

CPSC 340: Machine Learning and Data Mining

Regularization

Fall 2021

Admin

- Midterm is Thursday, October 21st, 6-7:30pm.
 - On Canvas, take it anywhere, but [SCRF 100 is available](#).
 - Swipe into the main door (off Main Mall), since it's after 5pm.
 - 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 **two types of questions on the midterm:**
 - Multiple choice questions that might be conceptual or more technical/specific.
 - Written questions involving code and/or math.
 - See the 2020W2 midterm which was in the same format (except 50 min)
 - Older midterms are good practice too!

Last Time: Feature Selection

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

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

A handwritten diagram showing a matrix X with two columns of zeros. A blue curly brace groups the two columns, with the word "relevant" written below it in blue, indicating that both features are 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 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.

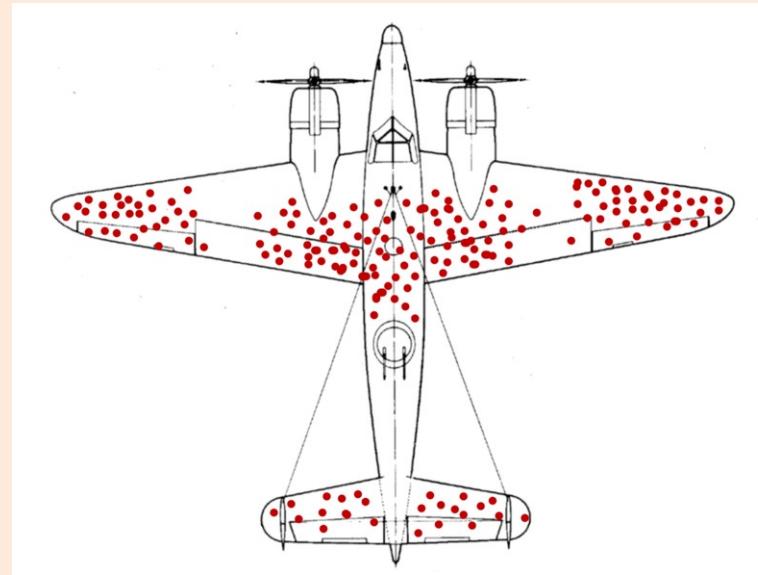
My advice if you want the “relevant” variables.

- Try the association approach.
- Maybe try forward selection with different values of λ .
- Try out a few other feature selection methods (Lasso – Wednesday!).
- 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.

bonus!

Related: Survivorship Bias

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

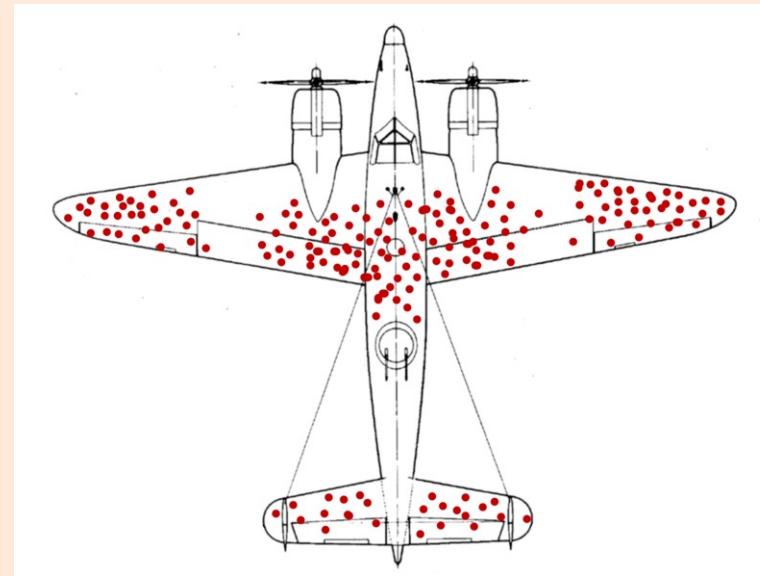


- Where are the “relevant” parts of the plane to protect?
 - “Relevant” parts are actually **where there are no bullets**.
 - **Planes shot in other places did not come back** (armor was needed).

bonus!

Related: Survivorship Bias

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

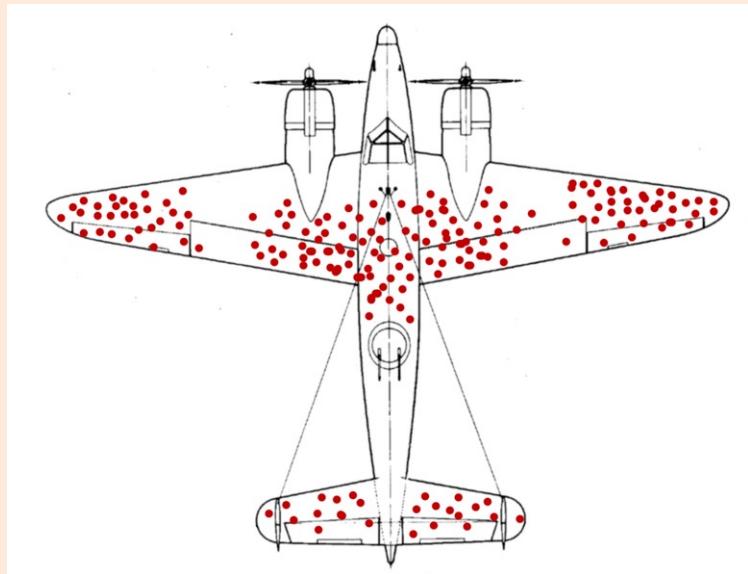


- This is an example of “survivorship bias”:
 - Data is not IID because you only sample the “survivors”.
 - Causes havoc for feature selection, and ML methods in general.

bonus!

Related: Survivorship Bias

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



- 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 people with the same traits.
 - Article hypothesizing about various topics (allergies, mental illness, etc.).

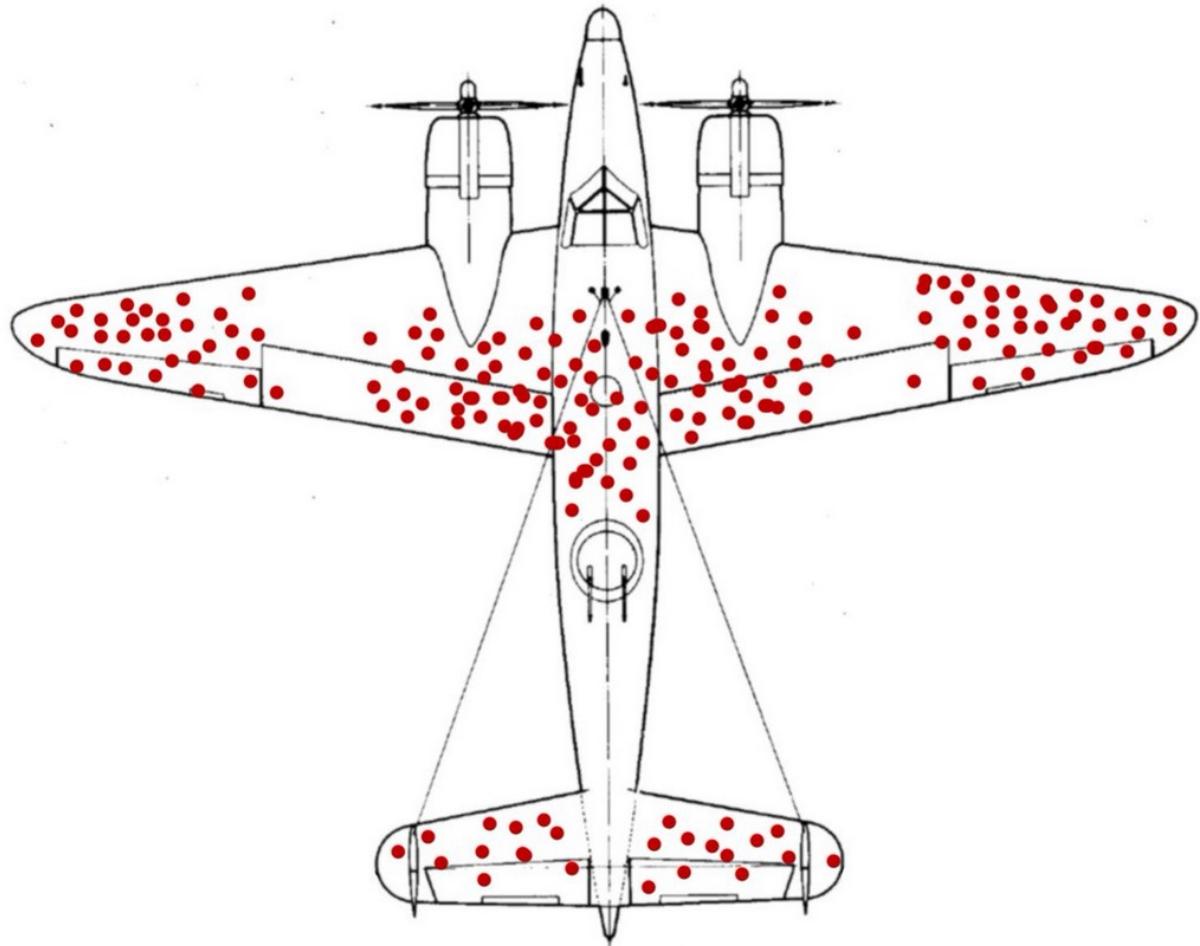


Jake VanderPlas
@jakevdp

...

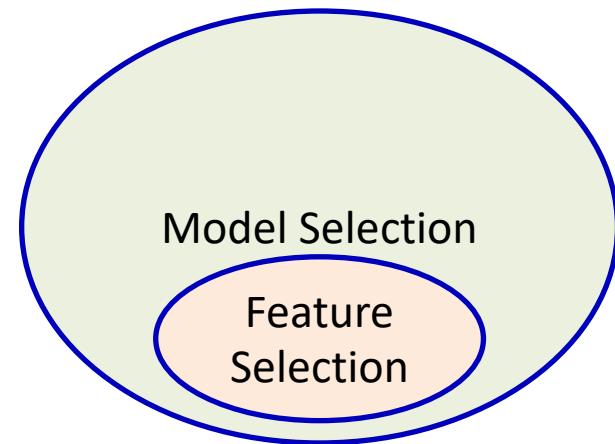
bonus!

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



“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.



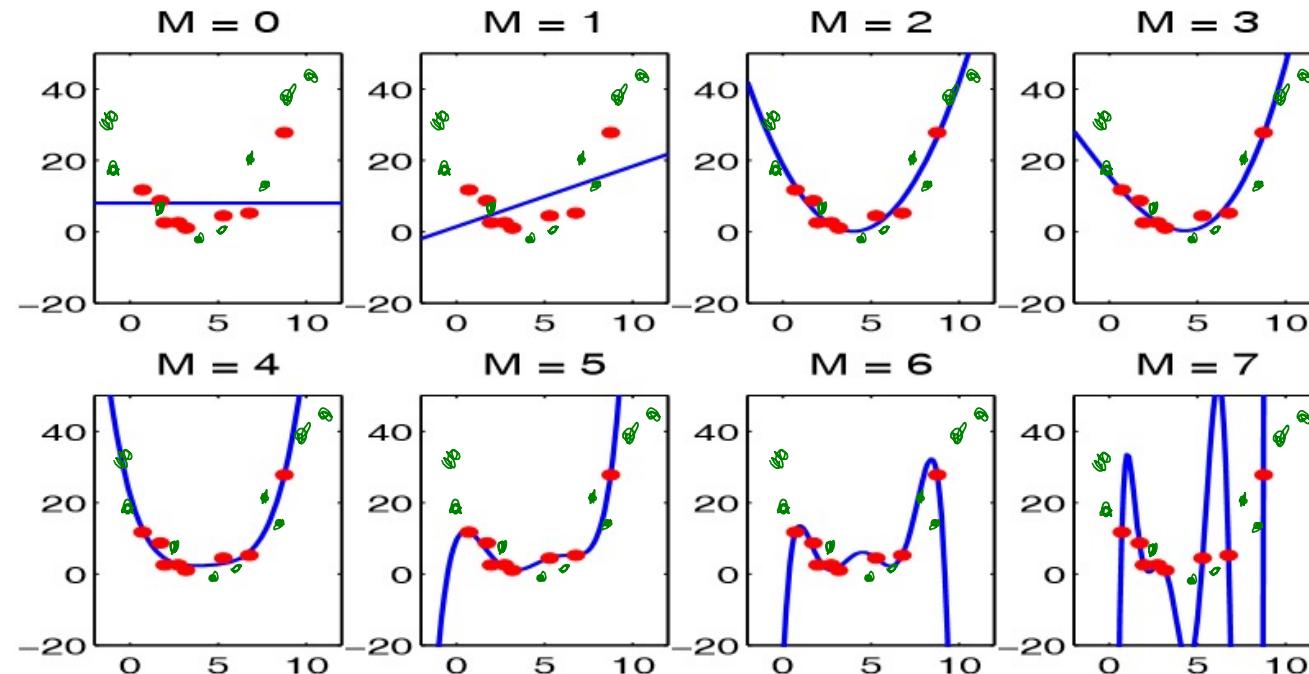
Can it help prediction to throw features away?

- 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.**



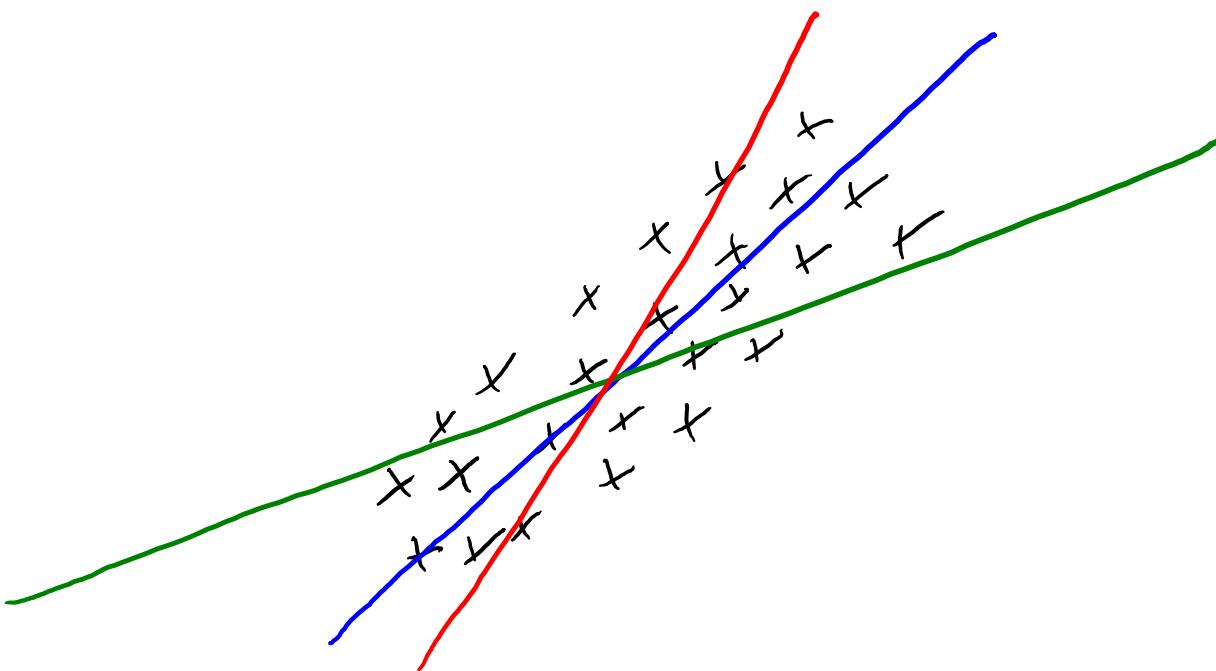
- But what if we **need** a complicated model?

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?

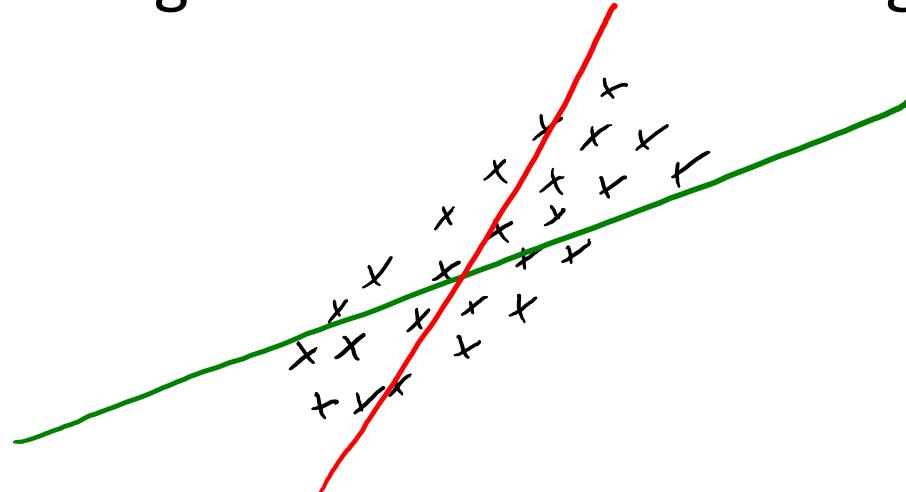
- Consider the following dataset and 3 linear regression models:



- Which line should we choose?

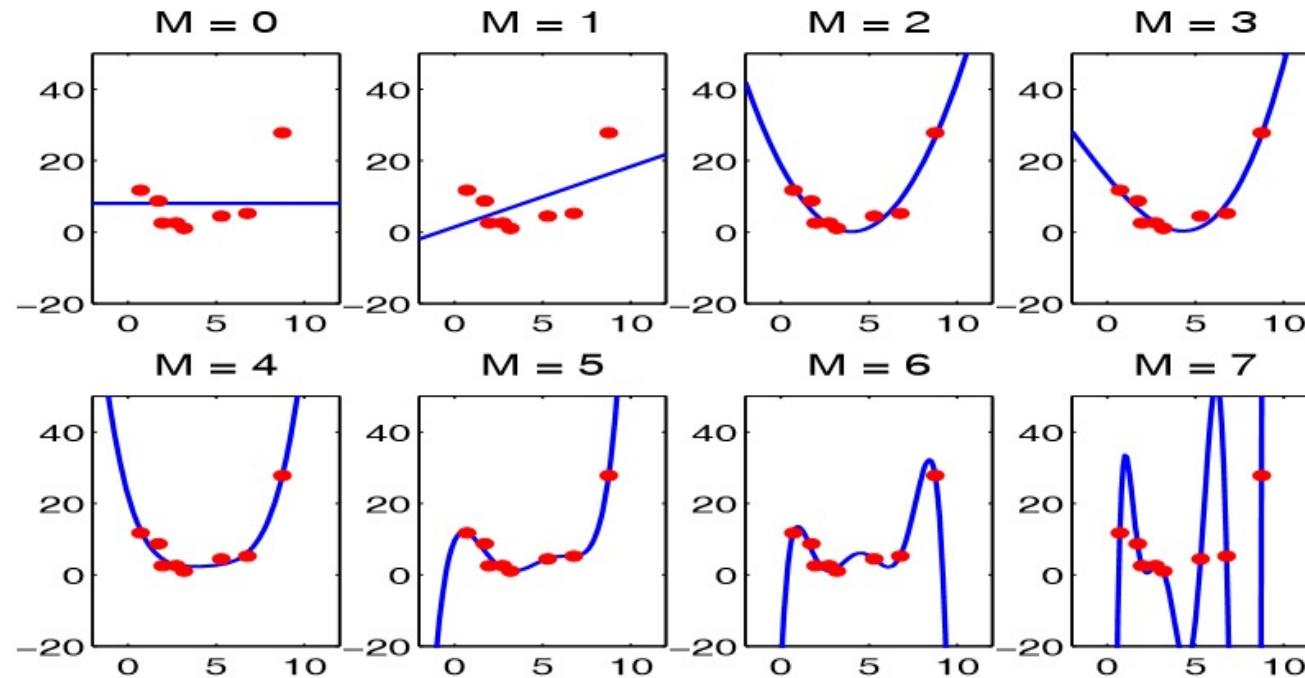
Would you rather?

- 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.

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

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 usually be $\Theta(\sqrt{n})$
 - 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

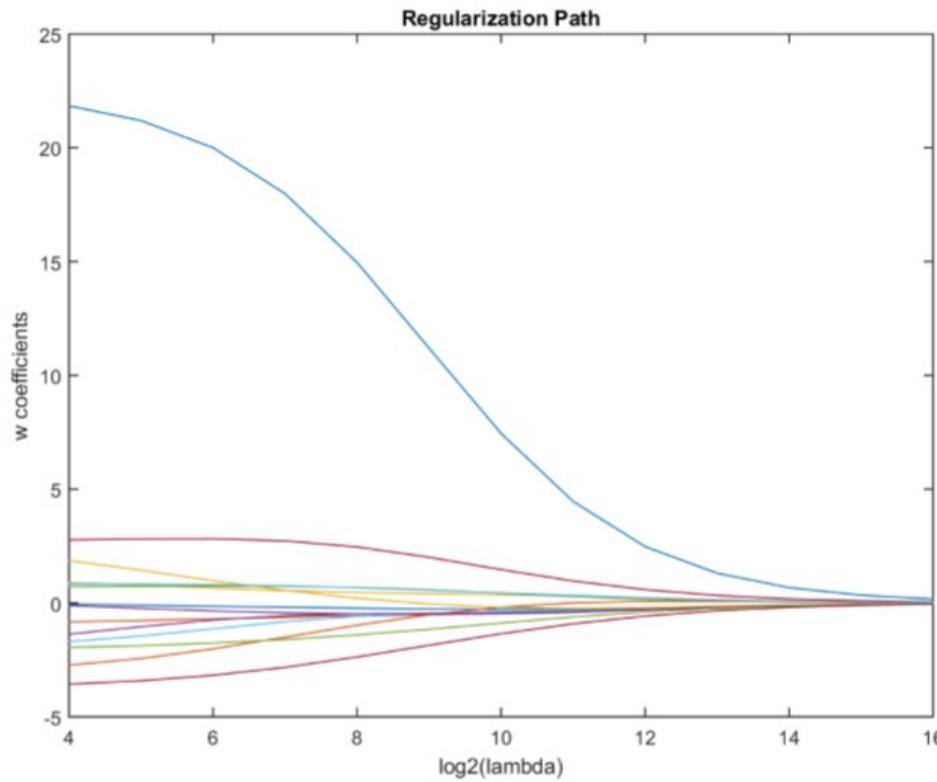
- Solution to a “least squares with L2-regularization” for different λ :

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
4096	-0.35	0.31	-0.42	0.18	-0.36	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 $\nabla f(w) = 0$** .
- 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: $w = (X^T X + \lambda I)^{-1} (X^T y)$

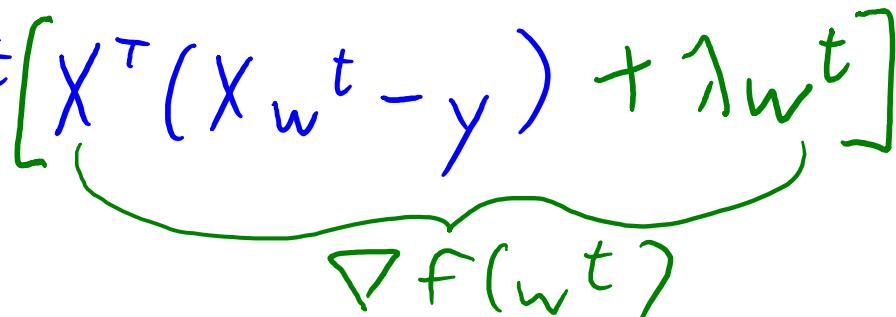
Gradient Descent for L2-Regularized Least Squares

- The L2-regularized least squares objective and gradient:

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

- Gradient descent iterations for L2-regularized least squares:

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



$\nabla f(w^t)$

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

bonus!

Why use L2-Regularization?

- The 340 Team™ 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. $X^T X$ 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:
 - $w_j^*(100 \text{ mL})$ gives the same model as $w_j^*(0.1 \text{ L})$ with a different w_j .

Features with Different Scales

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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 **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:

- Compute mean and standard deviation:

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

- 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.

$$X = \left[\begin{array}{c} \text{average of column 'j'} \\ \vdots \end{array} \right]$$

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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.

$$X = \left[\begin{array}{c} \text{average of column 'j'} \\ \vdots \end{array} \right]$$

Standardizing Target

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

Replace y_i 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/trig functions:

Use $\log(y_i)$ or $\exp(\gamma y_i)$

- Makes sense for geometric/exponential processes.

bonus!

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.

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

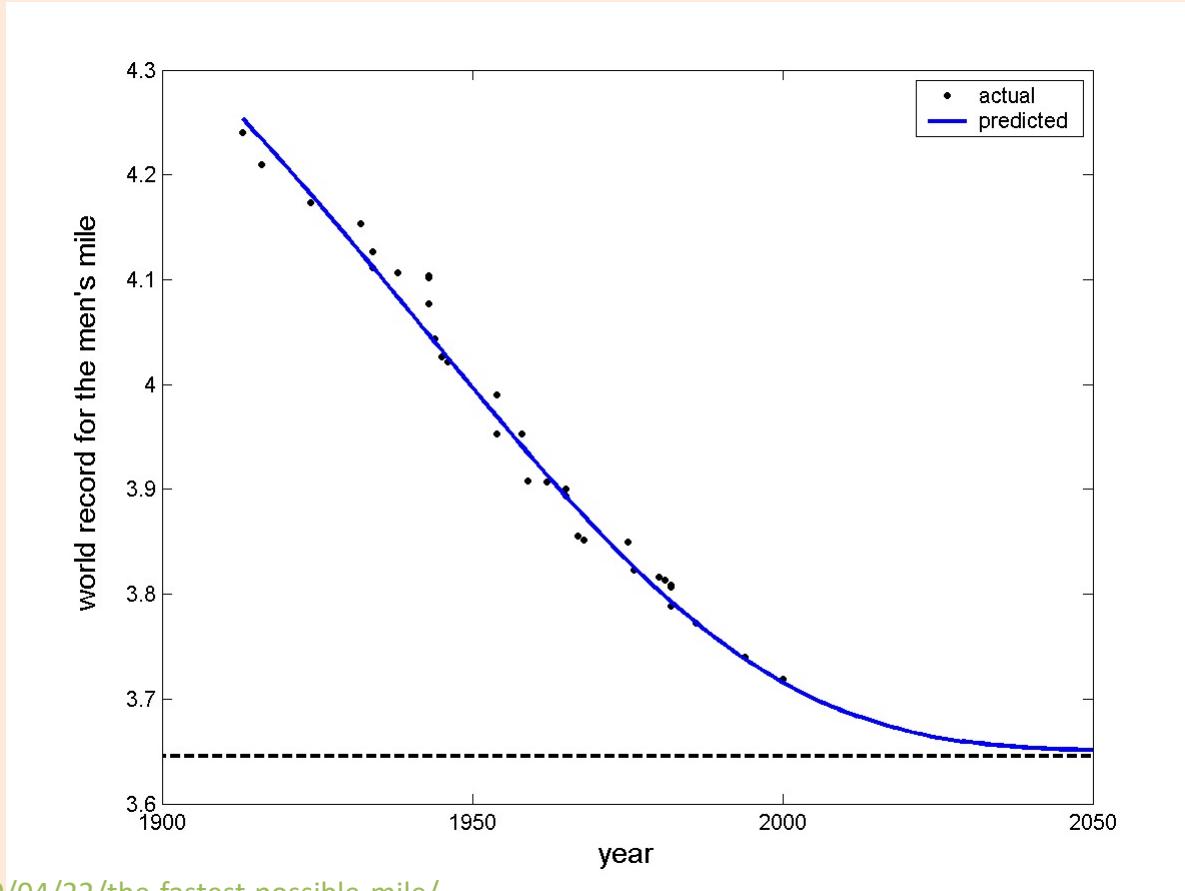
- With a constant z feature: replace 1 by $\text{sqrt}(\lambda/\lambda_0)$.
 - Don’t standardize it!

(pause)

bonus!

Predicting the Future

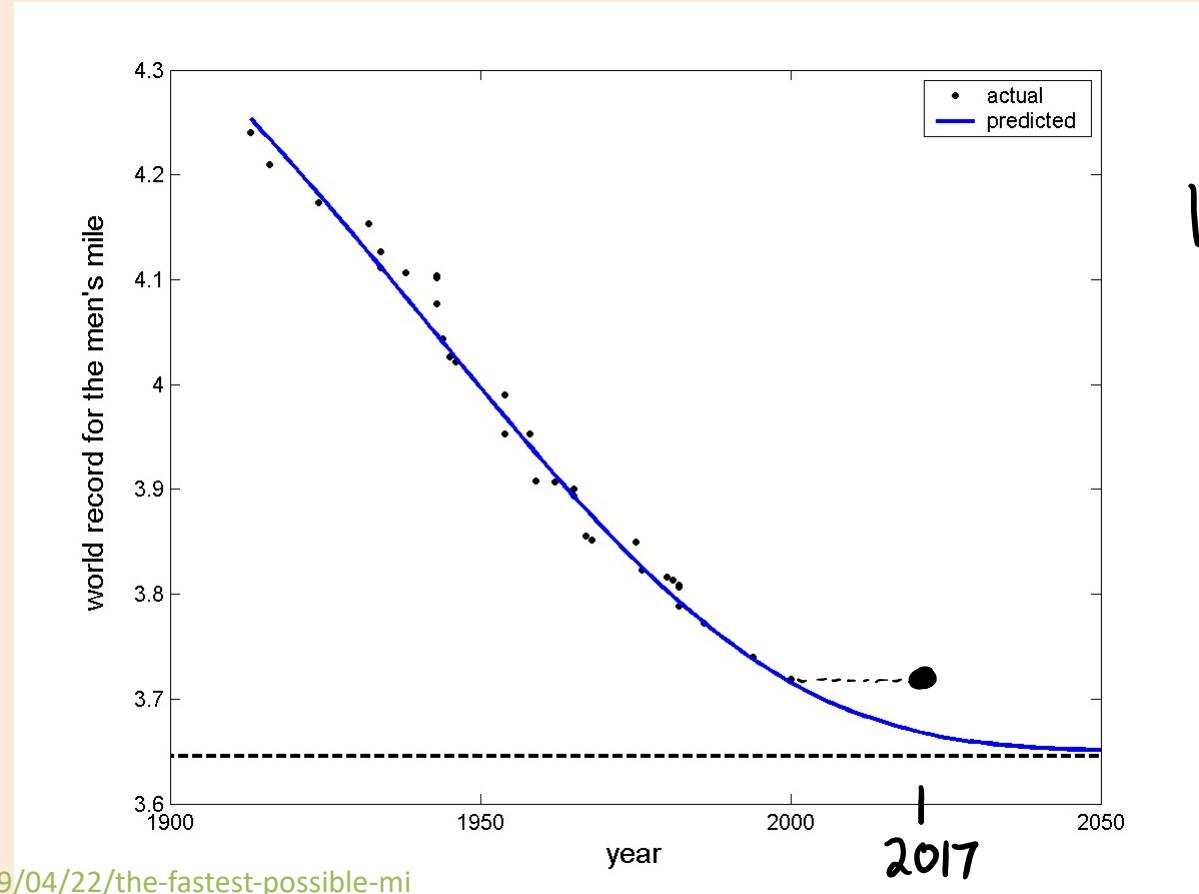
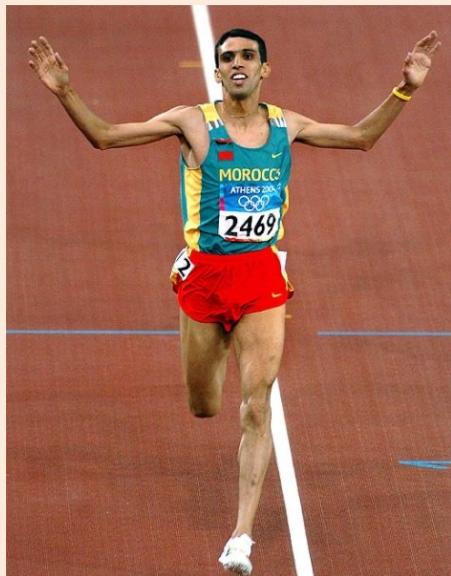
- In principle, we can use any features x_i that we think are relevant.
- This makes it tempting to use **time** as a feature, and predict future.



bonus!

Predicting the Future

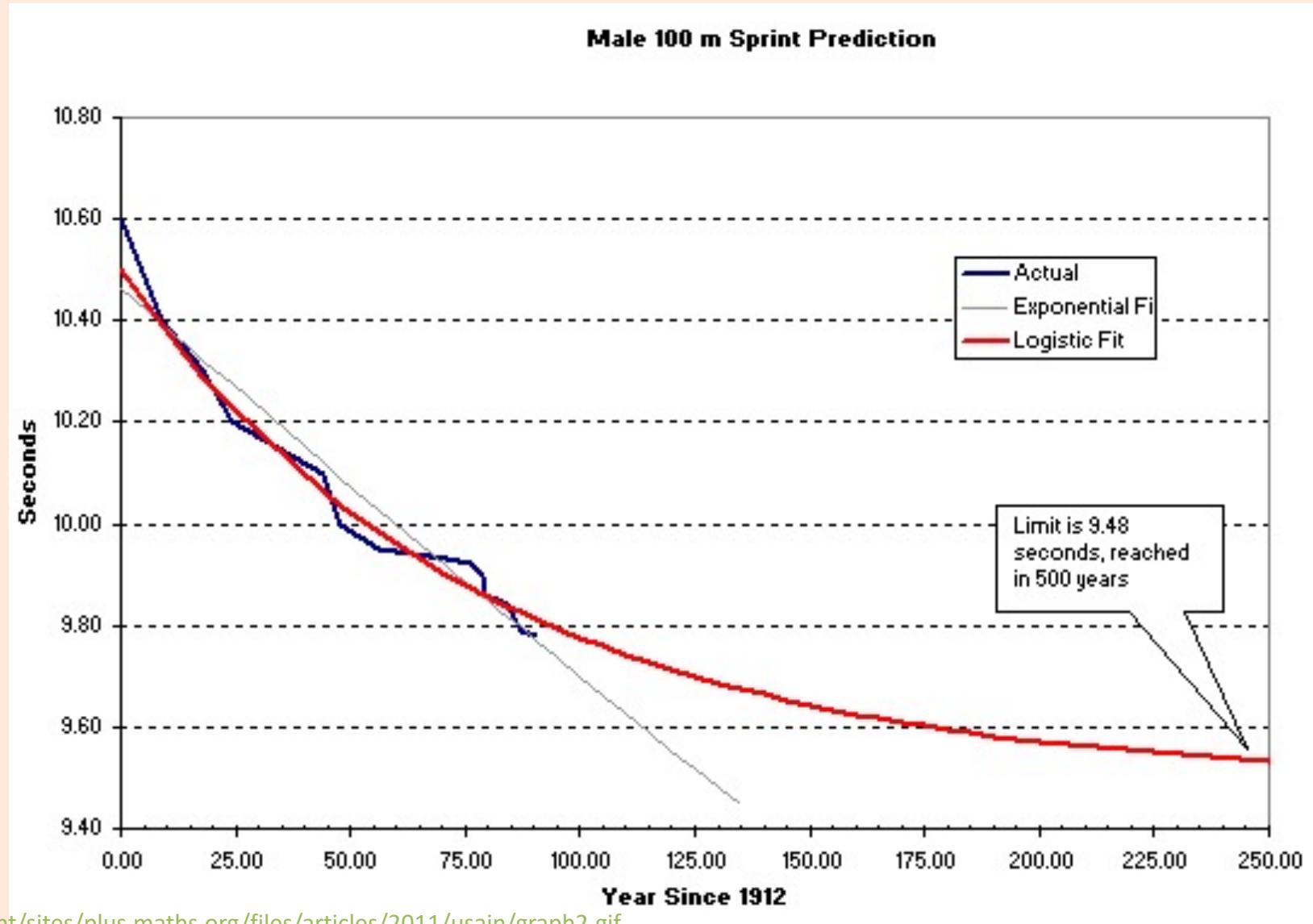
- In principle, we can use any features x_i that we think are relevant.
- This makes it tempting to use **time as a feature**, and predict future.



We need to be
Cautious about
doing this.

Predicting 100m times 400 years in the future?

bonus!

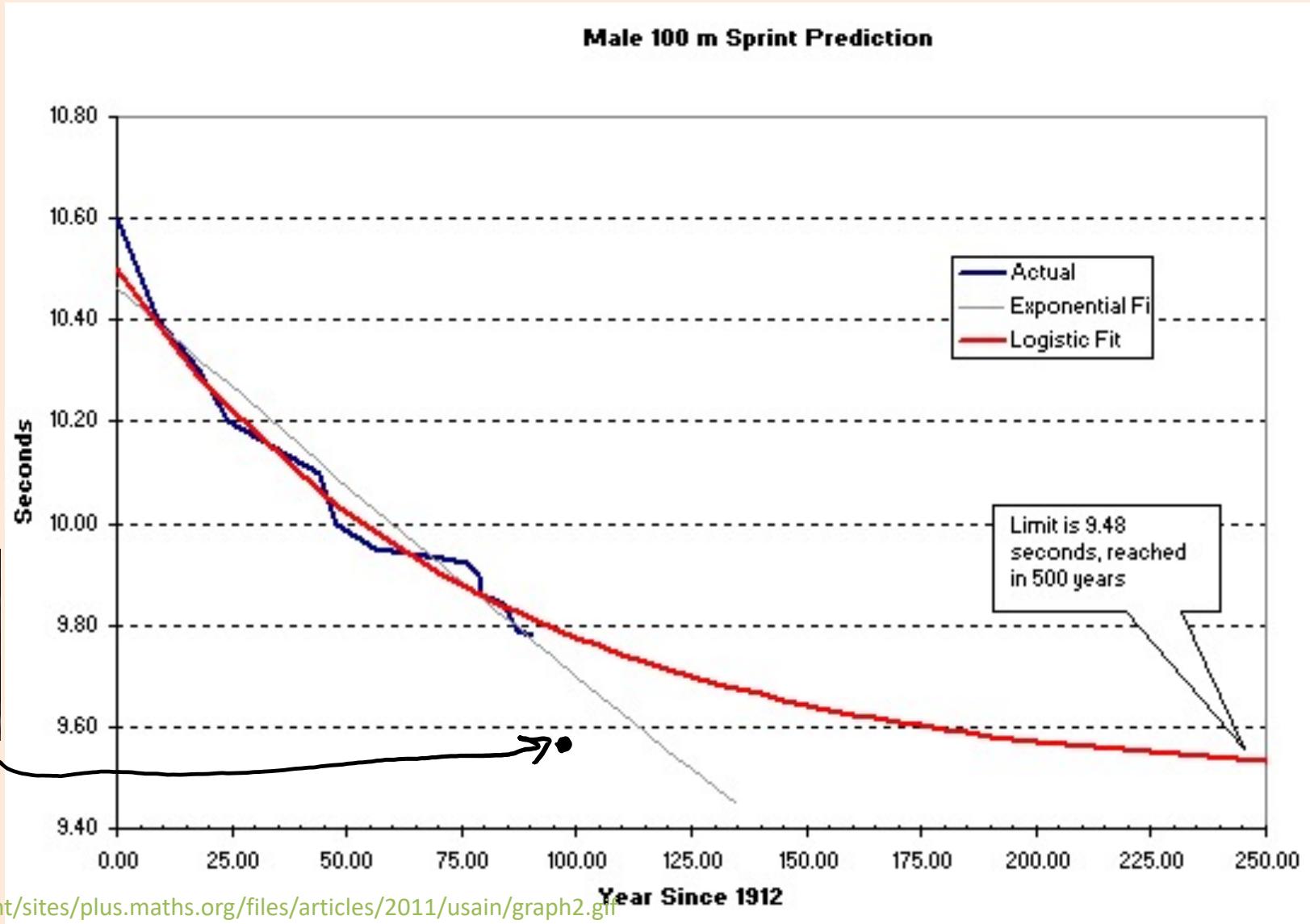


Predicting 100m times 400 years in the future?

bonus!



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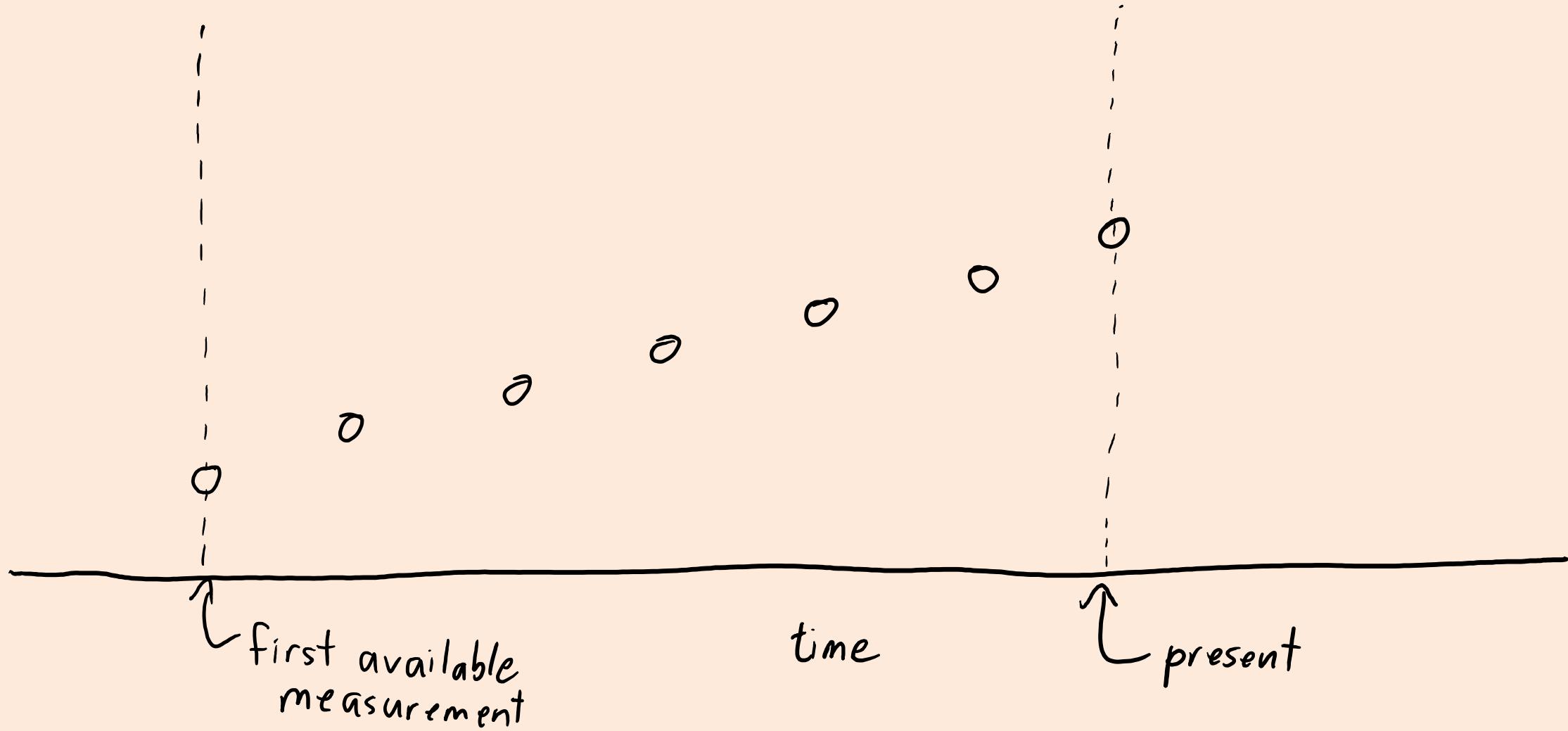
bonus!

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

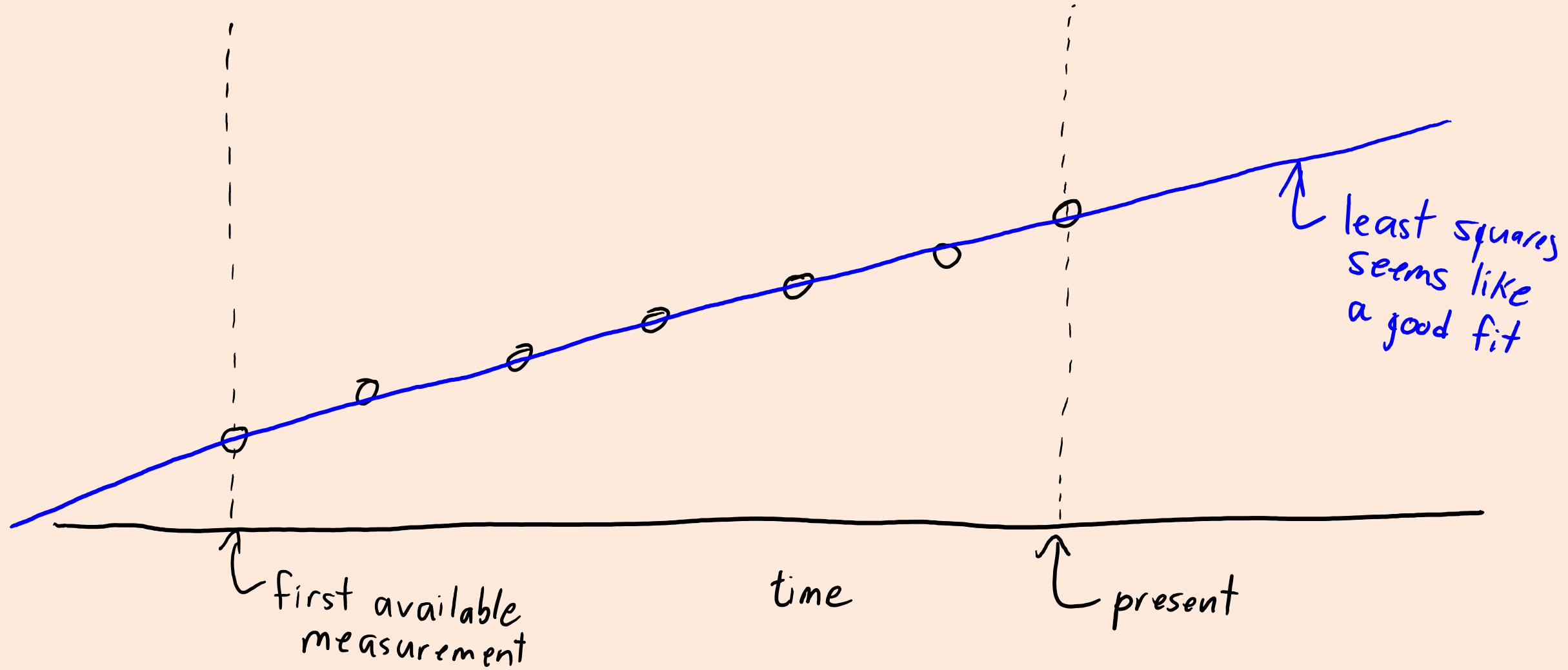
bonus!

No Free Lunch, Consistency, and the Future



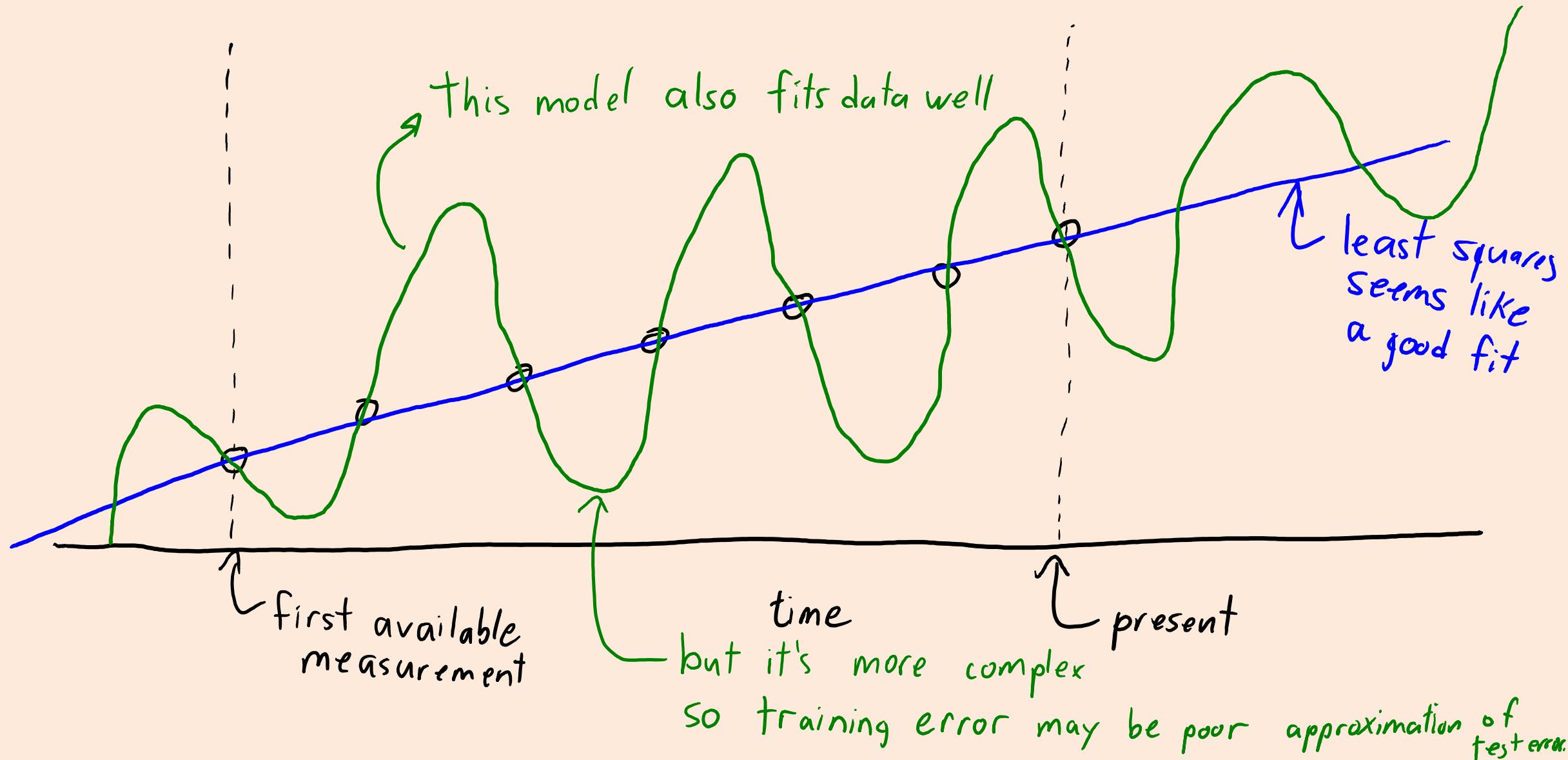
bonus!

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bonus!

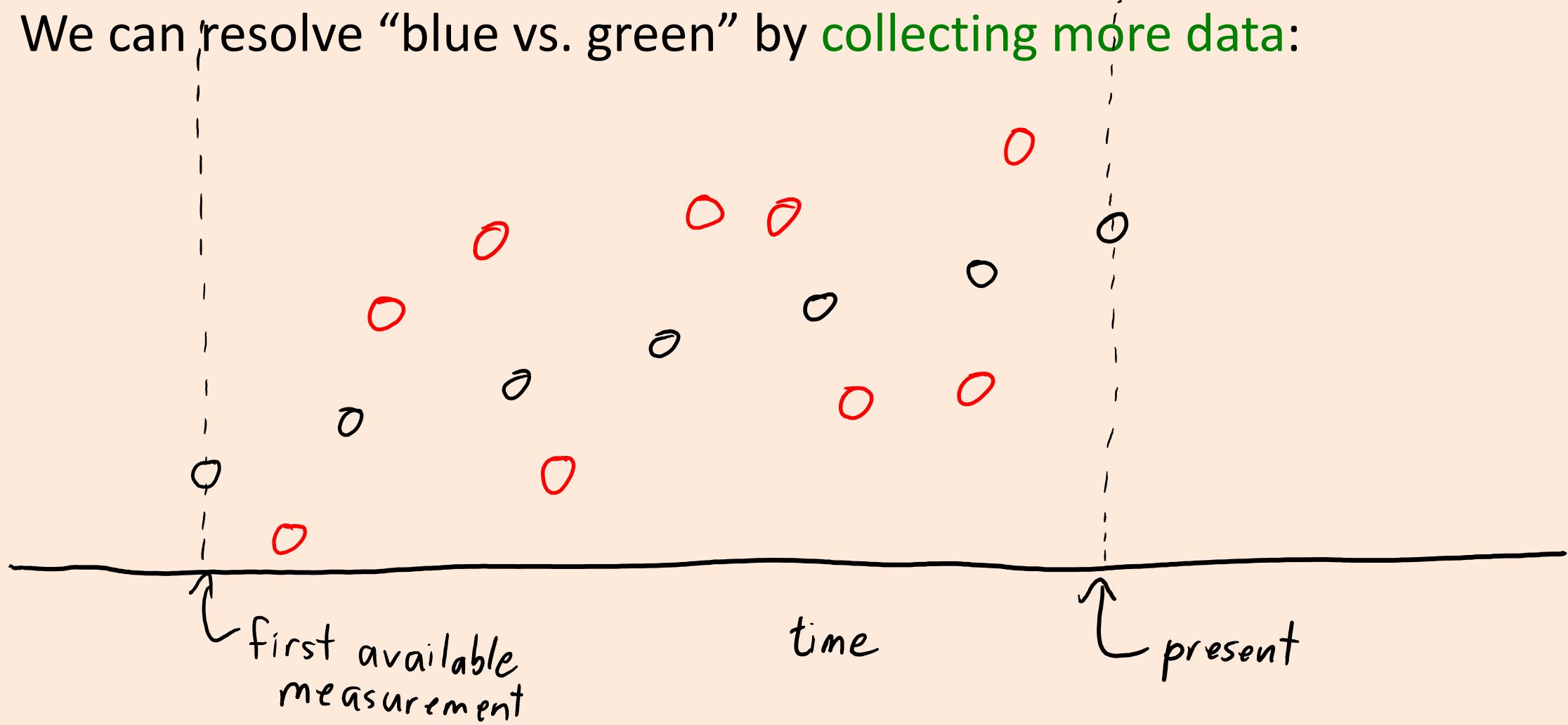
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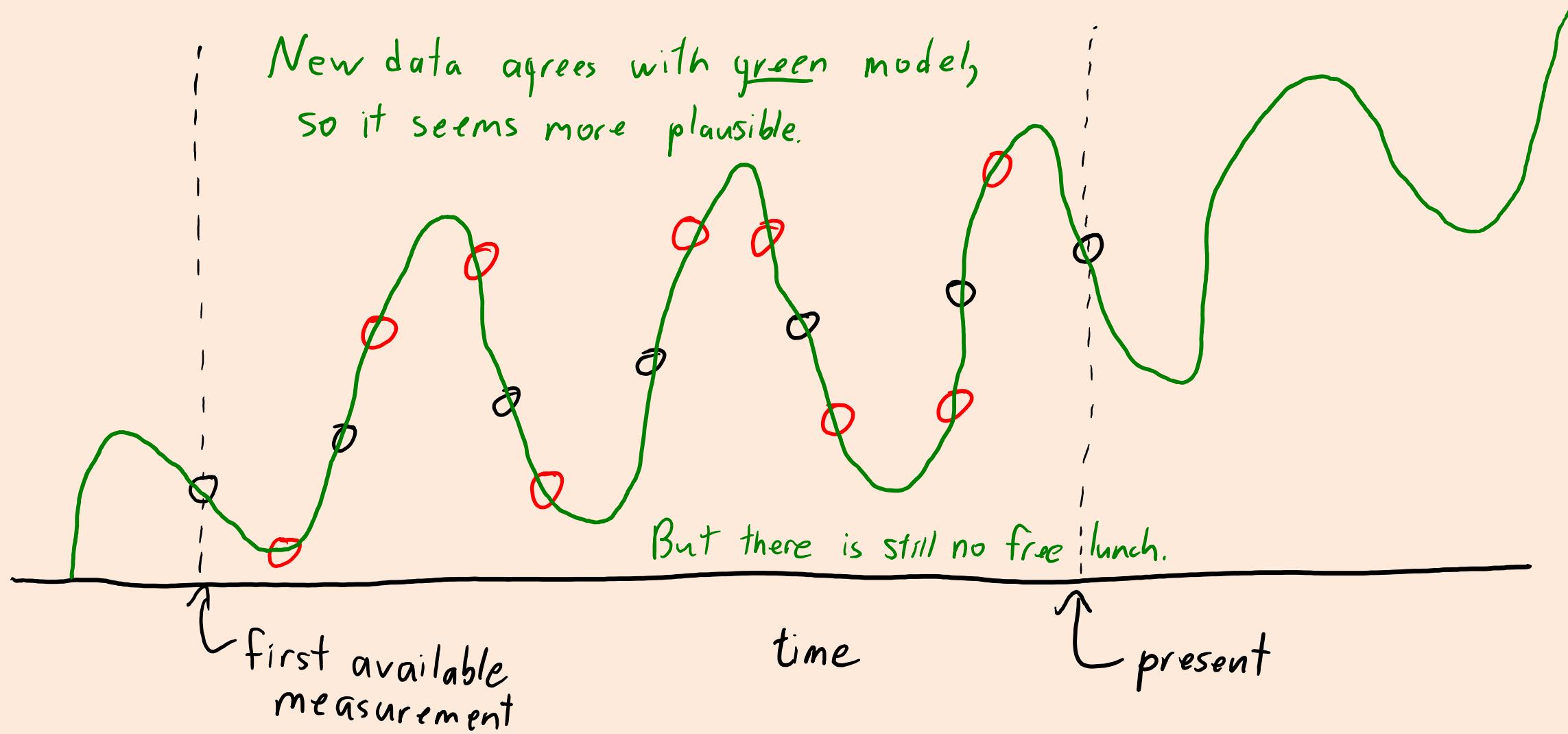
No Free Lunch, Consistency, and the Future

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



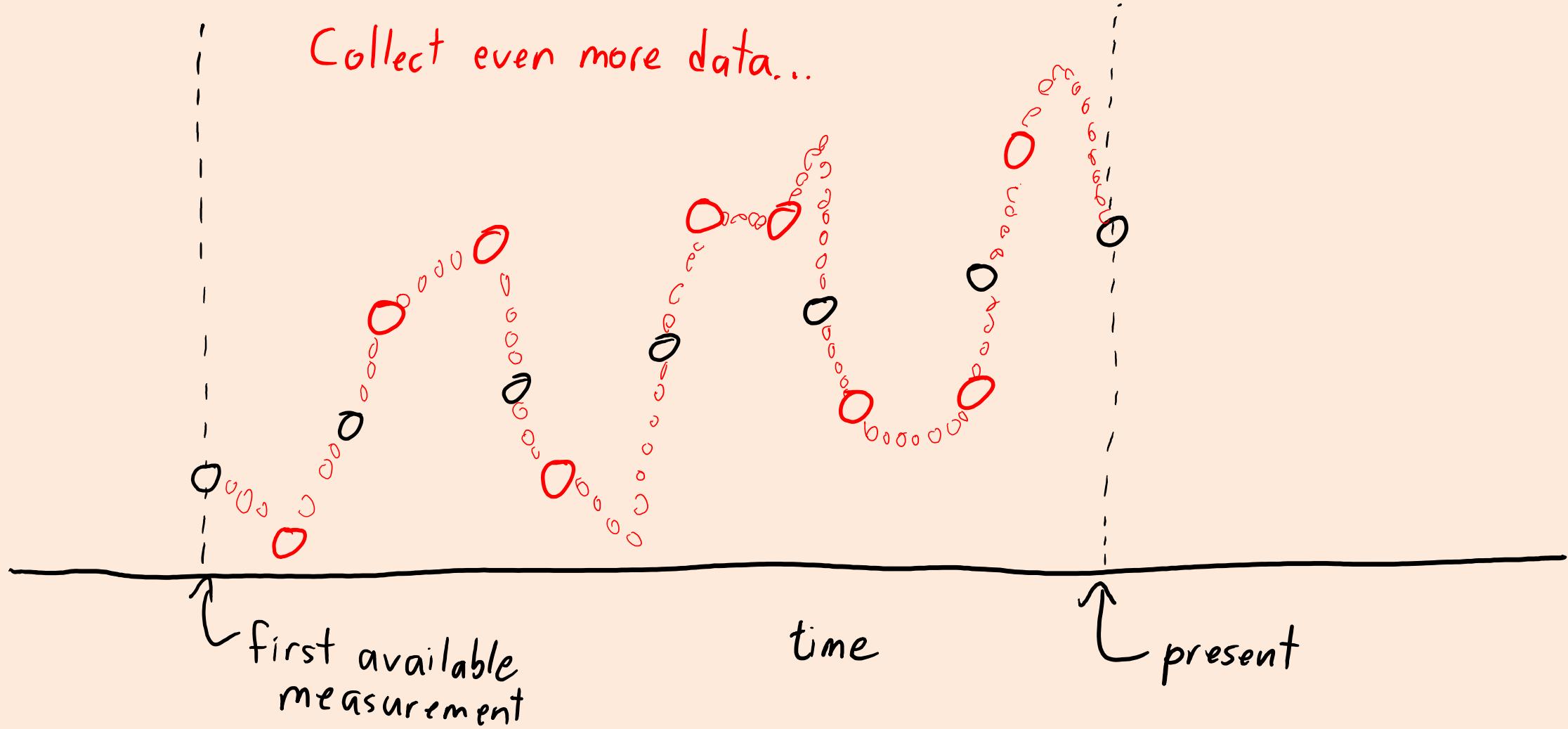
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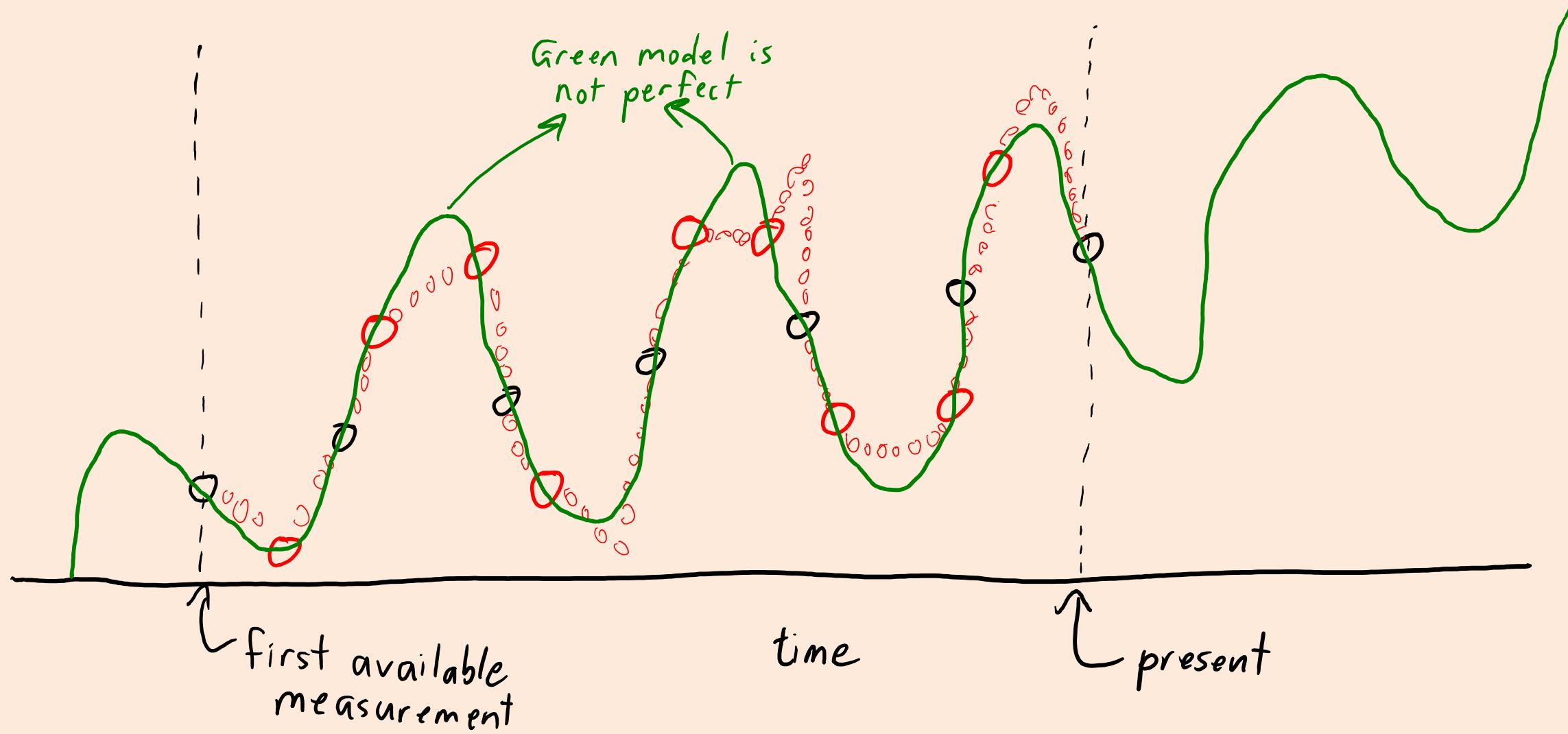
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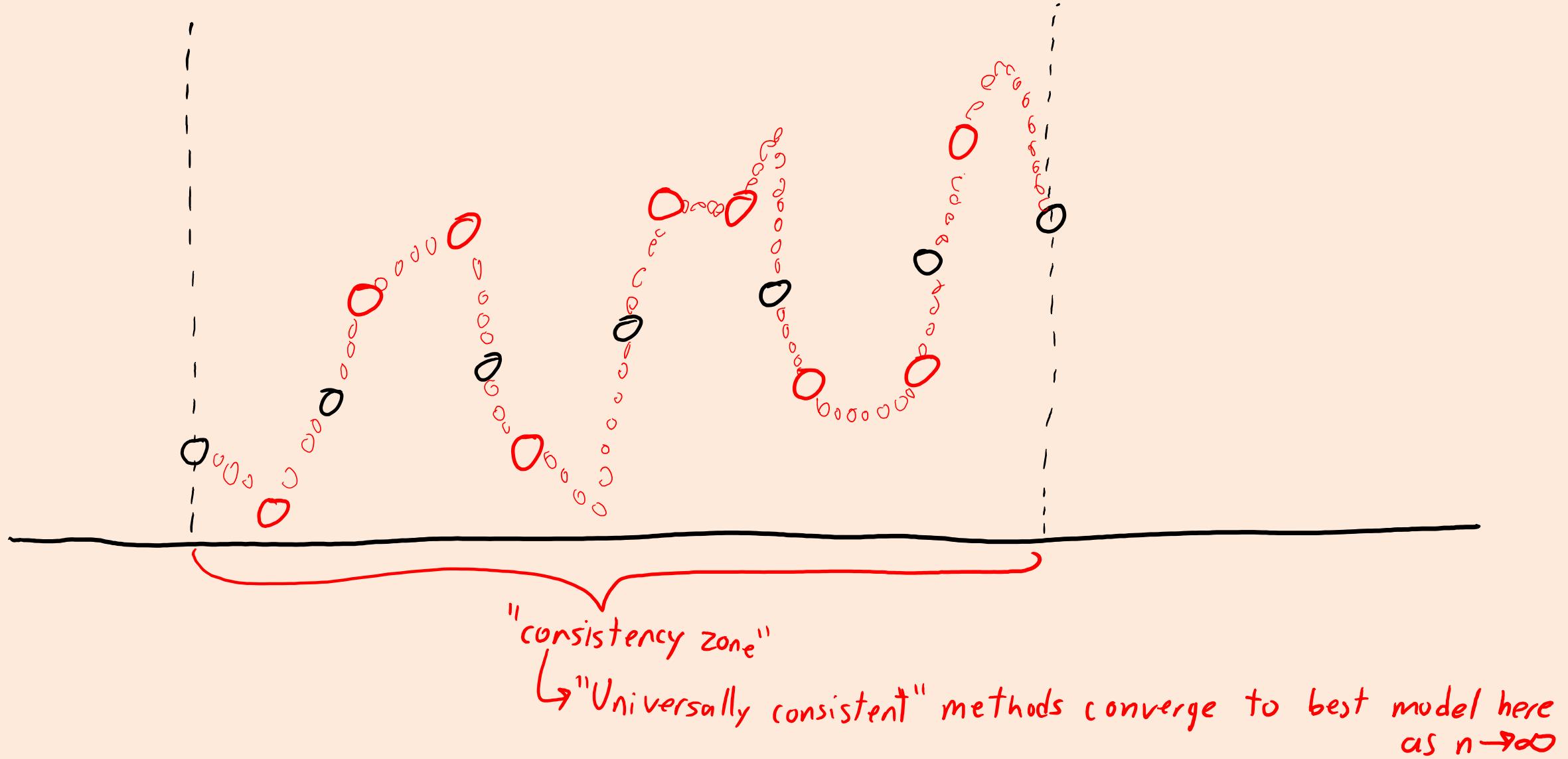
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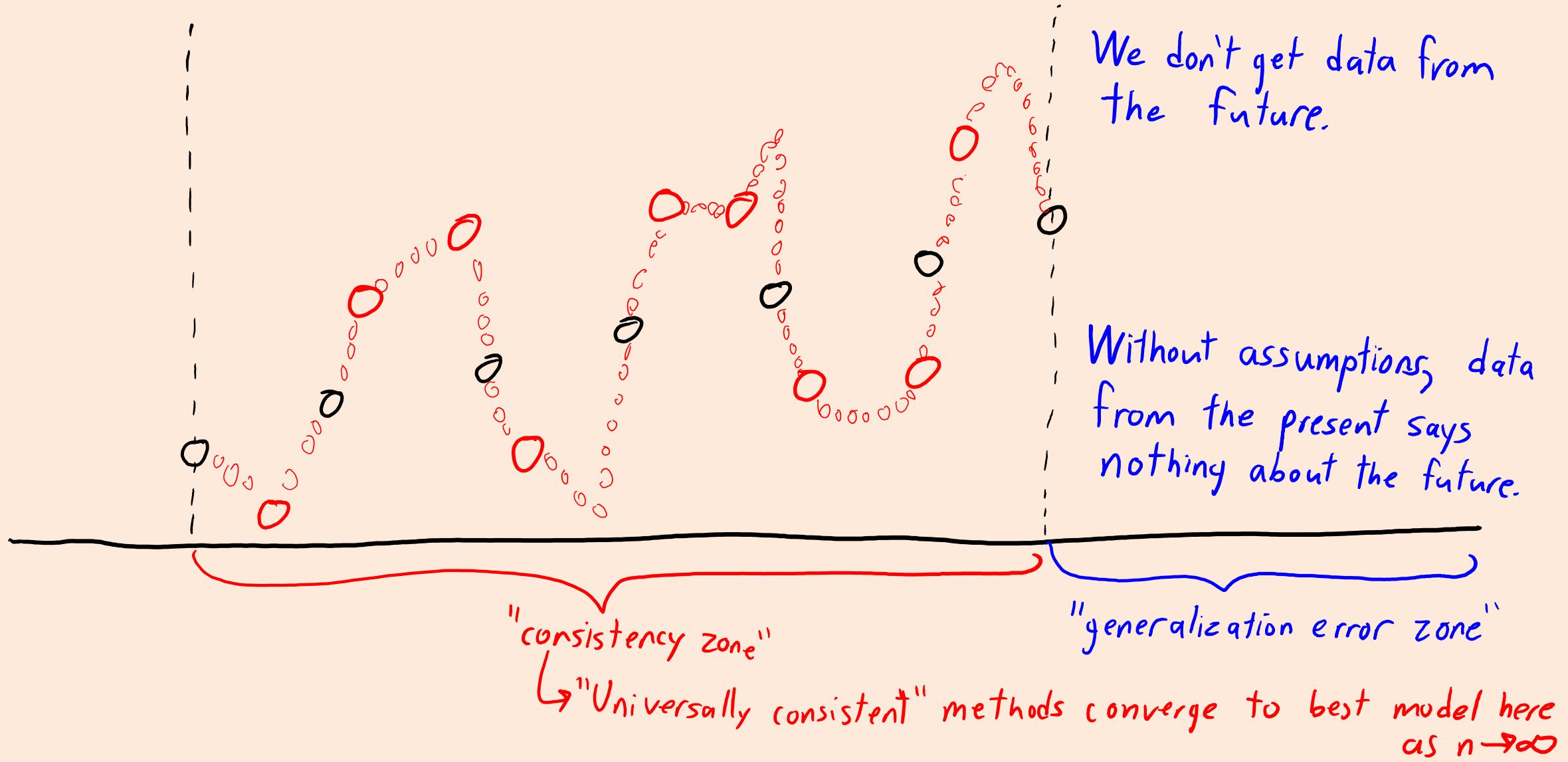
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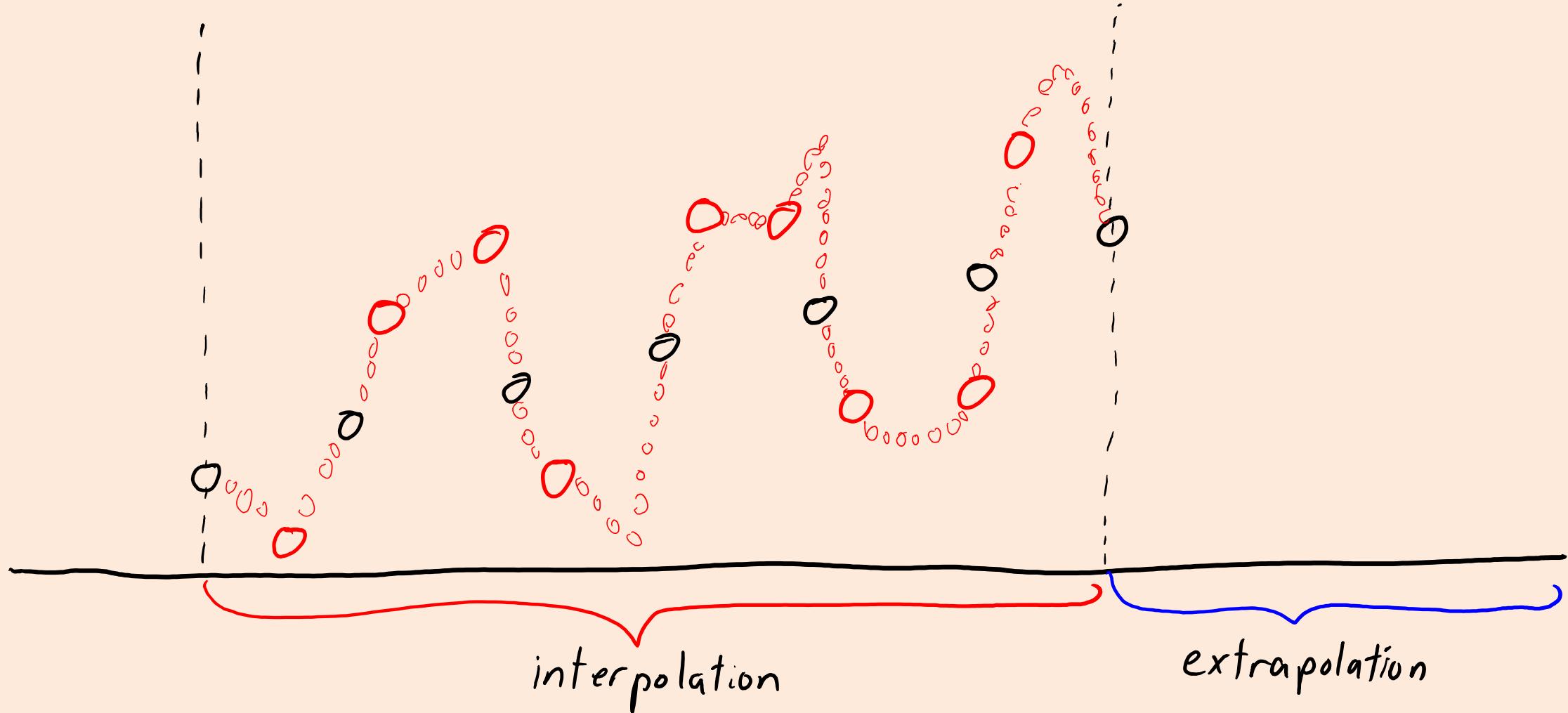
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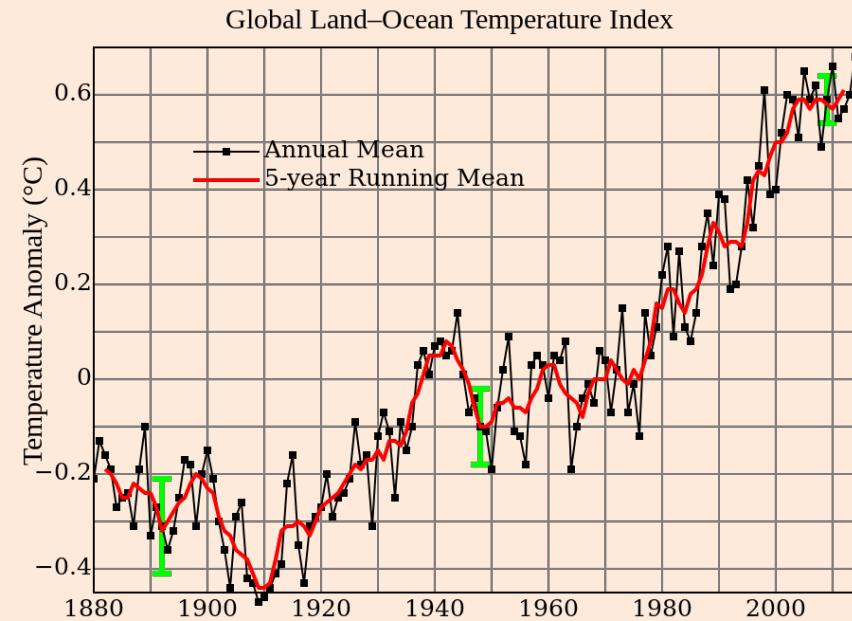
No Free Lunch, Consistency, and the Future



bonus!

Discussion: Climate Models

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

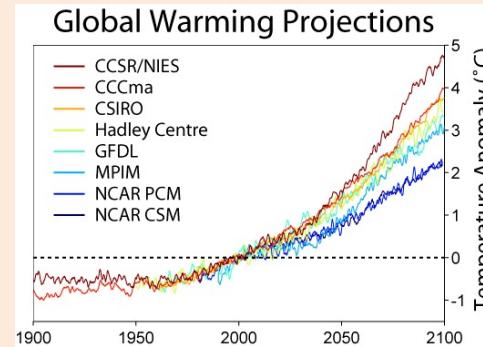


- Will Earth continue to warm over next 100 years? (generalization error)
 - We should be more skeptical about models that predict future events.

bonus!

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:

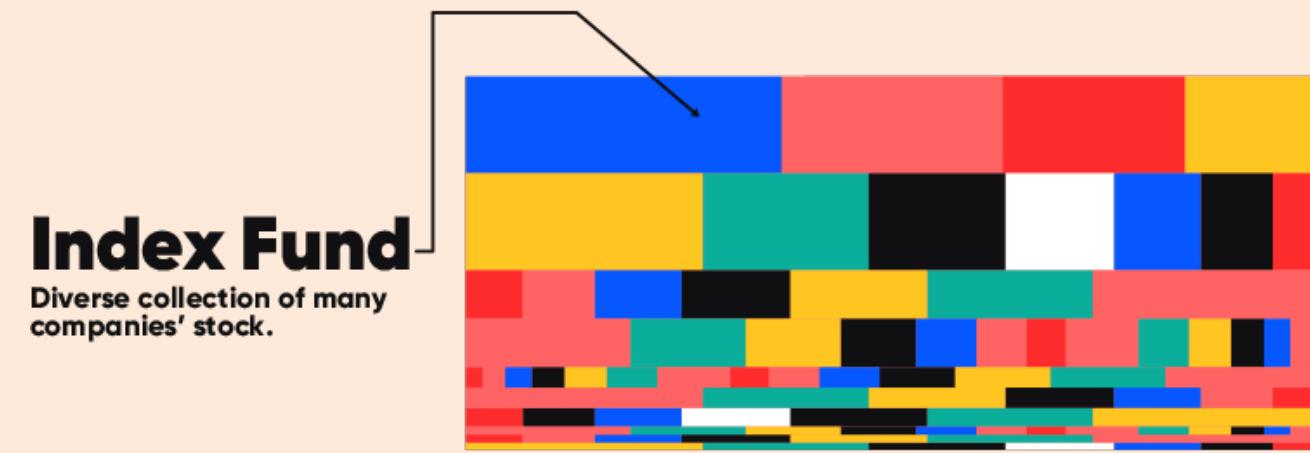


- We should be skeptical of individual models, but agreeing predictions made by models with different data/assumptions are more likely be true.
- All the near-future predictions agree, so they are likely to be accurate.
 - And it's probably reasonable to assume fairly **continuous change** (no big “jumps”).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

Index Funds: Ensemble Extrapolation for Investing

bonus!

- 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.



GOAL = Match the Market (Index)



- This simple investing strategy **outperforms most fund managers.**

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.

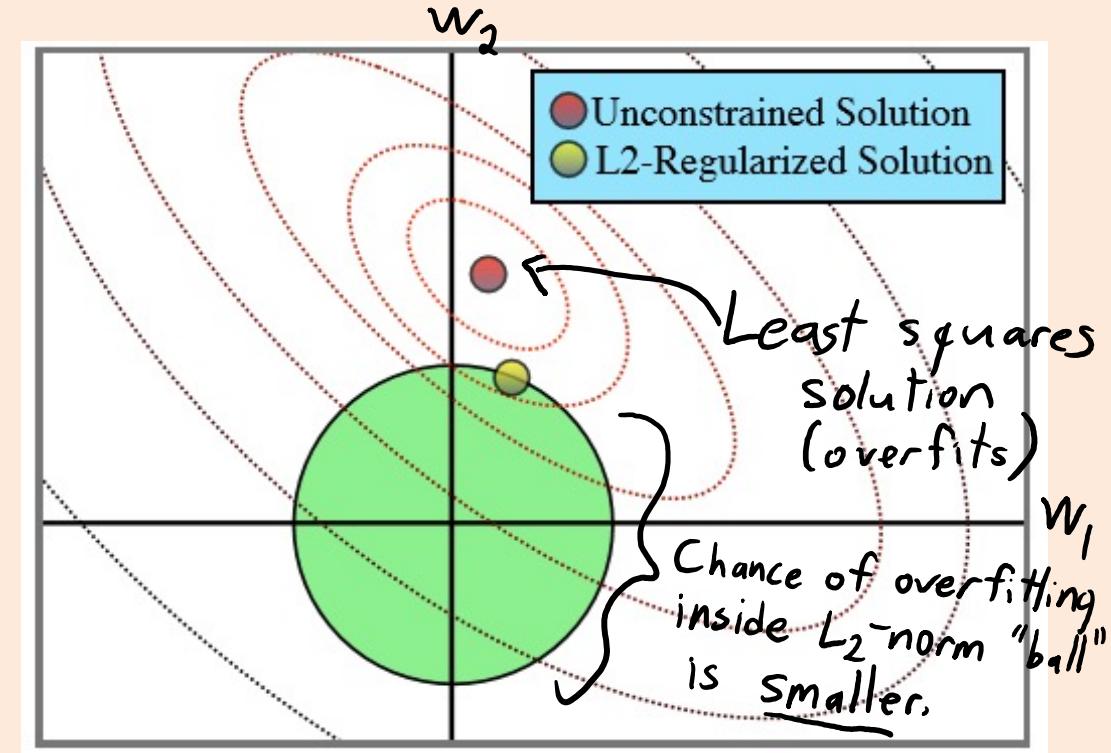
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L2-Regularization

- Standard **regularization** strategy is **L2-regularization**:

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

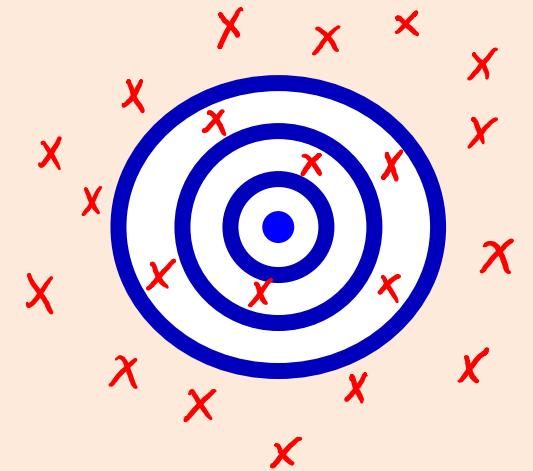
- Equivalent to minimizing squared error but keeping L2-norm small.



bonus!

Regularization/Shrinking Paradox

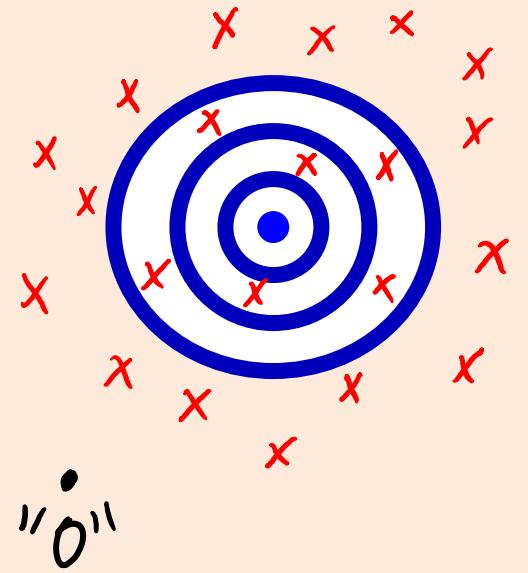
- We throw darts at a target:
 - Assume we don't always hit the exact center.
 - Assume the darts follow a symmetric pattern around center.



bonus!

Regularization/Shrinking Paradox

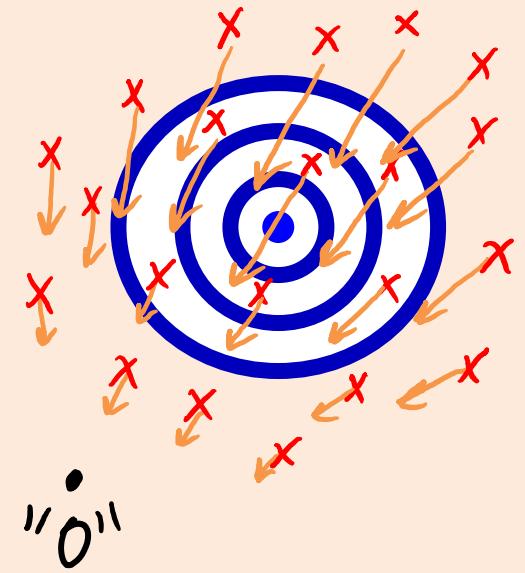
- We throw darts at a target:
 - Assume we don't always hit the exact center.
 - Assume the darts follow a symmetric pattern around center.
- Shrinkage of the darts :
 1. Choose some **arbitrary** location '0'.
 2. Measure distances from darts to '0'.



bonus!

Regularization/Shrinking Paradox

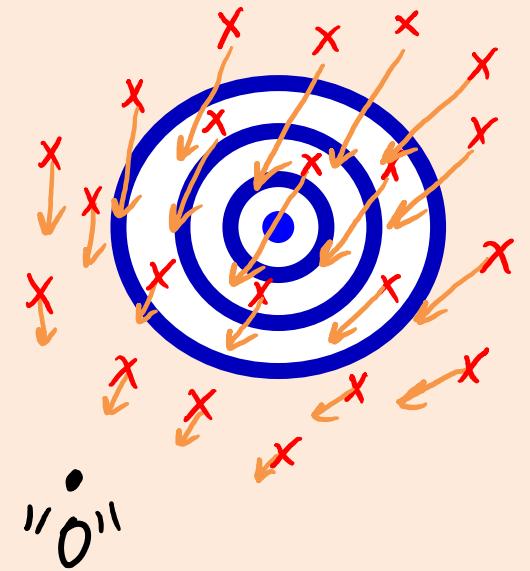
- We throw darts at a target:
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 1. Choose some **arbitrary** location '0'.
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 3. **Move misses towards '0'**, by *small* amount proportional to distance from 0.
- If small enough, **darts will be closer to center on average.**



bonus!

Regularization/Shrinking Paradox

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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>

bonus!

Occam's Razor vs. No Free Lunch

- Occam'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.

