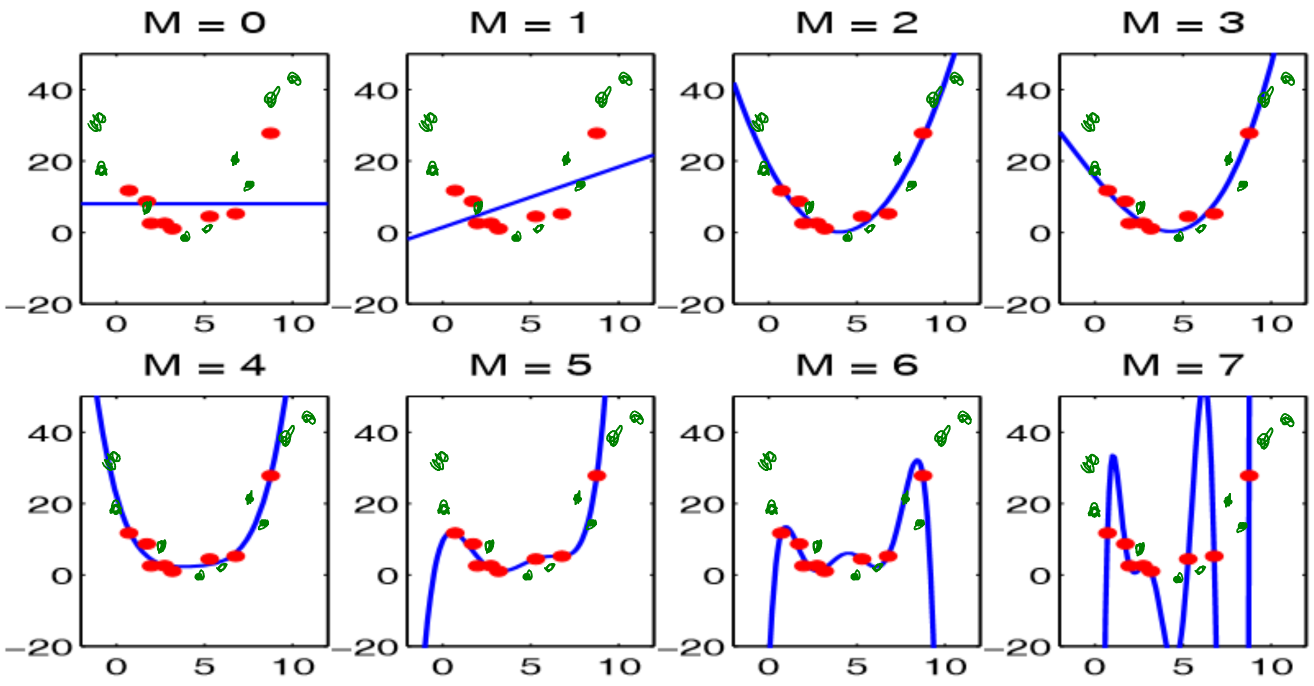
Recall: Polynomial Degree and Training vs. Testing



http://www.cs.ubc.ca/~arnaud/stat535/slides5_revised.pdf

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.
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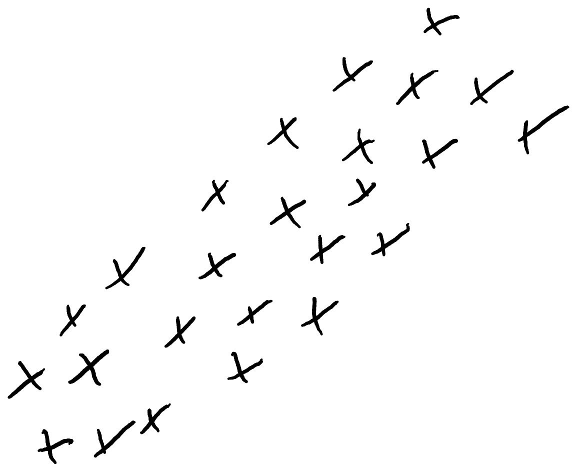
Controlling Complexity

- 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?



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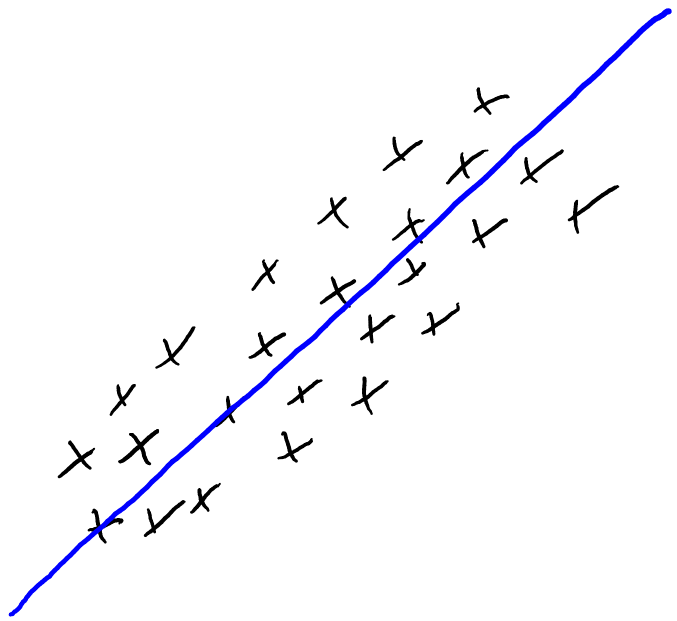

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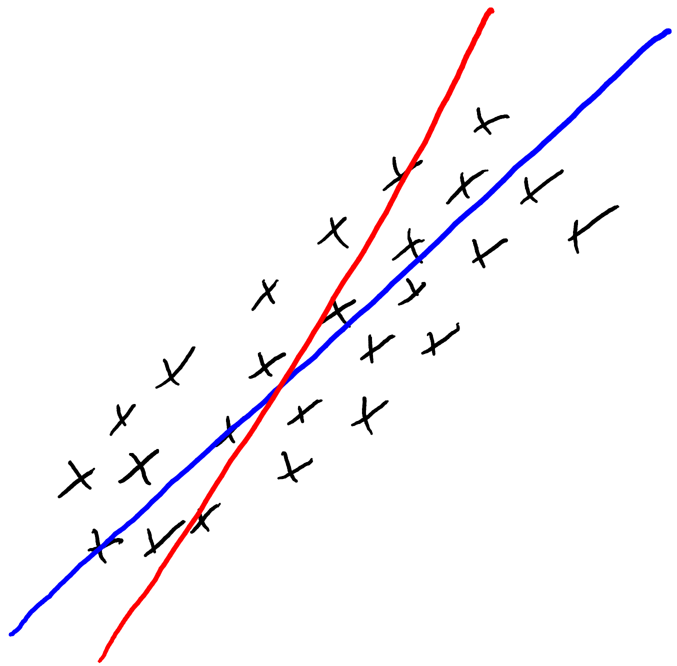

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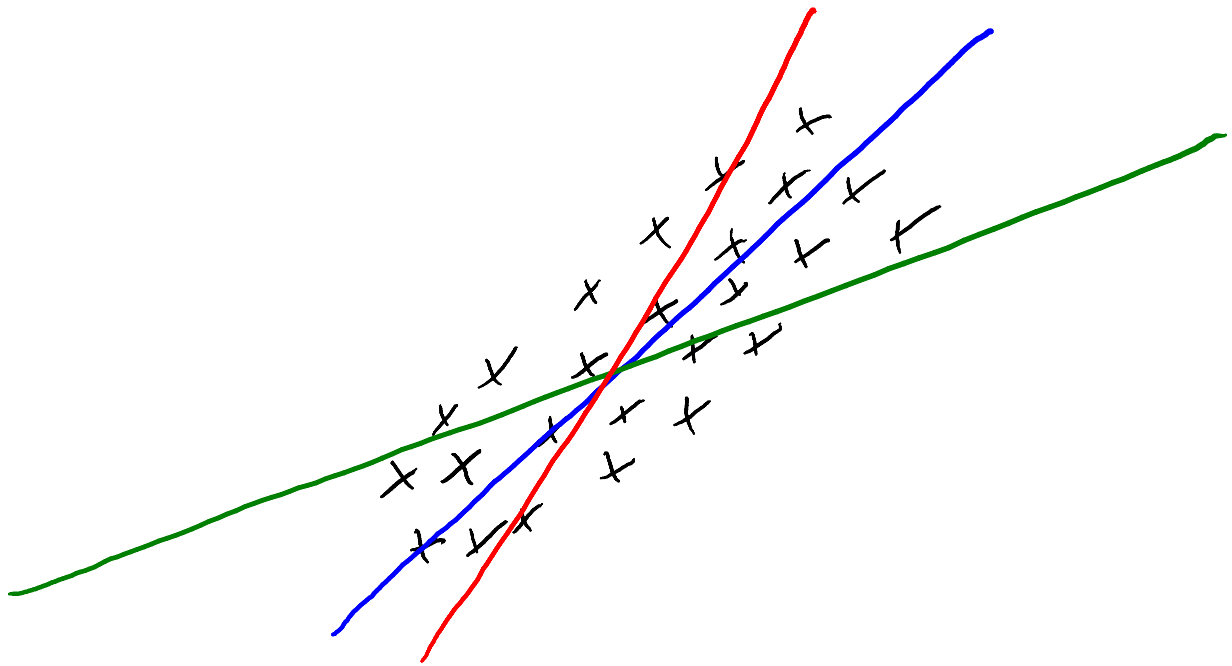
- Consider the following dataset and 3 linear regression models:



- Which line should we choose?

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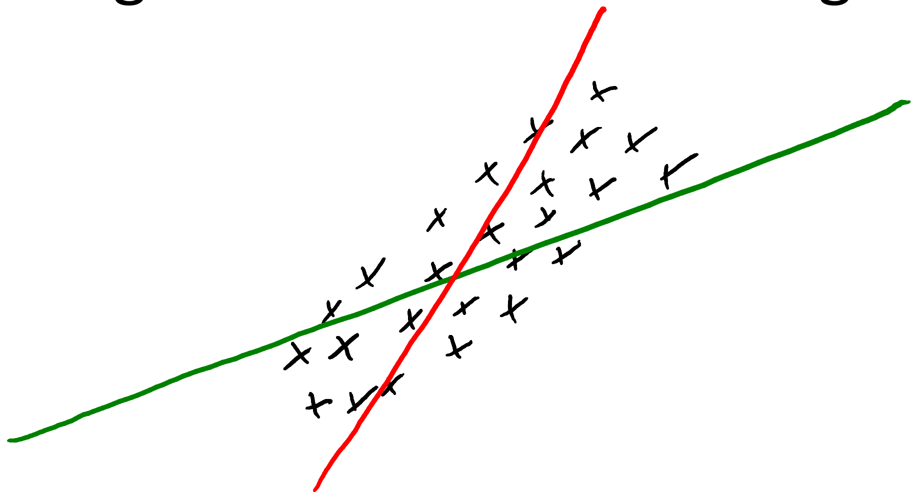

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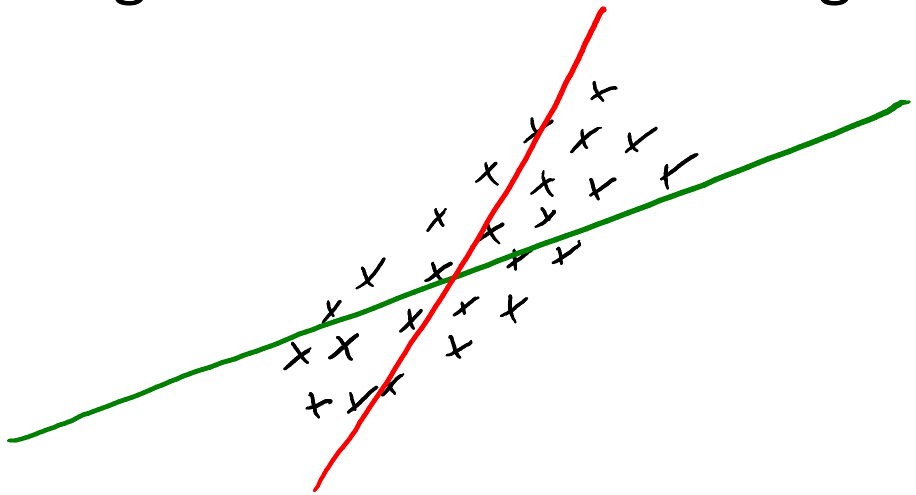

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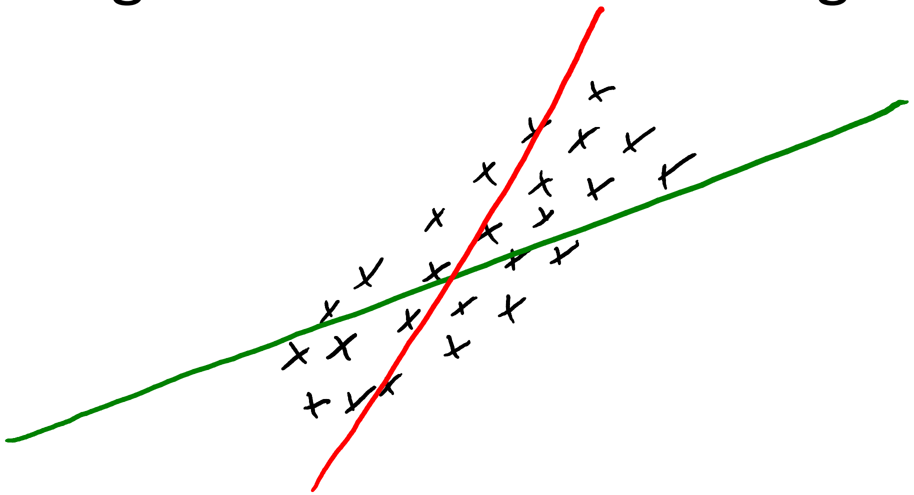
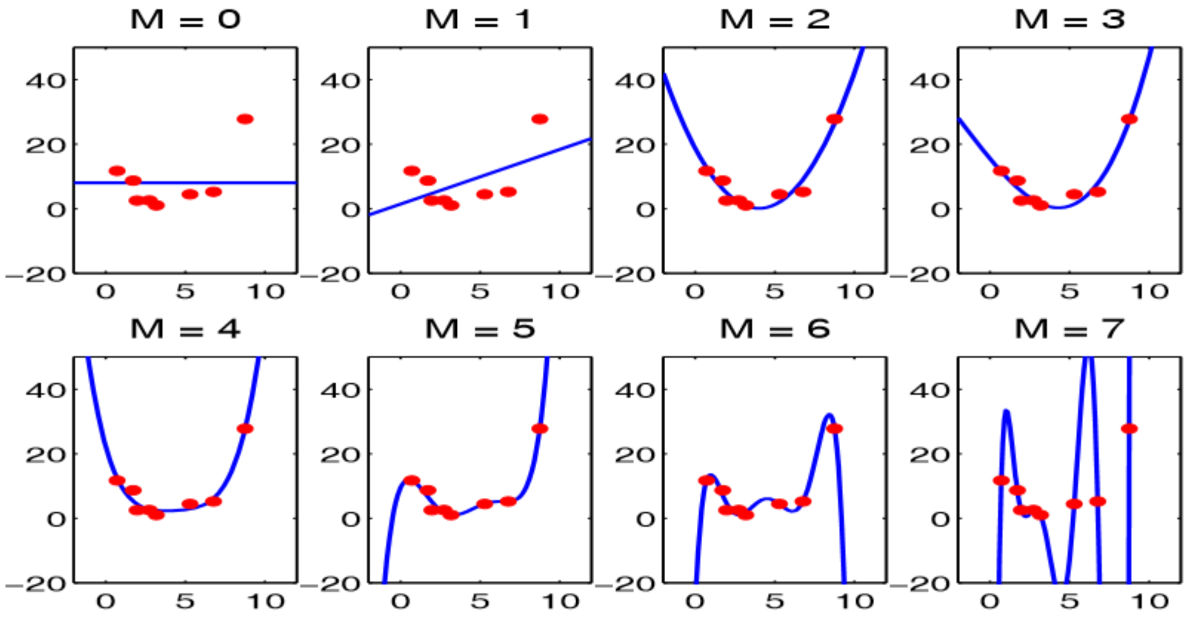


- What if you are forced to choose between red and green?
  - And assume they have the same training error.
- You should pick green.
  - Since slope is smaller, small change in x_i has a smaller change in prediction y_i.
    - Green line's predictions are less sensitive to having 'w' exactly right.
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

Large Regression Weights are Overfitting



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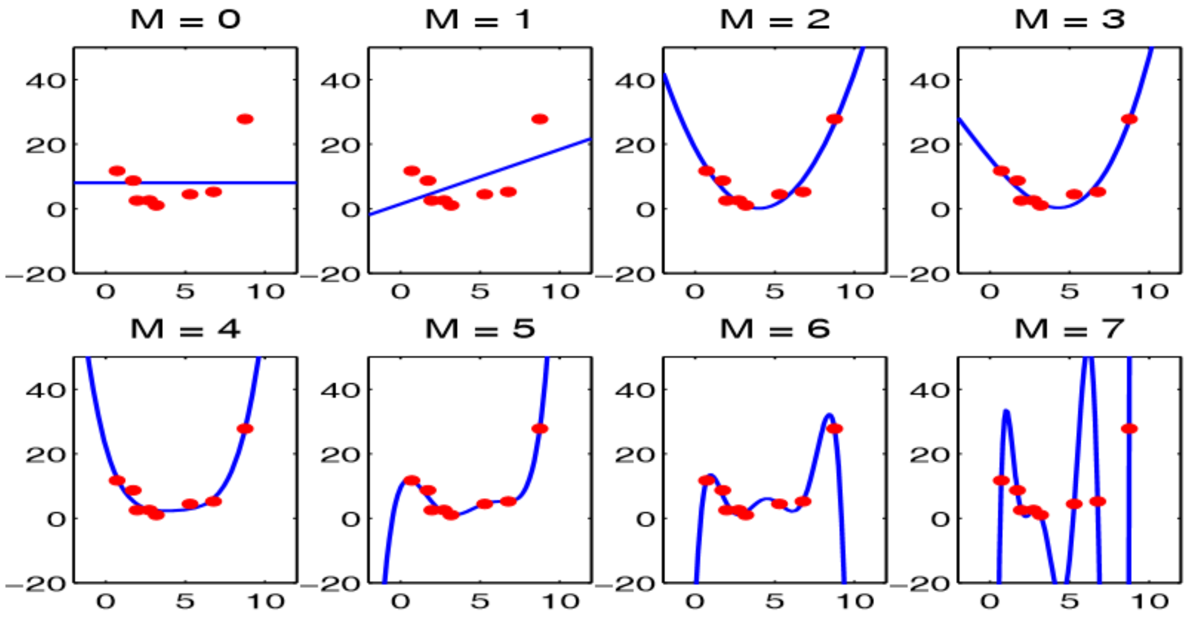

- The regression weights with degree-7 are huge in this example (small change in x_i has a large change in prediction y_i).
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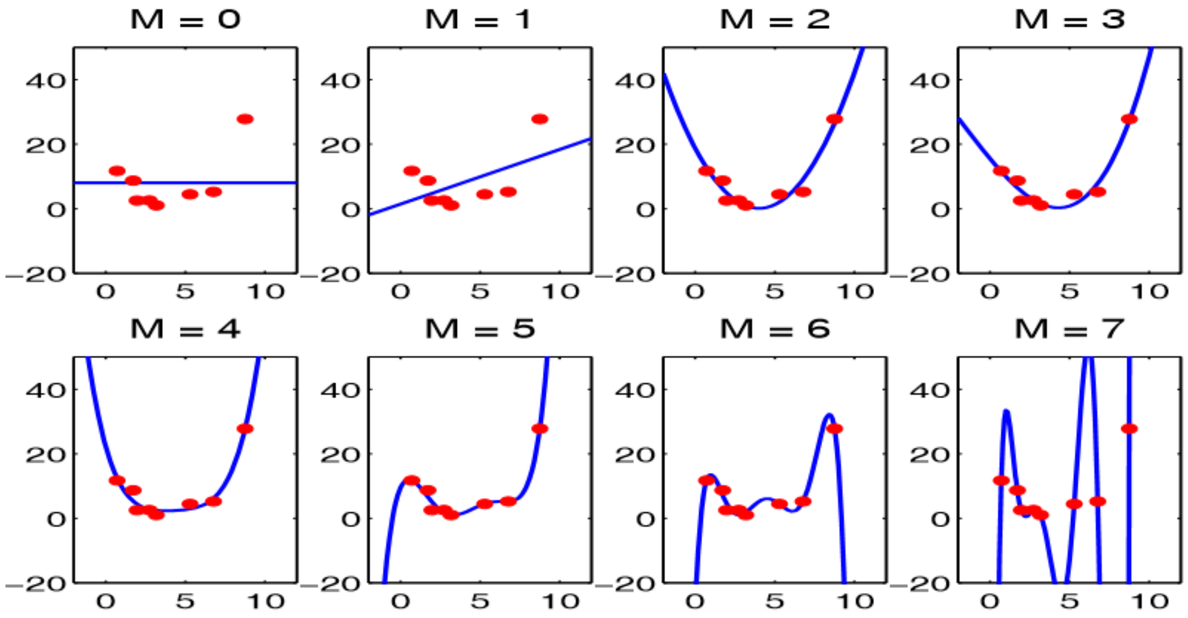

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$\hat{y}_i = 0.0001(x_i)^7 + 0.03(x_i)^3 + 3$ vs. $\hat{y}_i = 1000(x_i)^7 - 500(x_i)^6 + 890x_i$

L2-Regularization

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

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    - different in some cases (e.g. bigger if 'd' grows with 'n', smaller if there's no noise)
  - 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	$\|\|Xw - y\|\|^2$	$\|\|w\|\|^2$
0	-1.88	1.29	-2.63	1.78	-0.63	285.64	15.68
1	-1.88	1.28	-2.62	1.78	-0.64	285.64	15.62
4	-1.87	1.28	-2.59	1.77	-0.66	285.64	15.43
16	-1.84	1.27	-2.50	1.73	-0.73	285.71	14.76
64	-1.74	1.23	-2.22	1.59	-0.90	286.47	12.77
256	-1.43	1.08	-1.70	1.18	-1.05	292.60	8.60
1024	-0.87	0.73	-1.03	0.57	-0.81	321.29	3.33
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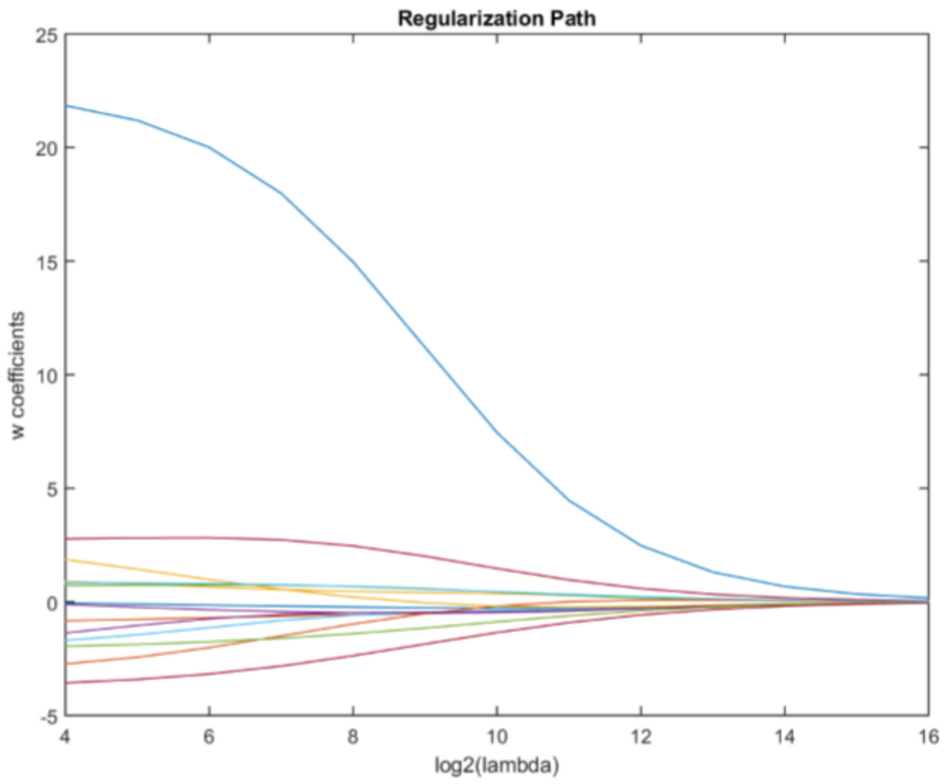
- We get least squares with $\lambda = 0$.
  - But we can achieve similar training error with smaller $||w||$.
- $||X w - y||$ increases with λ, and $||w||$ decreases with λ.
  - Though individual w_j can increase or decrease with lambda.
  - Because we use the L2-norm, the large ones decrease the most.

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 $\nabla f(w) = 0$.
- Loss before: $f(w) = \frac{1}{2}\|Xw - y\|^2$
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- 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^TX, the matrix $(X^TX + \lambda I)$ 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:

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

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  - Can show number of iterations decreases as λ increases (not obvious).

bonus!

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  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
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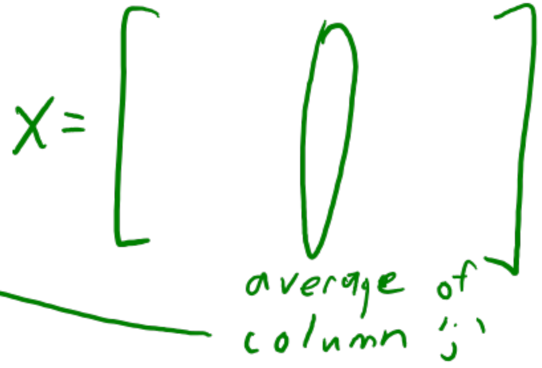

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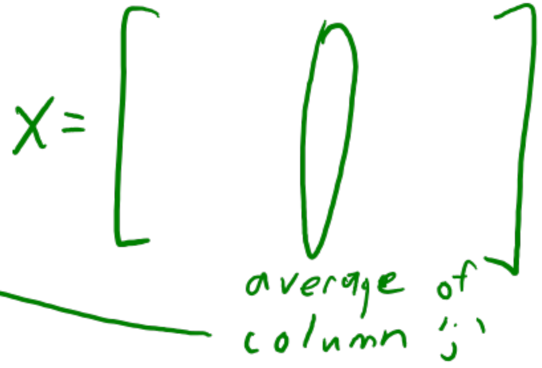

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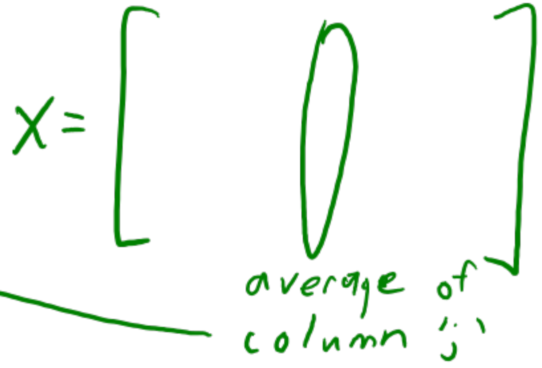

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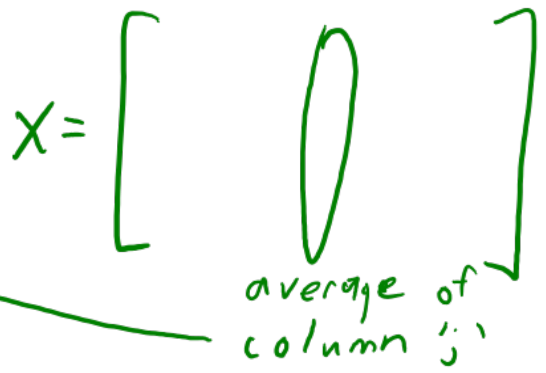

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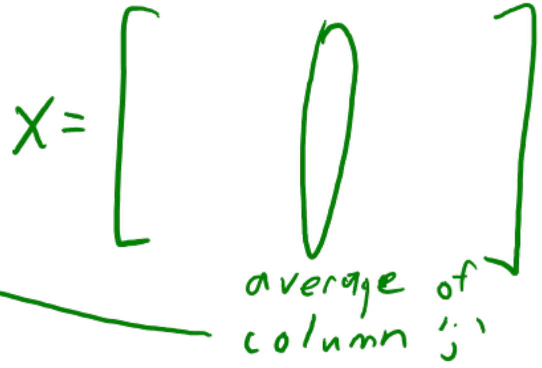

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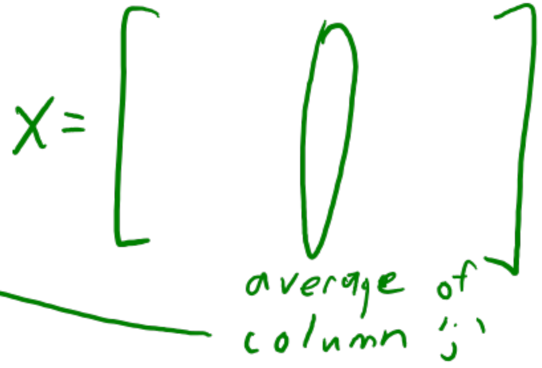

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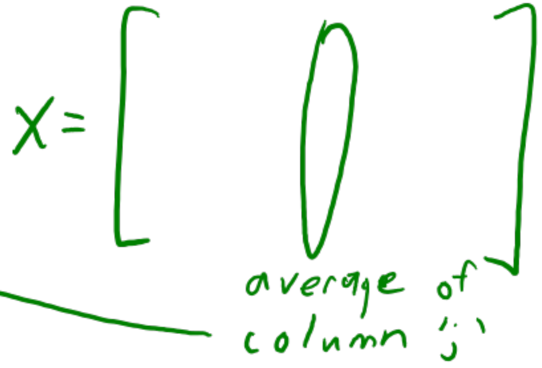

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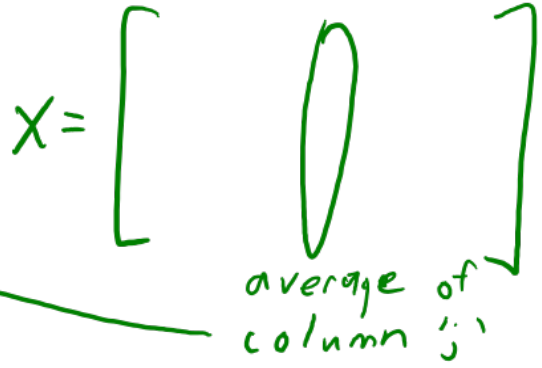

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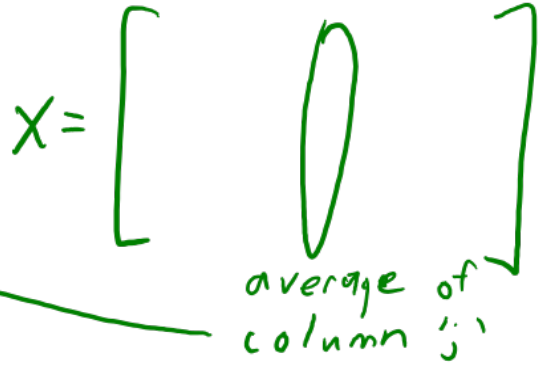

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- Other common transformations of y_i are logarithm/trig functions:
  - Makes sense for geometric/exponential processes.

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

Regularizing the y-Intercept?

bonus!

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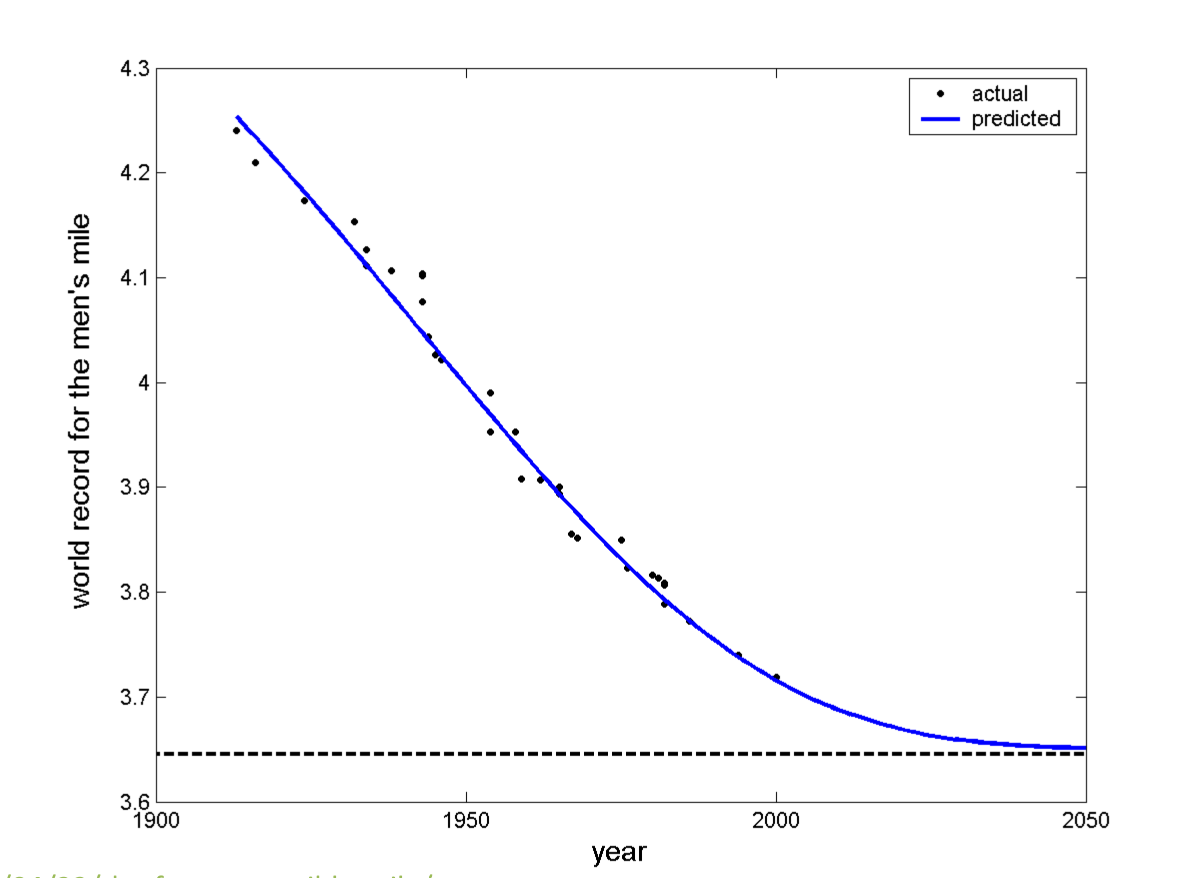

https://gravityandlevity.wordpress.com/2009/04/22/the-fastest-possible-mile/

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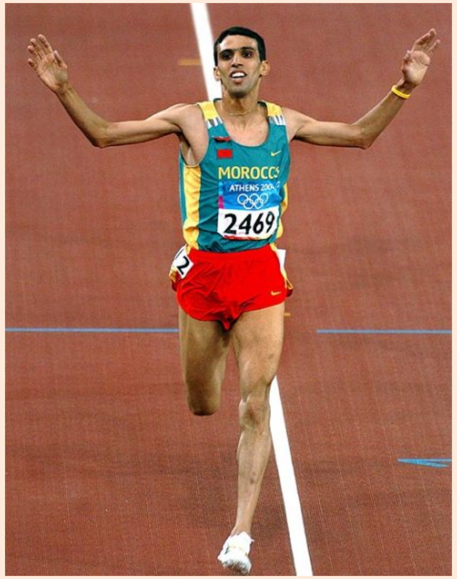
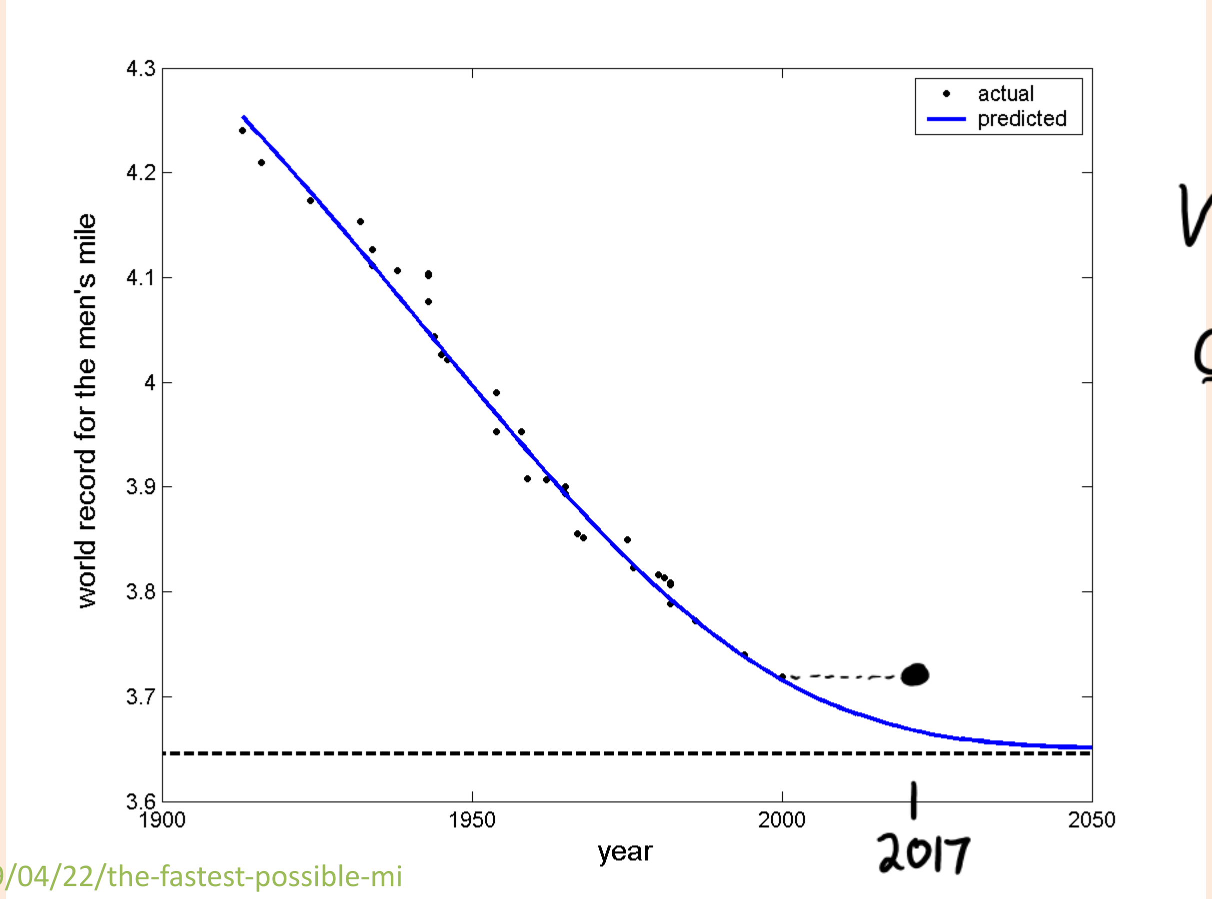


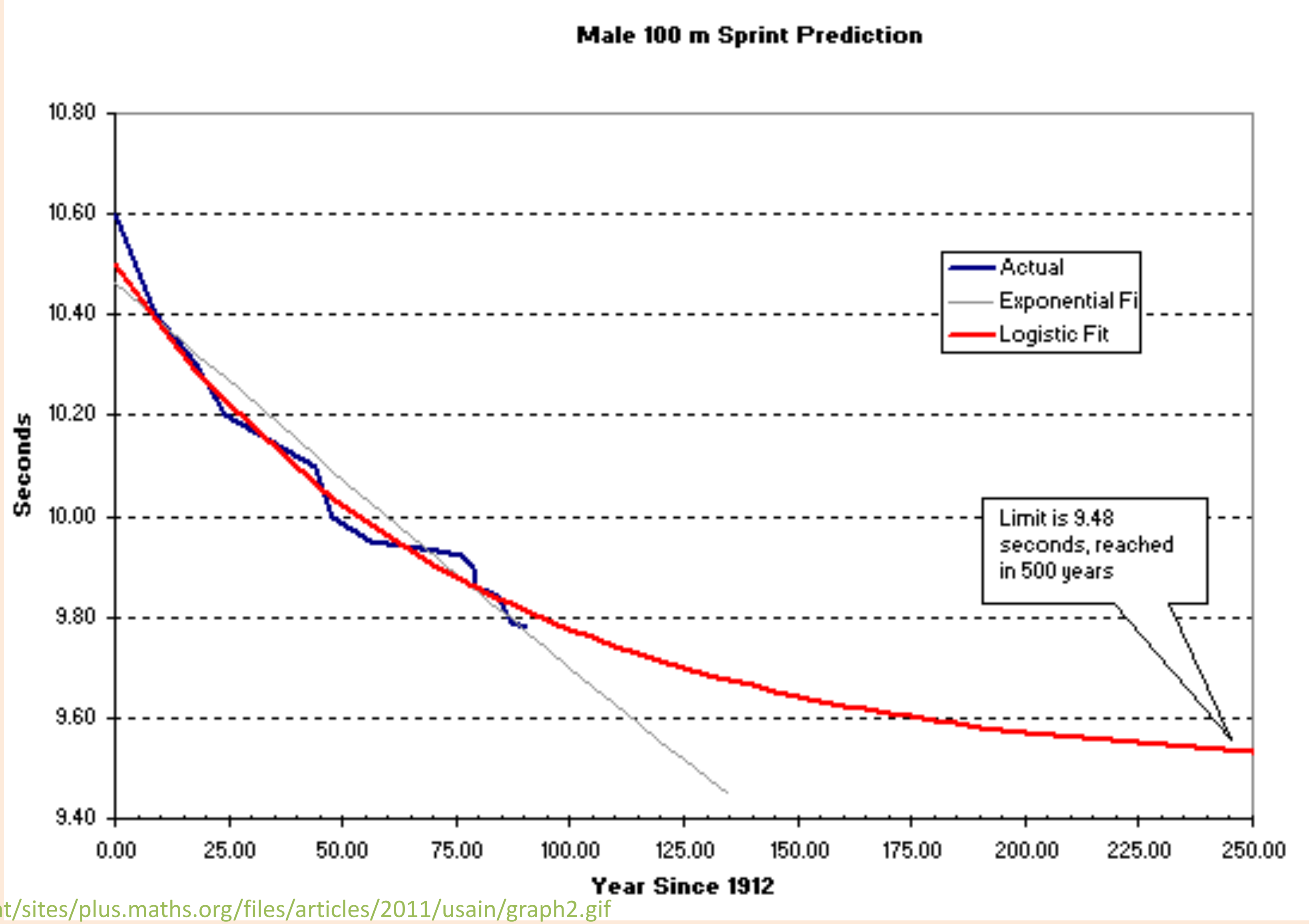


We need to be cautious about doing this.

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?

bonus!



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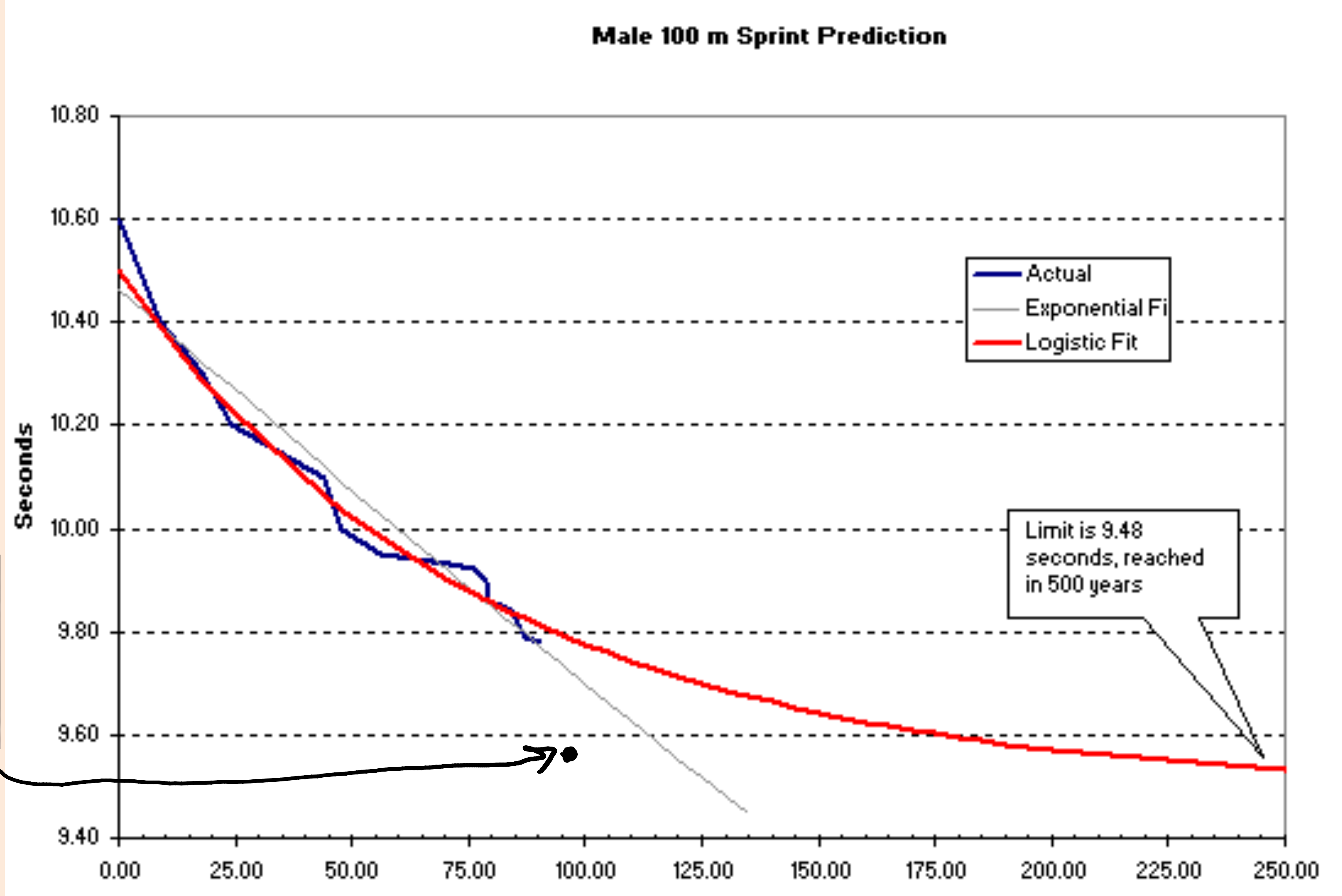

9.58

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bonus!

Interpolation vs Extrapolation

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

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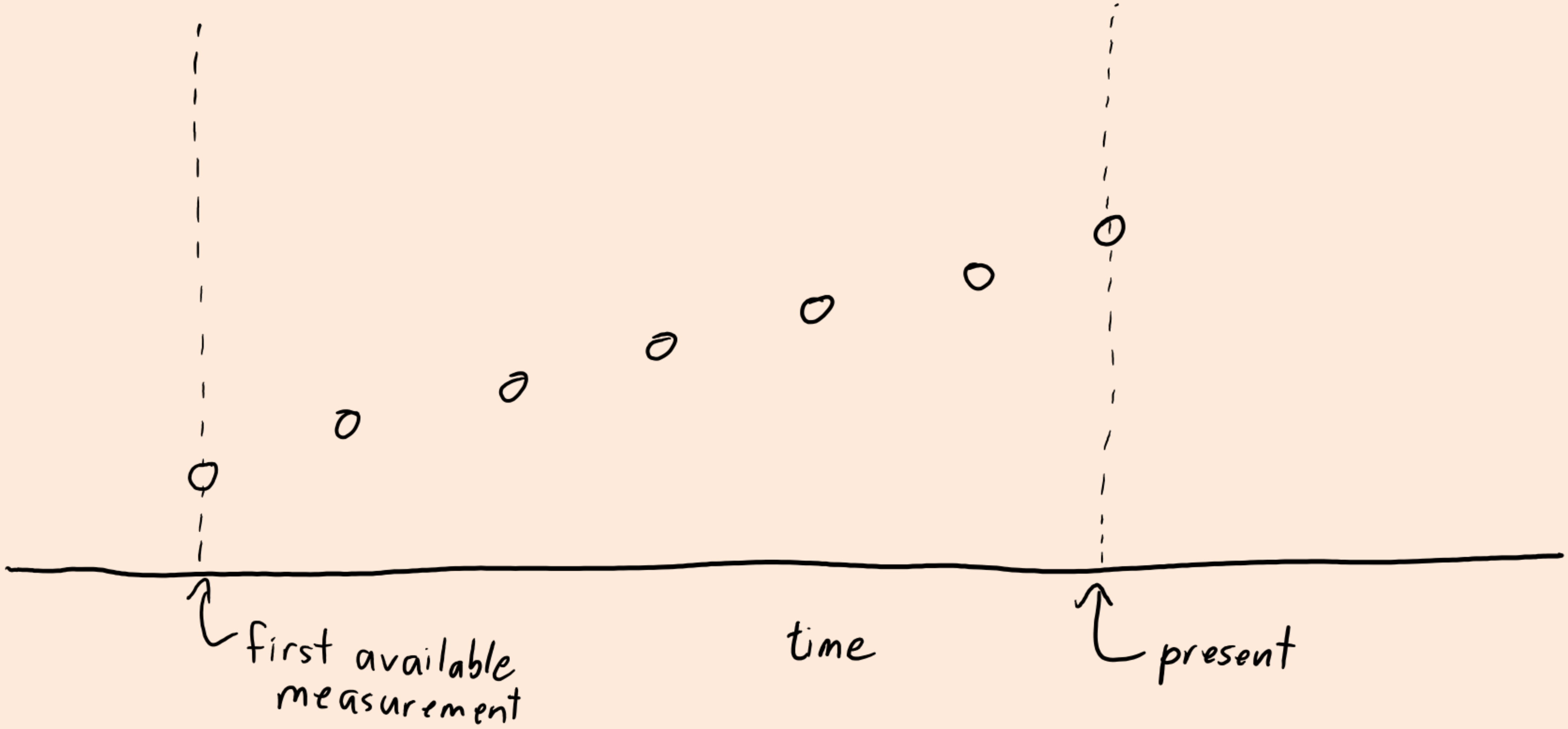
No Free Lunch, Consistency, and the Future

bonus!



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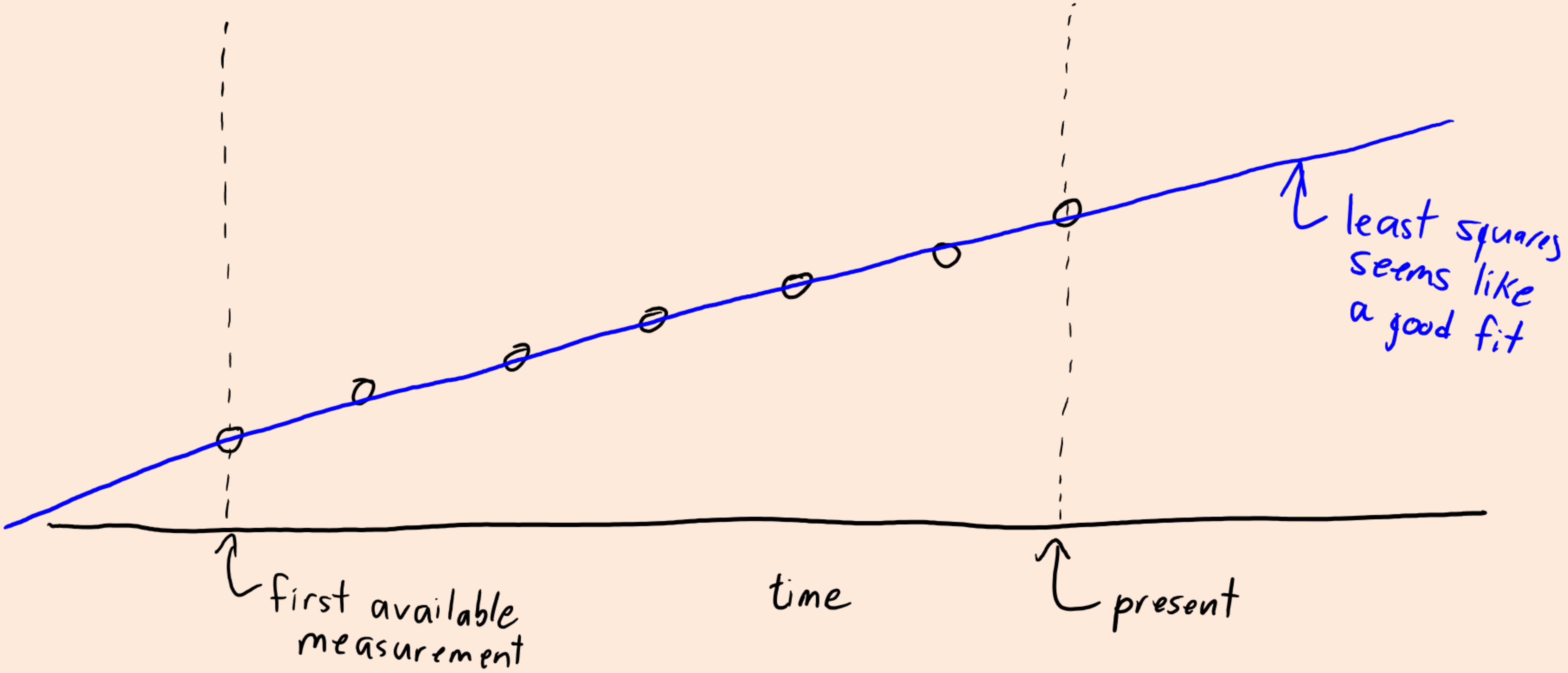

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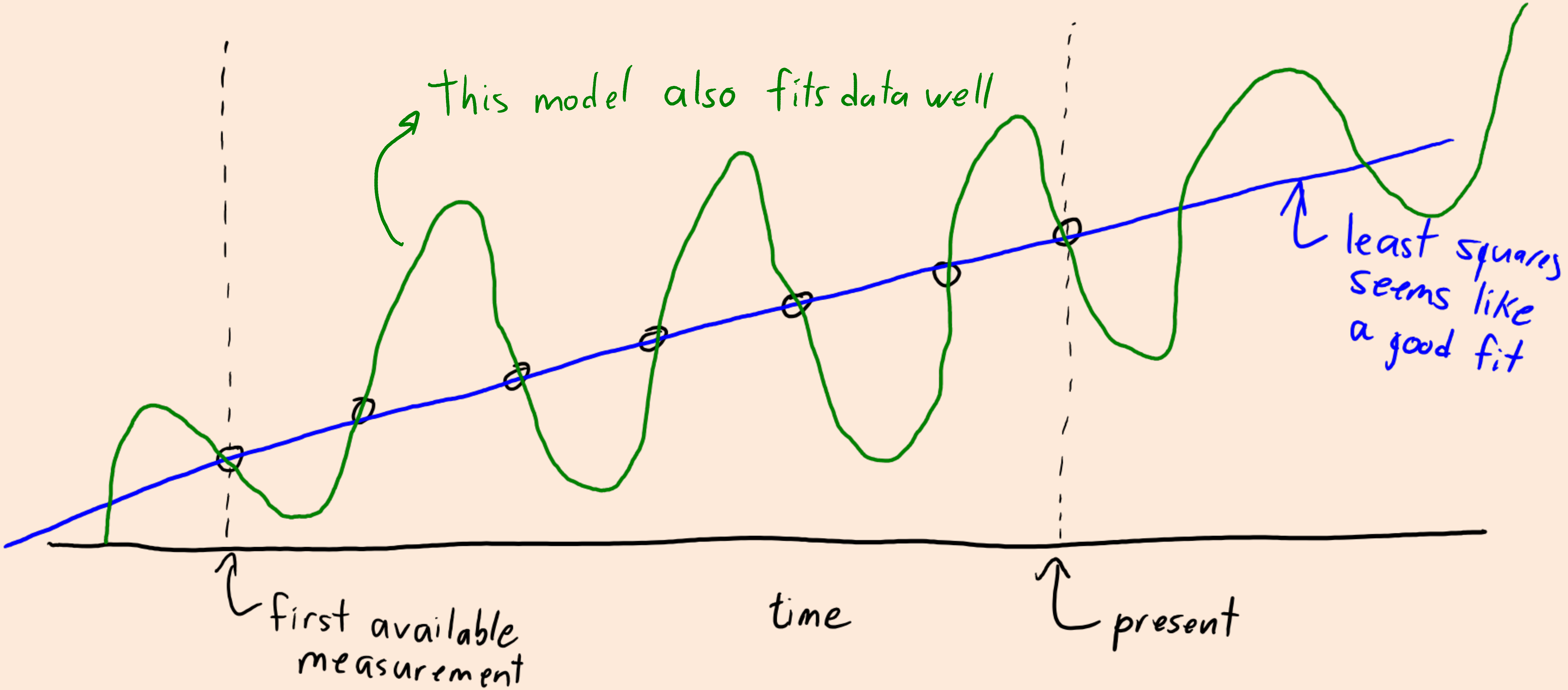

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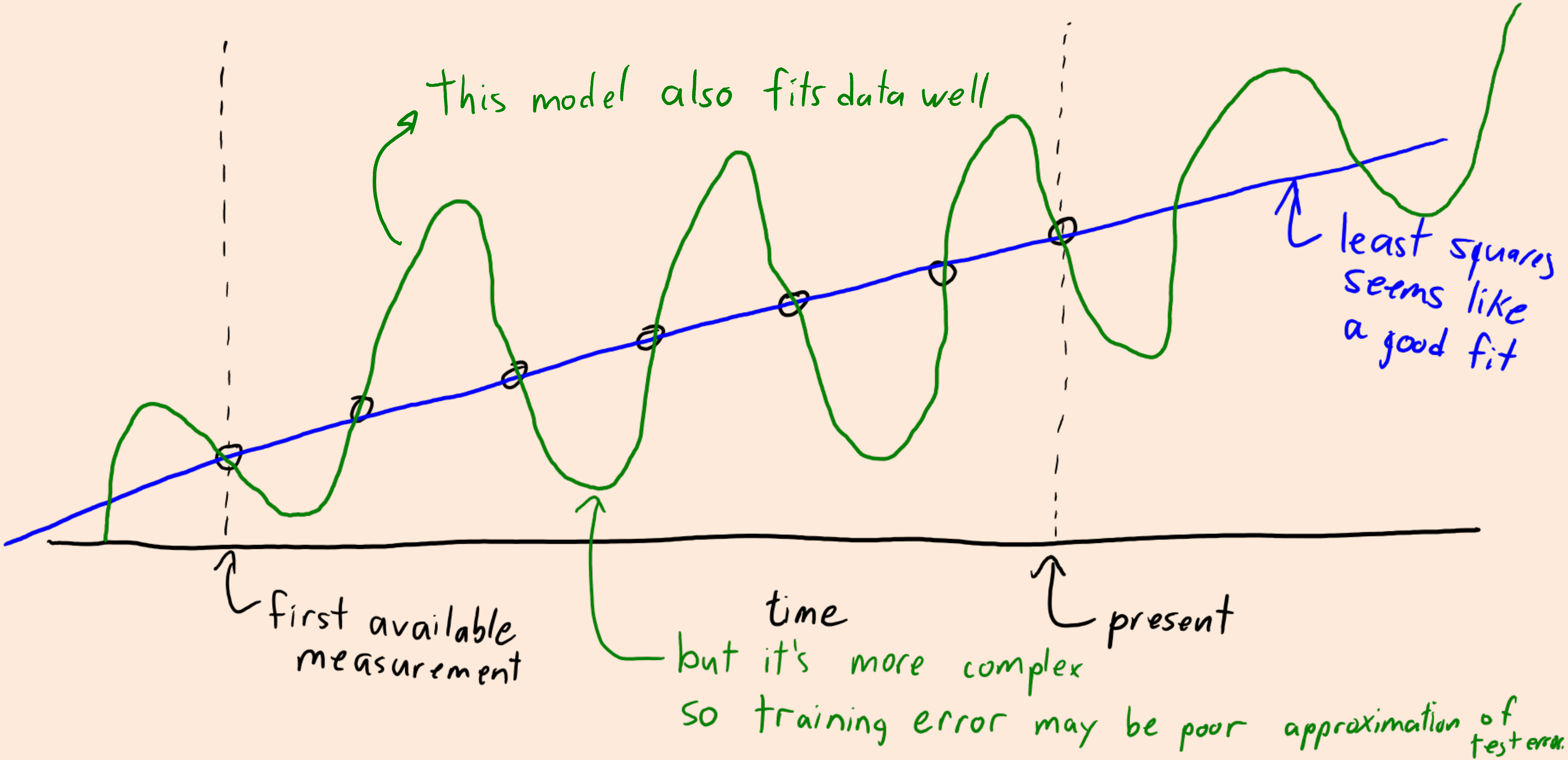

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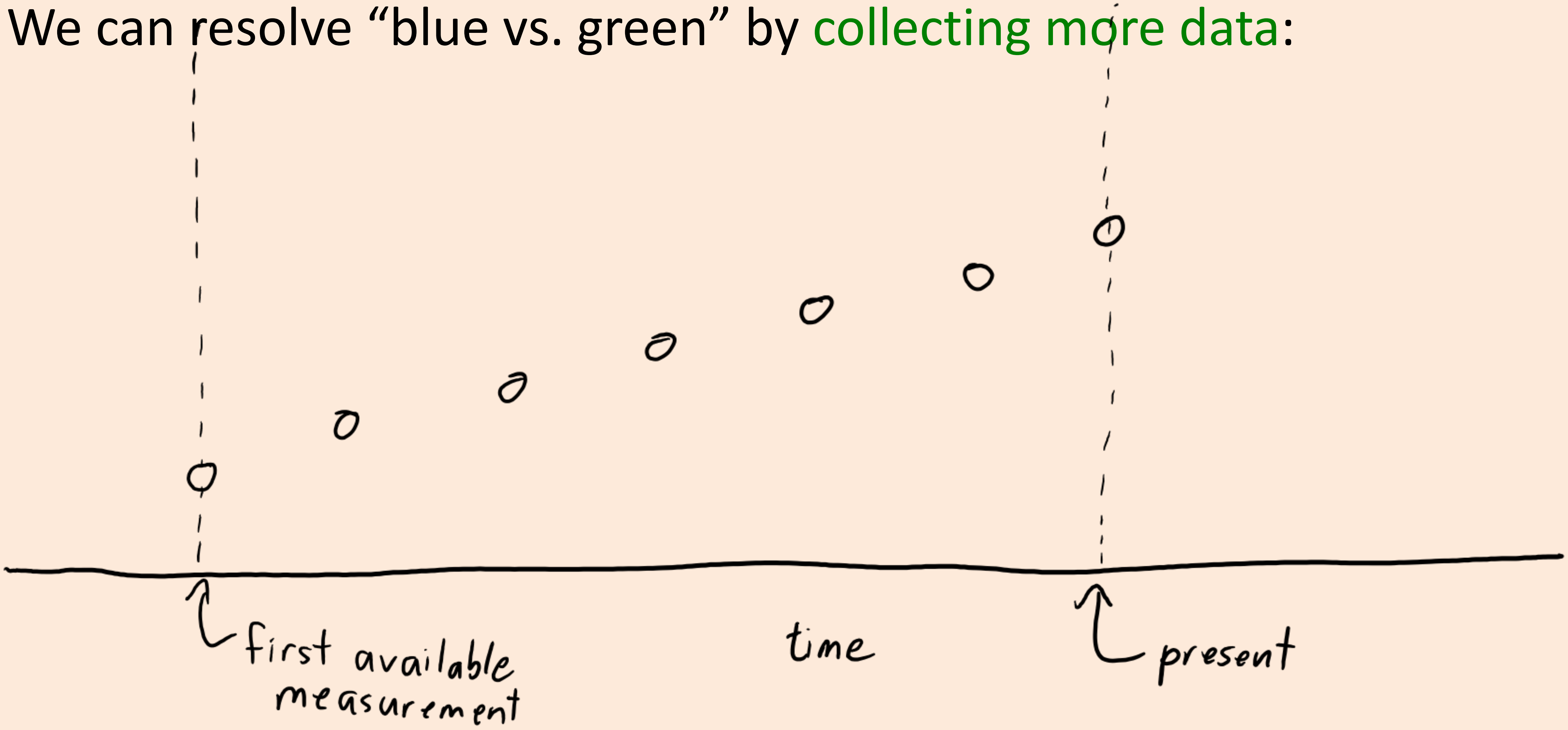

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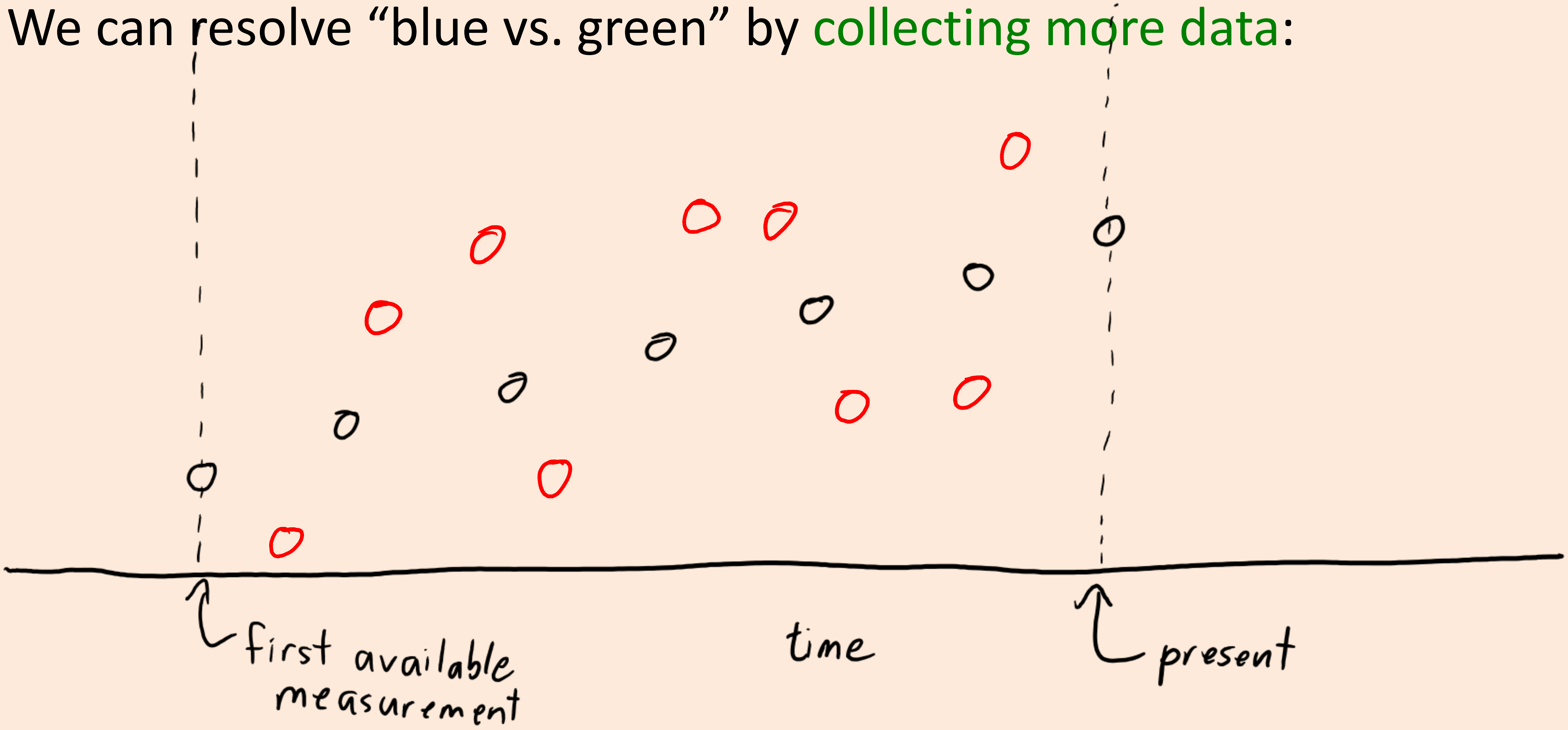

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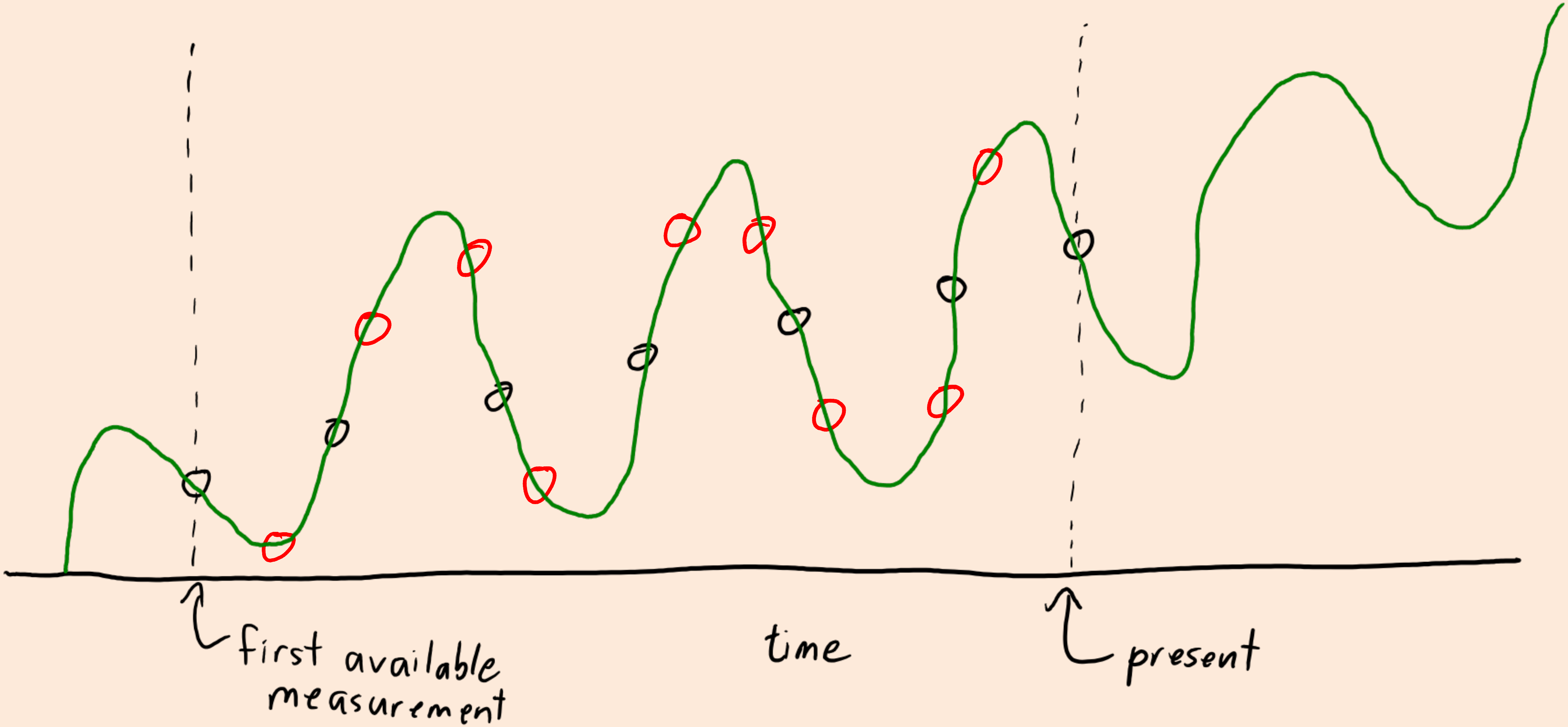

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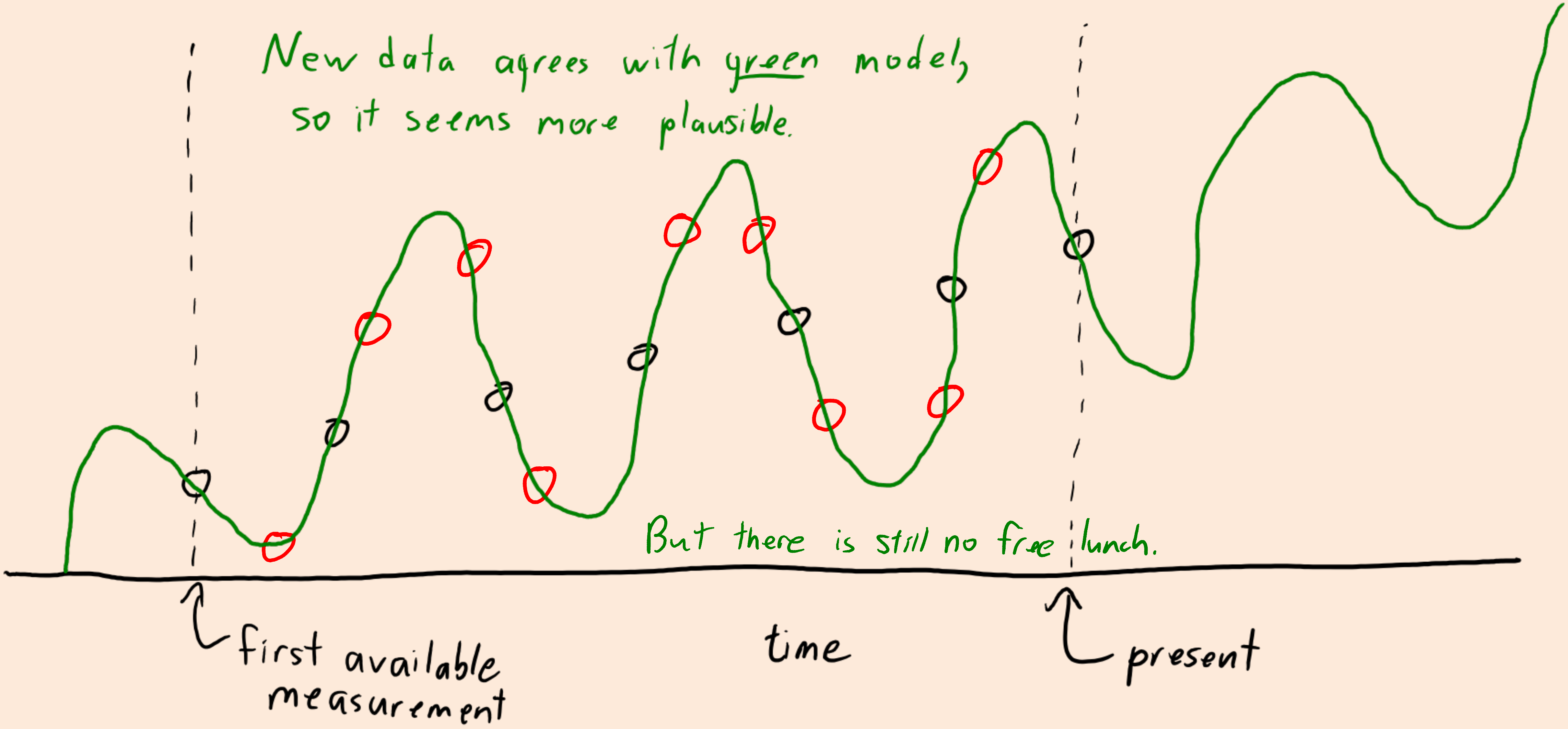

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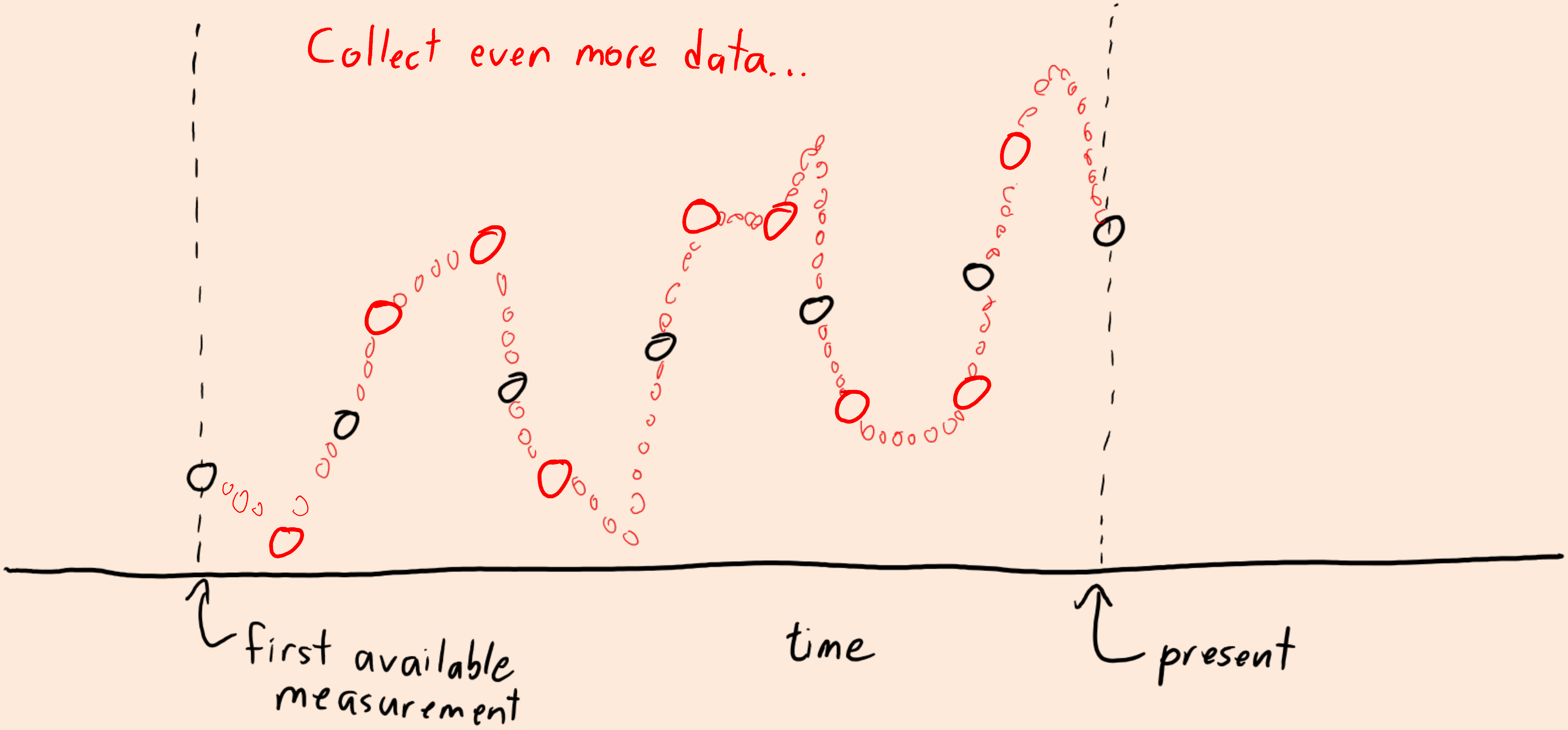

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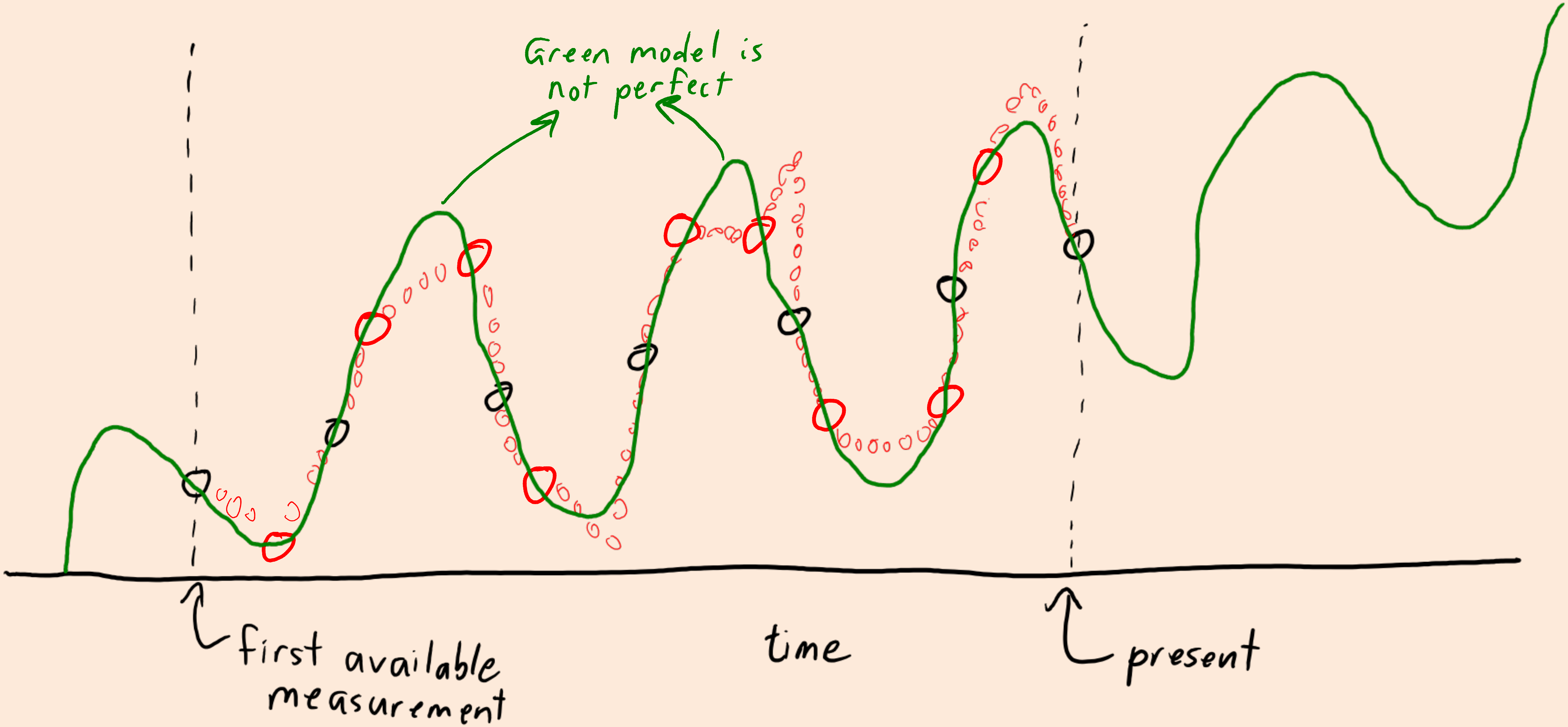

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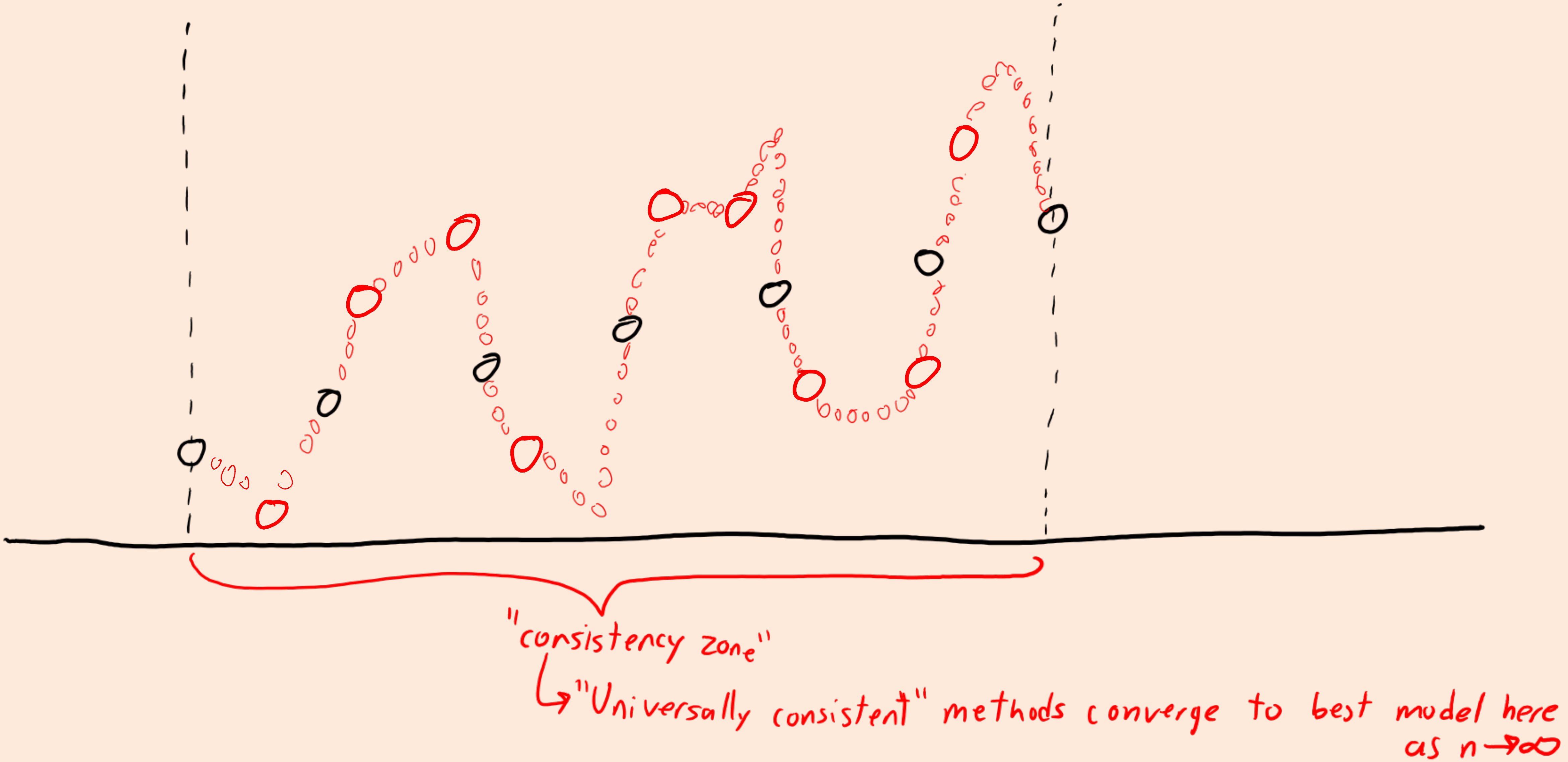

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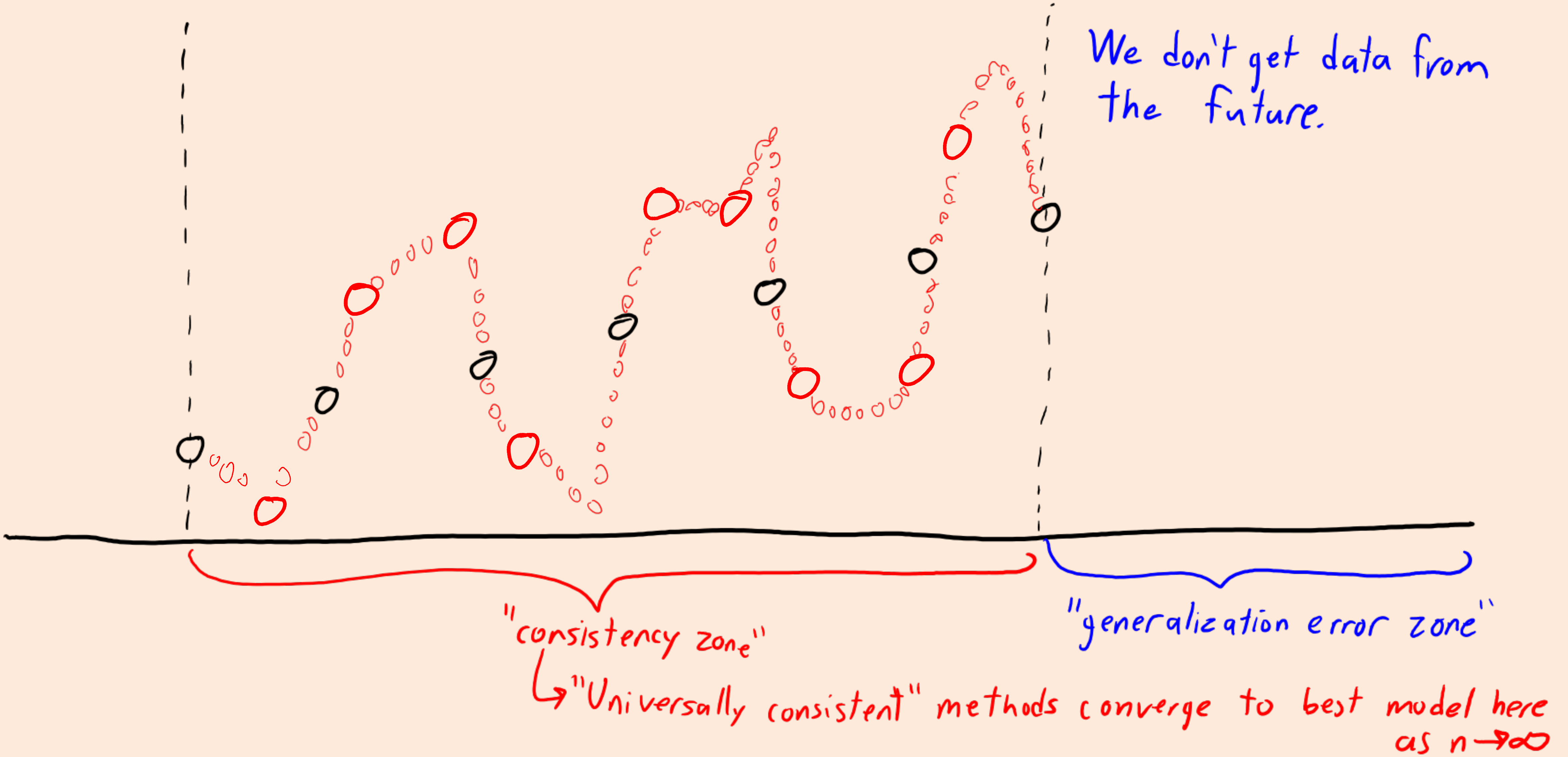

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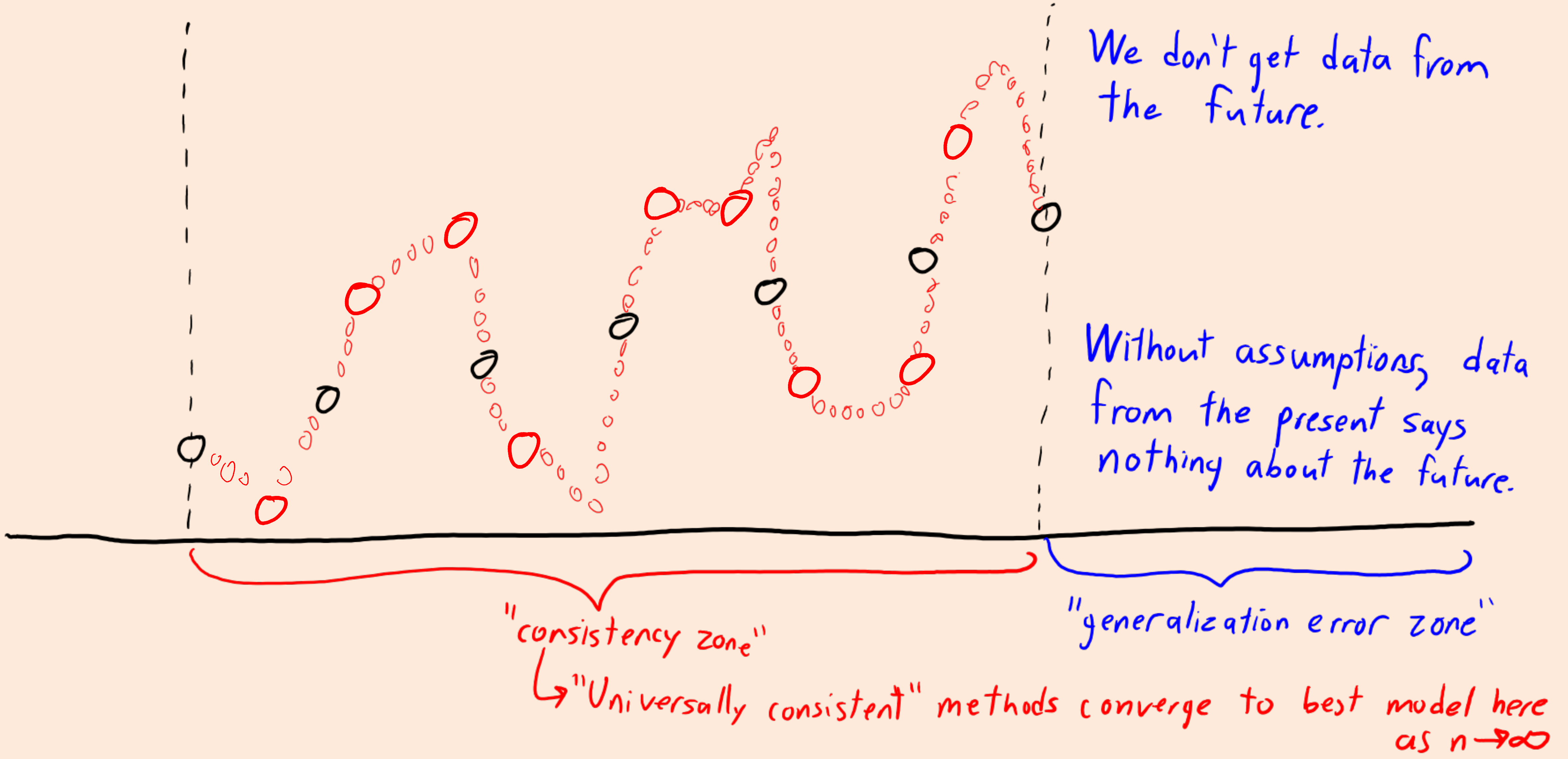

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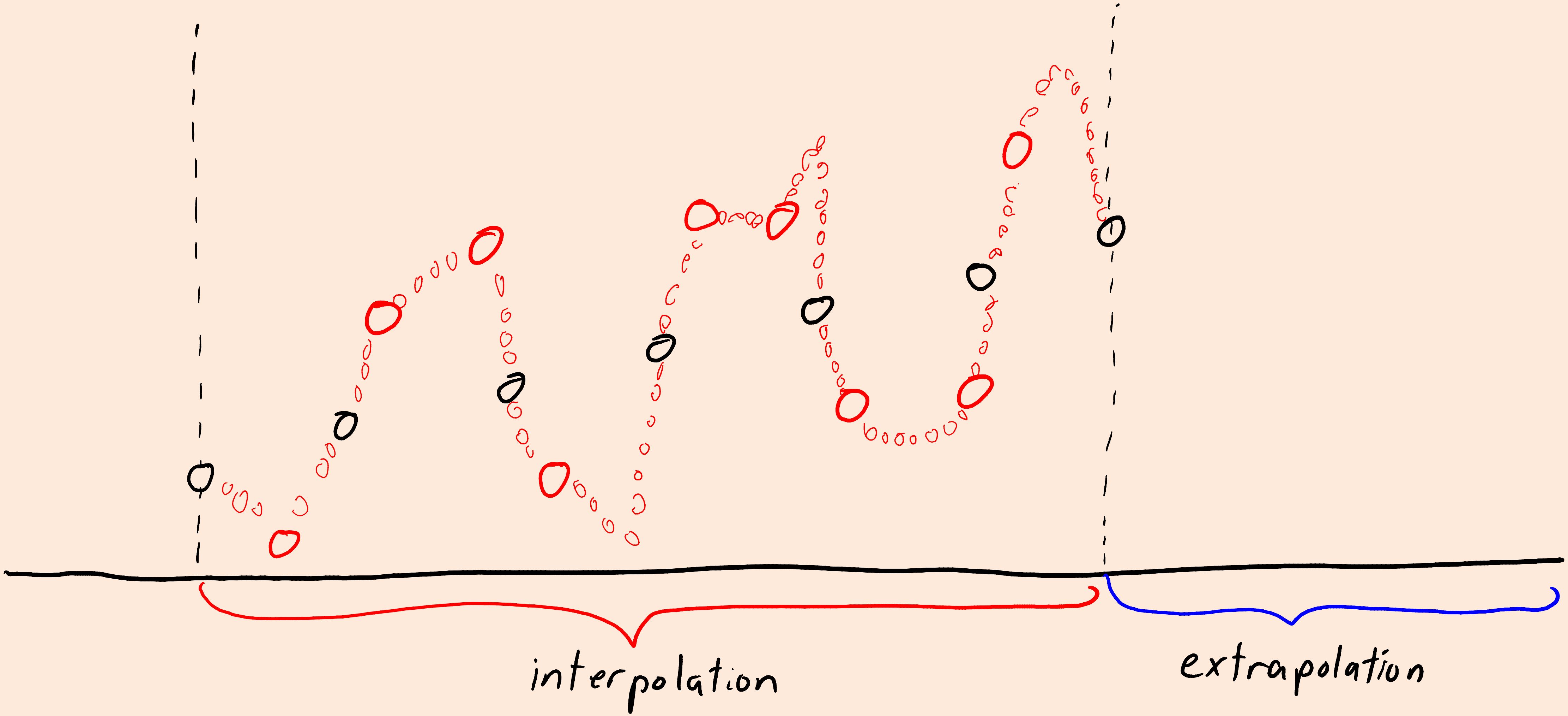

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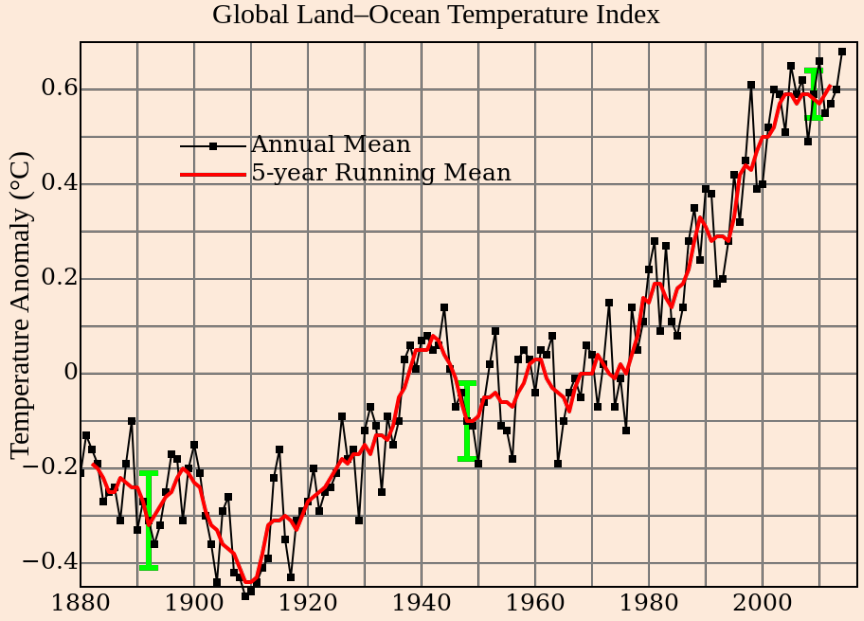
Discussion: Climate Models

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



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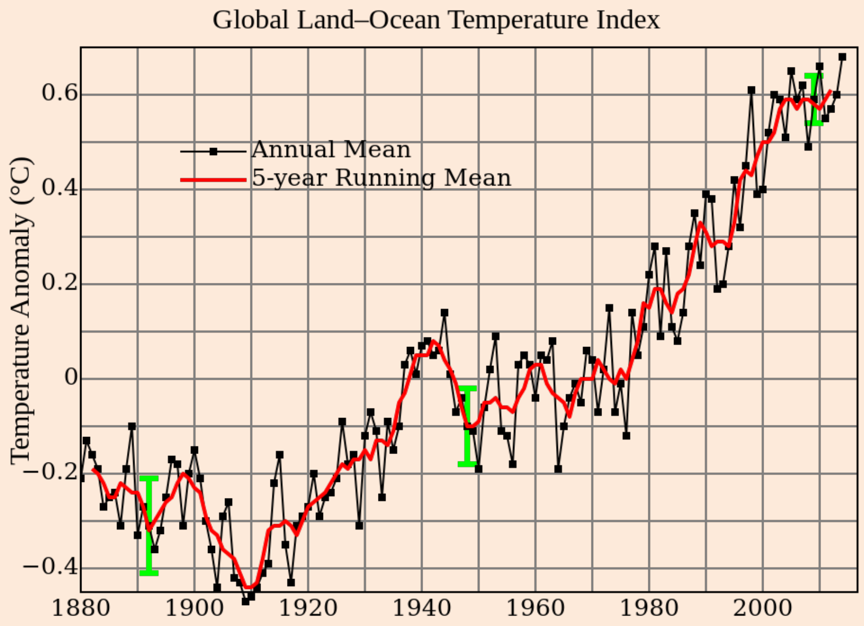

- Will Earth continue to warm over next 100 years? (generalization error)
  - We should be more skeptical about models that predict future events.

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Discussion: Climate Models

- So should we all become global warming skeptics?

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- 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:

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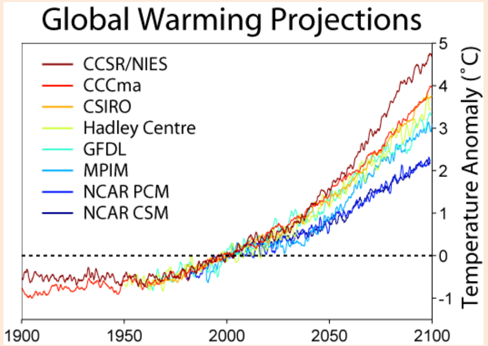

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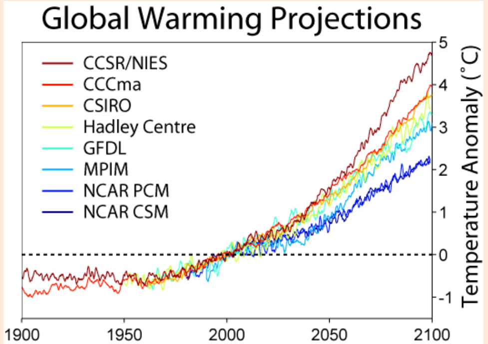

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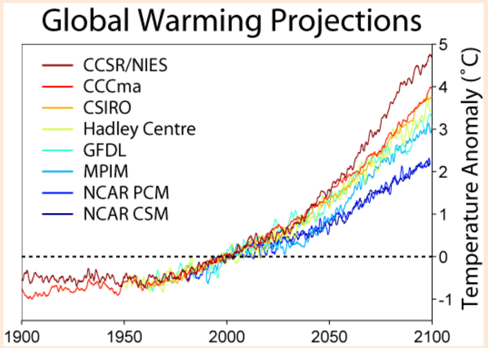

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- All the near-future predictions agree, so they are likely to be accurate.
  – And it's probably reasonable to assume fairly continuous change (no big "jumps").
- Variance is higher further into future, so predictions are less reliable.
  – Relying more on assumptions and less on data.

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Index Funds: Ensemble Extrapolation for Investing

bonus!

- Want to do extrapolation when investing money.
  - What will this be worth in the future?

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

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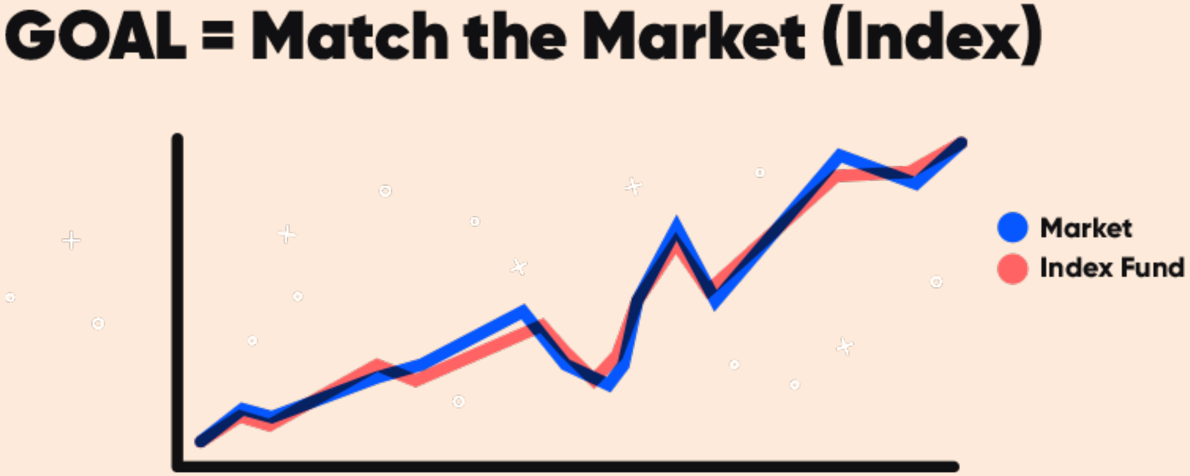

  - This simple investing strategy outperforms most fund managers.

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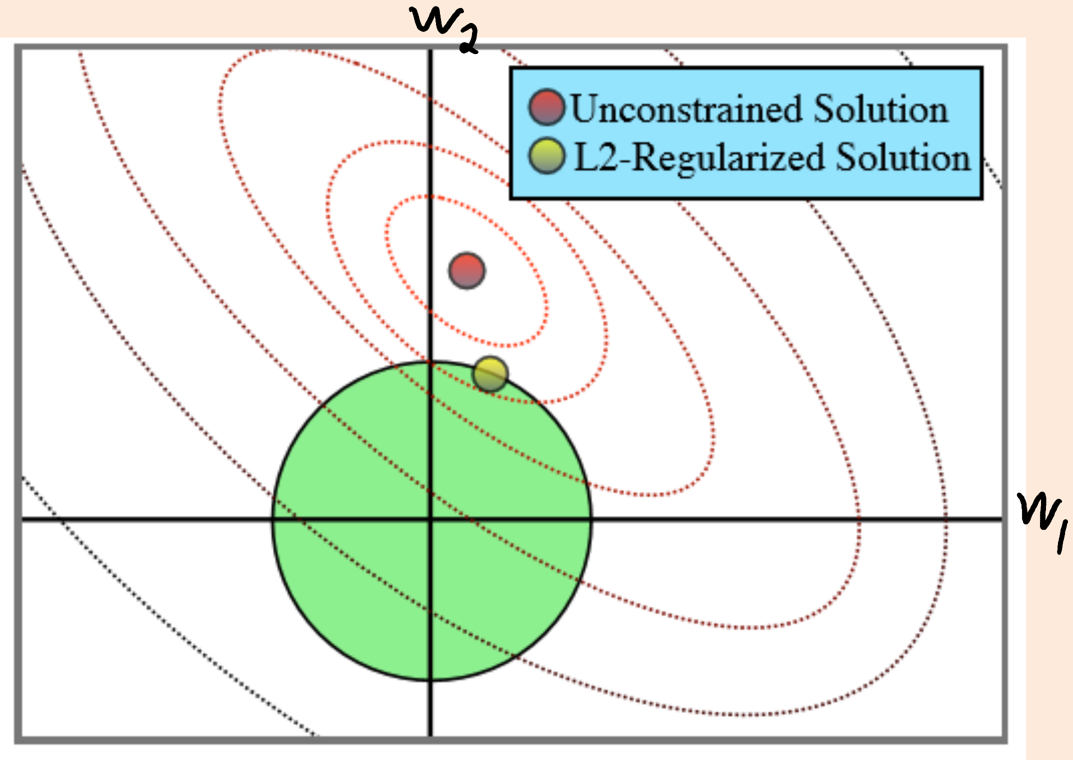
L2-Regularization

- 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.



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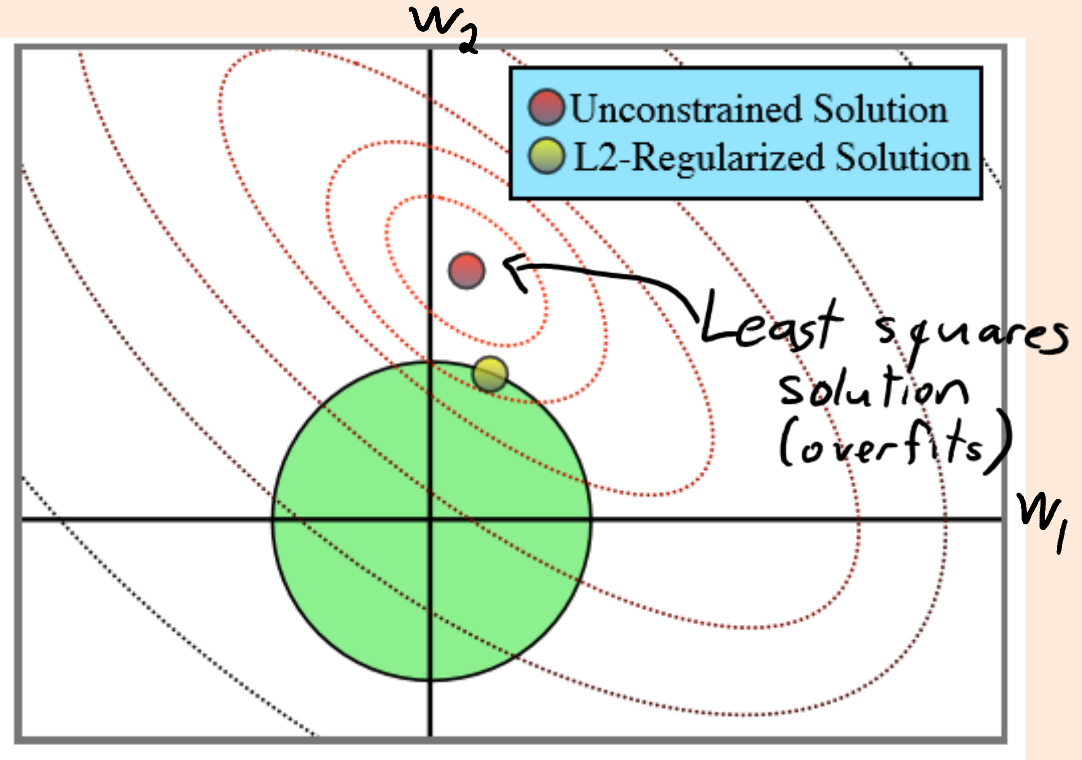

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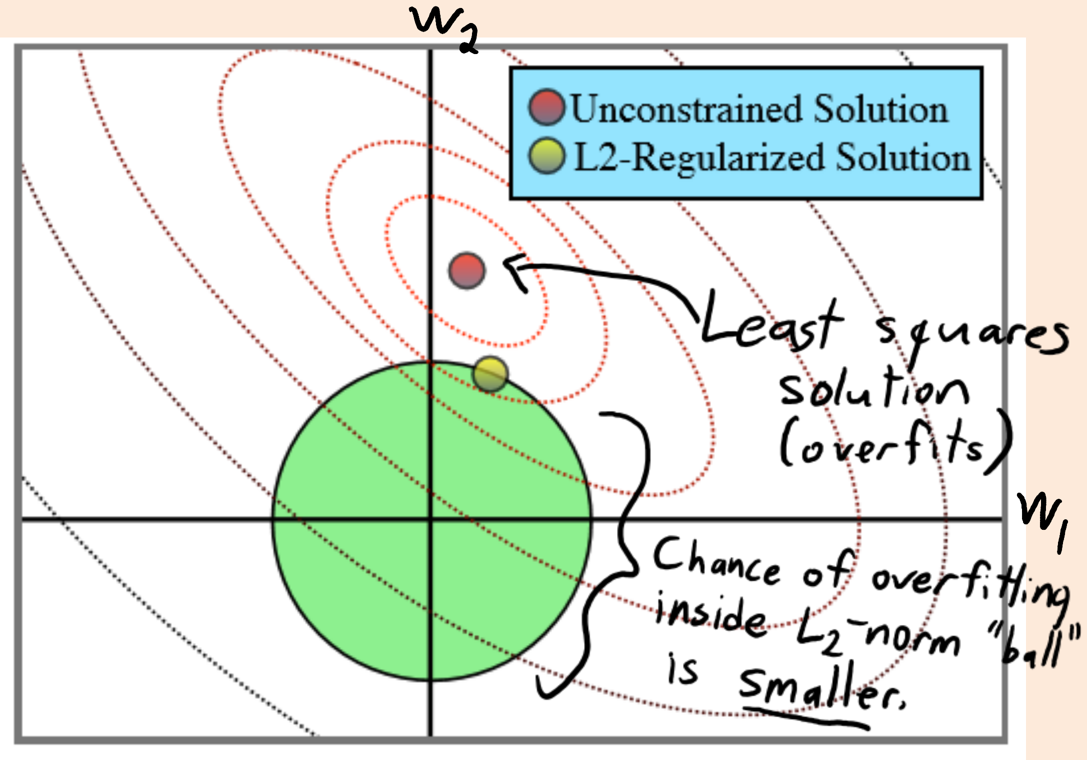

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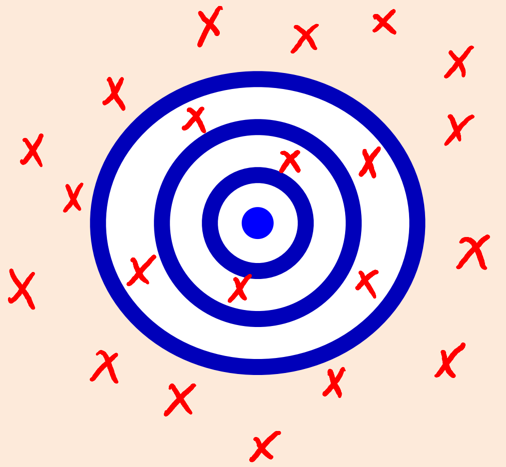

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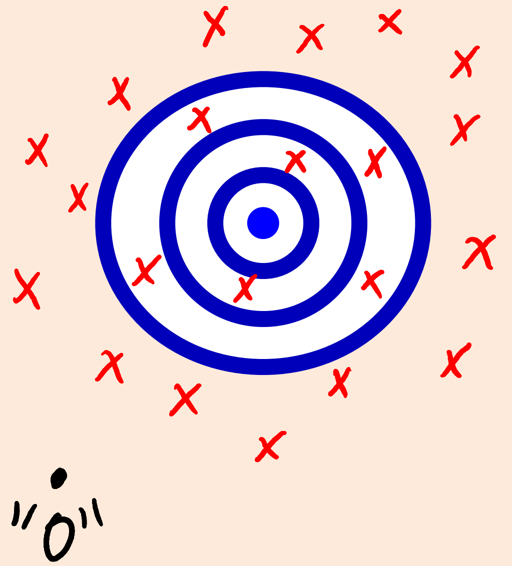

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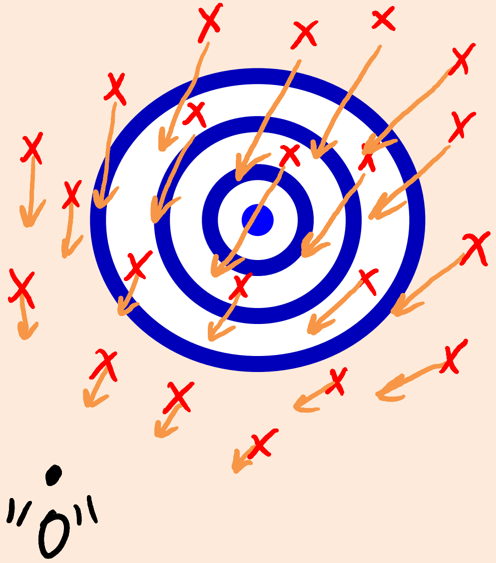

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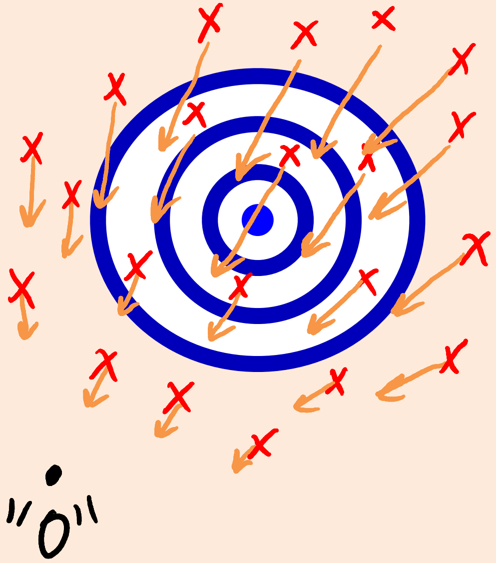

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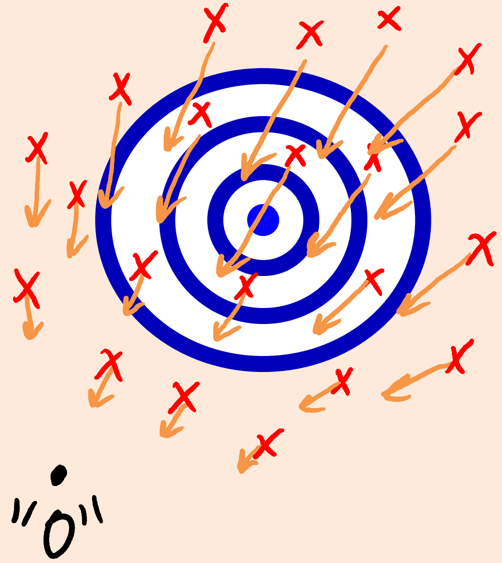

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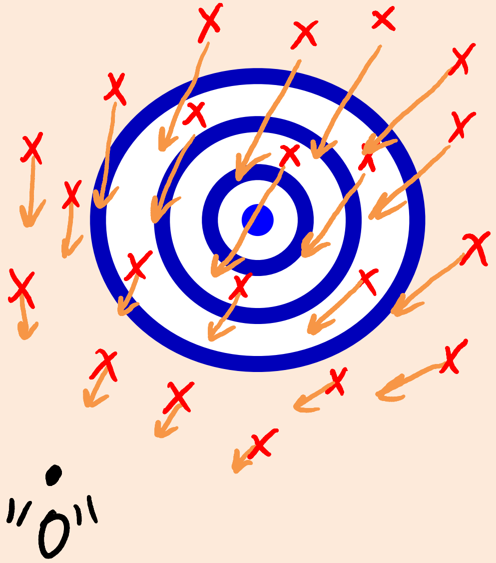

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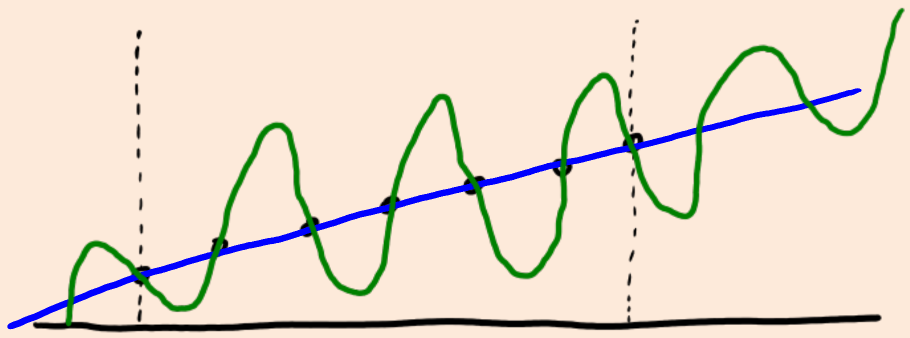

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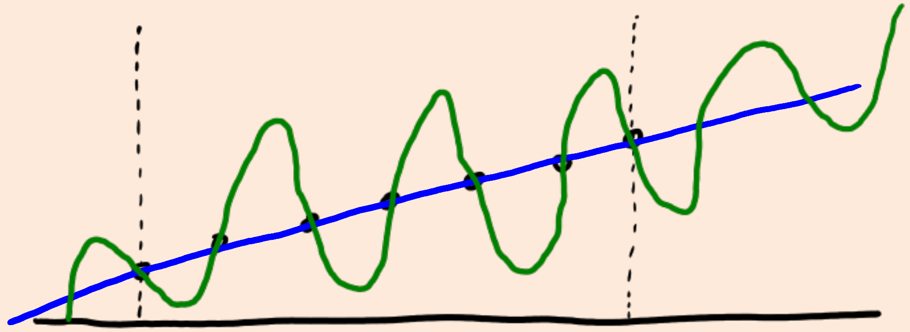

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- No free lunch theorem:
  - There *exists possible datasets* where you should select the green model.