CPSC 340: Machine Learning and Data Mining

More Regularization

Original version of these slides by Mark Schmidt, with modifications by Mike Gelbart.

Admin

- Assignment 3
  - Due tonight

- Midterm
  - Feb 14 in class (this is the next time we'll meet because of Monday holiday)
  - If your surname starts with the letters A-G, room DMP 201
  - If your surname starts with the letters H-Z, room DMP 110 (this room)
  - Plenty of practice exams on course homepage
  - Extra office hours added on Tuesday (see calendar)

- Tutorials
  - Cancelled next week (due to Monday holiday)

Last Time: L2-Regularization

- We discussed regularization:
  - Adding a continuous penalty on the model complexity:

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

  - Best parameter λ almost always leads to improved test error.
    - L2-regularized least squares is also known as "ridge regression".
    - Can be solved as a linear system like least squares.
  - Numerous other benefits:
    - Solution is unique, less sensitive to data, gradient descent converges faster.

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

- 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 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

$X = \left[\quad 0 \quad \right]$

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:

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

  - Now changes in 'w_j' have similar effect for any feature 'j'.
- Should we regularize the y-intercept?
  - No! The y-intercept can be anywhere, why encourage it to be close to zero?
  - Yes! Regularizing all variables makes solution unique and it easier to compute 'w'.
  - Compromise: regularize the bias by a smaller amount than other variables?

$\hookrightarrow \frac{1}{2}\|Xw - y\|^2 + \sum_{j=1}^{d} \lambda_j w_j$ (λ_j small for bias)

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.
- 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.

(pause)

RBFs, Regularization, and Validation

- Radial basis functions (RBFs):
  - With 'n' data points RBFs have 'n' basis functions.
- How do we avoid overfitting with this huge number of features?
  - We regularize 'w' and use validation error to choose σ and λ.
- A model that is hard to beat:
  - RBF basis with L2-regularization and cross-validation to choose σ and λ.
  - Flexible non-parametric basis, magic of regularization, and tuning for test error!
  - Can add bias or linear/poly basis to do better away from data.
  - But expensive at test time: needs distance to all training examples.

Hyperparameter Optimization

- In this setting we have 2 hyperparameters (σ and λ).
- More complicated models have even more hyperparameters.
  - This makes searching all values expensive (and increases overfitting risk).

- Leads to the problem of hyperparameter optimization.
  - Try to efficiently find "best" hyperparameters.

- Simplest approaches:
  - Exhaustive search: try all combinations among a fixed set of σ and λ values.
    - In scikit-learn, GridSearchCV
  - Random search: try random values.
    - In scikit-learn, RandomizedSearchCV

Hyperparameter Optimization (bonus slide)

- Other common hyperparameter optimization methods:
  - Coordinate search:
    - Optimize one hyperparameter at a time, keeping the others fixed.
    - Repeatedly go through the hyperparameters
  - Generic global optimization methods:
    - simulated annealing, genetic algorithms, etc.
  - Bayesian optimization (Mike's PhD topic):
    - Use regression to build model of how hyper-parameters affect validation error.
    - Try the best guess based on the model.
    - Tends to be worth the hassle if each function evaluation is very expensive (slow).
- See bonus slides for a list of hyperparameter optimization software

(pause)

Previously: Search and Score

- We talked about search and score for feature selection:
  - Define a "score" and "search" for features with the best score.
- Usual scores count the number of non-zeroes ("L0-norm"):

$$f(w) = \frac{1}{2}\|X_w - y\|^2 + \lambda \underbrace{\|w\|_0}_{\text{number of non-zeroes in 'w'}}$$

- But it's hard to find the 'w' minimizing this objective.
- We discussed forward selection, but requires fitting $O(d^2)$ models.

L1-Regularization

- Consider regularizing by the L1-norm:

$$f(w) = \frac{1}{2}\|Xw - y\|^2 + \lambda\|w\|_1$$

- Like L2-norm, it's convex and improves our test error.
- Like L0-norm, it encourages elements of 'w' to be exactly zero.

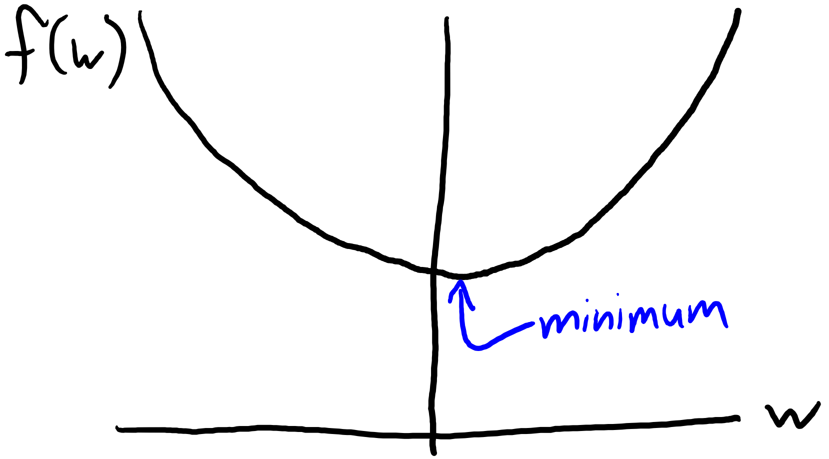
- L1-regularization simultaneously regularizes and selects features.
  - Very fast alternative to search and score.
  - Sometimes called "LASSO" regularization.

Sparsity and Least Squares

- Consider 1D least squares objective:

$$f(w) = \frac{1}{2}\sum_{i=1}^{n}(w x_i - y_i)^2$$

- This is a convex 1D quadratic function of ‘w’ (i.e., a parabola):



$f'(0) = 0$ only happens if $y^T x = 0$ (bonus)

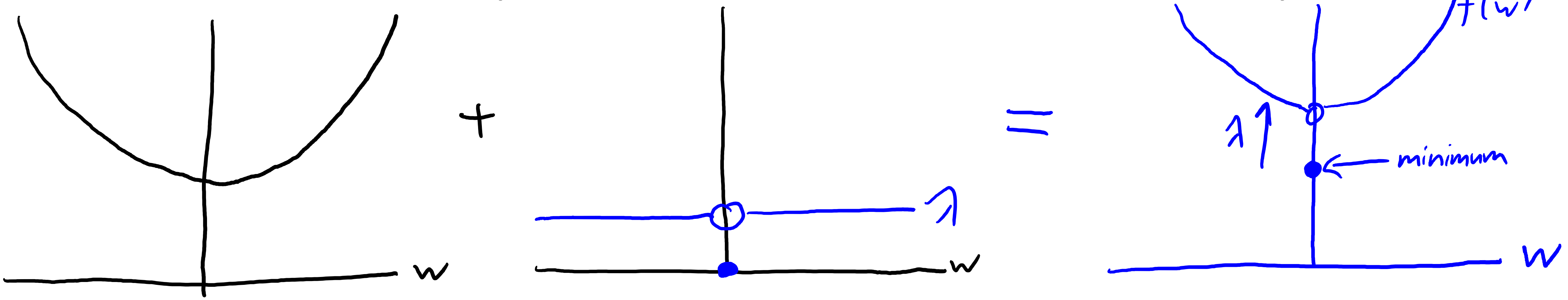
- This variable does not look relevant (minimum is close to 0).
  – But for finite ‘n’ the minimum is unlikely to be exactly zero.

Sparsity and L0-Regularization

- Consider 1D L0-regularized least squares objective:

$$f(w) = \frac{1}{2}\sum_{i=1}^{n}(w x_i - y_i)^2 + \underbrace{\lambda \|w\|_0}_{\begin{cases}\lambda & \text{if } w \neq 0 \\ 0 & \text{if } w = 0\end{cases}}$$

- This is a convex 1D quadratic function but with a discontinuity at 0:



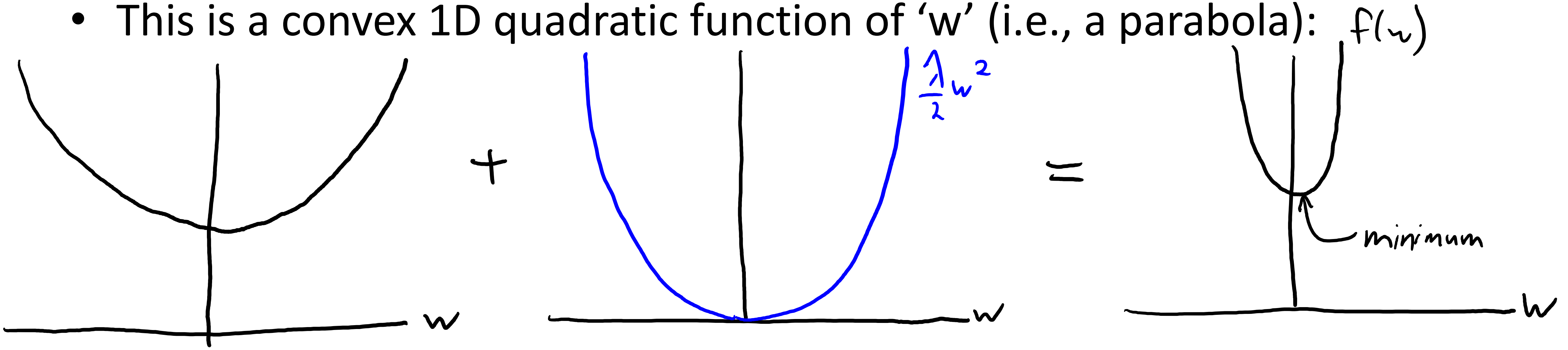
- L0-regularized minimum is often exactly at the 'discontinuity' at 0:
  - Sets the feature to exactly 0 (does feature selection), but is non-convex.

Sparsity and L2-Regularization

- Consider 1D L2-regularized least squares objective:

$$f(w) = \frac{1}{2}\sum_{i=1}^{n}(wx_i - y_i)^2 + \frac{\lambda}{2}w^2$$

- This is a convex 1D quadratic function of ‘w’ (i.e., a parabola):



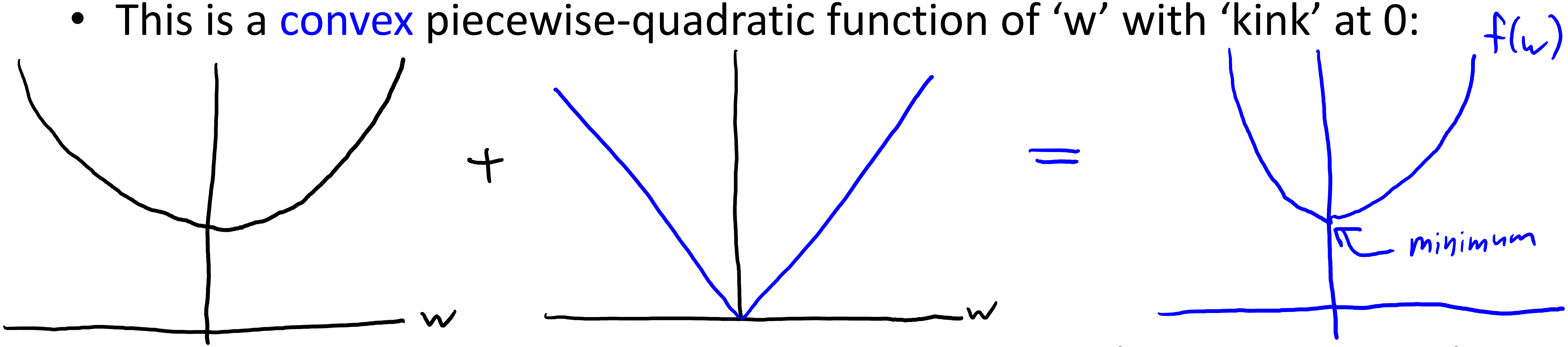
- L2-regularization moves it closer to zero, but not all the way to zero.
  – It doesn’t do feature selection (“penalty goes to 0 as slope goes to 0”).

Sparsity and L1-Regularization

- Consider 1D L1-regularized least squares objective:

$$f(w) = \frac{1}{2}\sum_{i=1}^{n}(w x_i - y_i)^2 + \lambda|w|$$

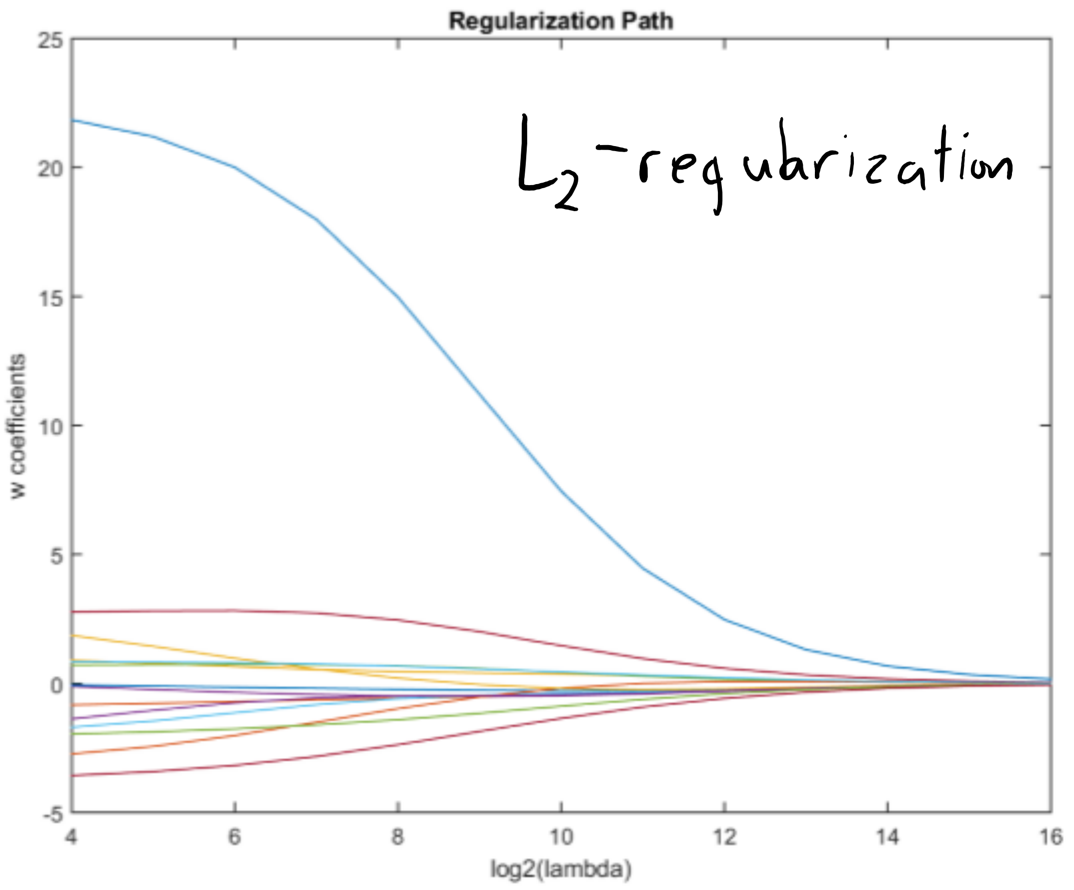
- This is a convex piecewise-quadratic function of 'w' with 'kink' at 0:

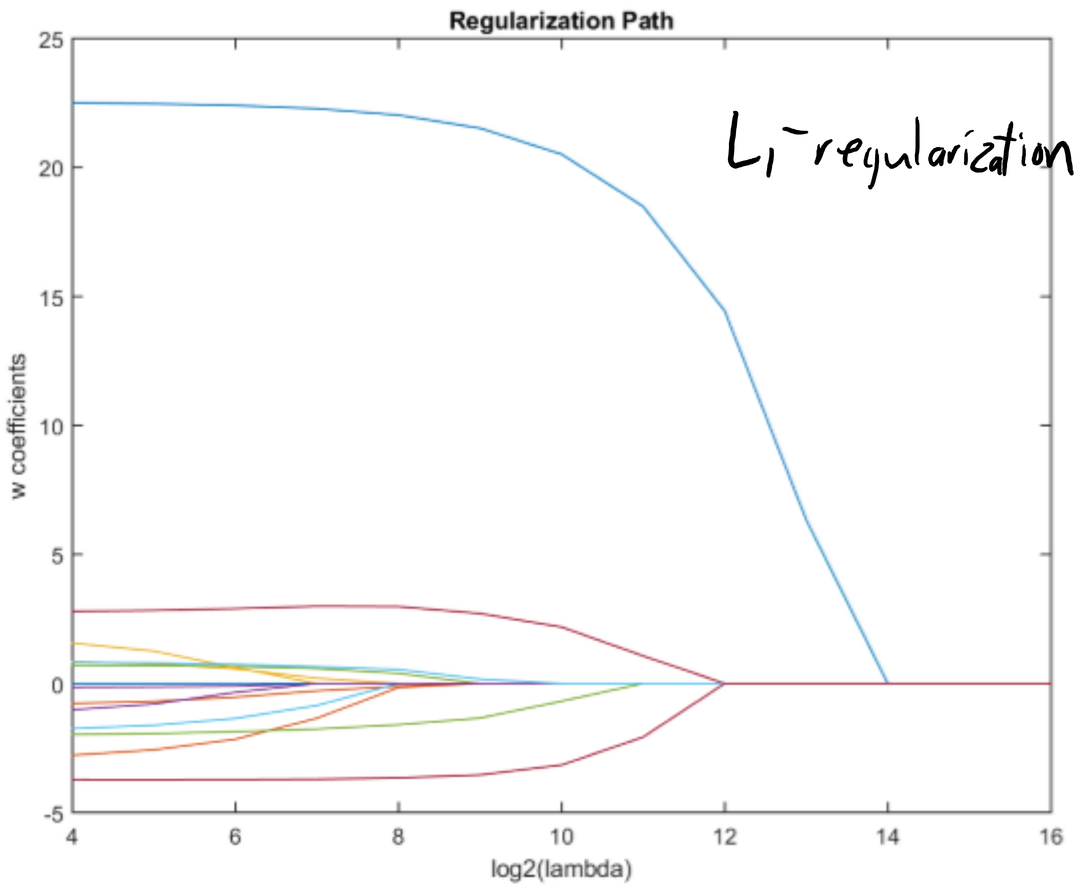


- L1-regularization tends to set variables to exactly 0 (feature selection).
  - Penalty on slope is λ even if you are close to zero.
  - Big λ selects few features, small λ allows many features.

L2-Regularization vs. L1-Regularization

- Regularization path of w_i values as ‘λ’ varies:





- Bonus slides: details on why only L1-regularization gives sparsity.

L2-Regularization vs. L1-Regularization

- L2-Regularization:
  - Insensitive to changes in data.
  - Decreased variance:
    - Lower test error.
  - Closed-form solution.
  - Solution is unique.
  - All ‘w’ tend to be non-zero.
- L1-Regularization:
  - Insensitive to changes in data.
  - Decreased variance:
    - Lower test error.
  - Requires iterative solver.
  - Solution is not unique.
  - Many ‘w’ tend to be zero.

- Can also do both (“elastic net regularization”)

L1-loss vs. L1-regularization

- Don't confuse the L1 loss with L1-regularization!!!
  - L1-loss is robust to outlier data points.
    - You can use instead of removing outliers.
    - "sparse residuals"
  - L1-regularization is robust to irrelevant features.
    - You can use instead of removing features.
    - "sparse coefficients/weights"
- And note that you can be robust to outliers and select features:

$$f(w) = \|Xw - y\|_1 + \lambda \|w\|_1$$

- Why aren't we smoothing and using "Huber regularization"?
  - With the L1 loss, we cared about its behavior far from 0.
  - With L1 regularization, we care about its behavior near 0.
    - It's precisely the non-smoothness that sets weights to exactly 0.

Summary

- Standardizing features:
  - For some models it makes sense to have features on the same scale.
- Hyperparameter optimization
  - A difficult but important task, especially with lots of hyperparameters.
- L1-regularization:
  - Simultaneous regularization and feature selection.
  - Robust to having lots of irrelevant features.
  - Not the same thing as using the L1 loss.

Why doesn't L2-Regularization set variables to 0?

- Consider an L2-regularized least squares problem with 1 feature:

$$f(w) = \frac{1}{2}\sum_{i=1}^{n}(wx_i - y_i)^2 + \frac{\lambda}{2}w^2$$

- Let's solve for the optimal 'w':

$$f'(w) = \sum_{i=1}^{n} x_i(wx_i - y_i) + \lambda w$$

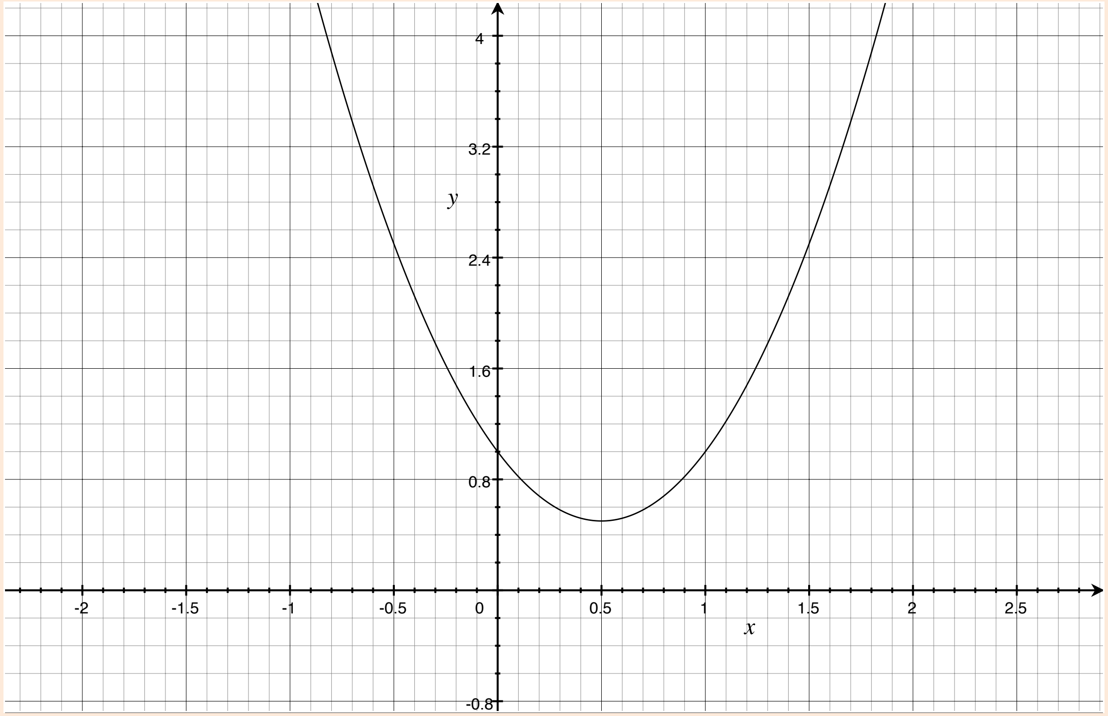
Set equal to 0: $\sum_{i=1}^{n} x_i^2 w - \sum_{i=1}^{n} x_i y_i + \lambda w = 0 \xrightarrow{\text{re-arrange}} w\Big(\underbrace{\sum_{i=1}^{n} x_i^2}_{\|x\|^2} + \lambda\Big) = \underbrace{\sum_{i=1}^{n} x_i y_i}_{y^Tx}$

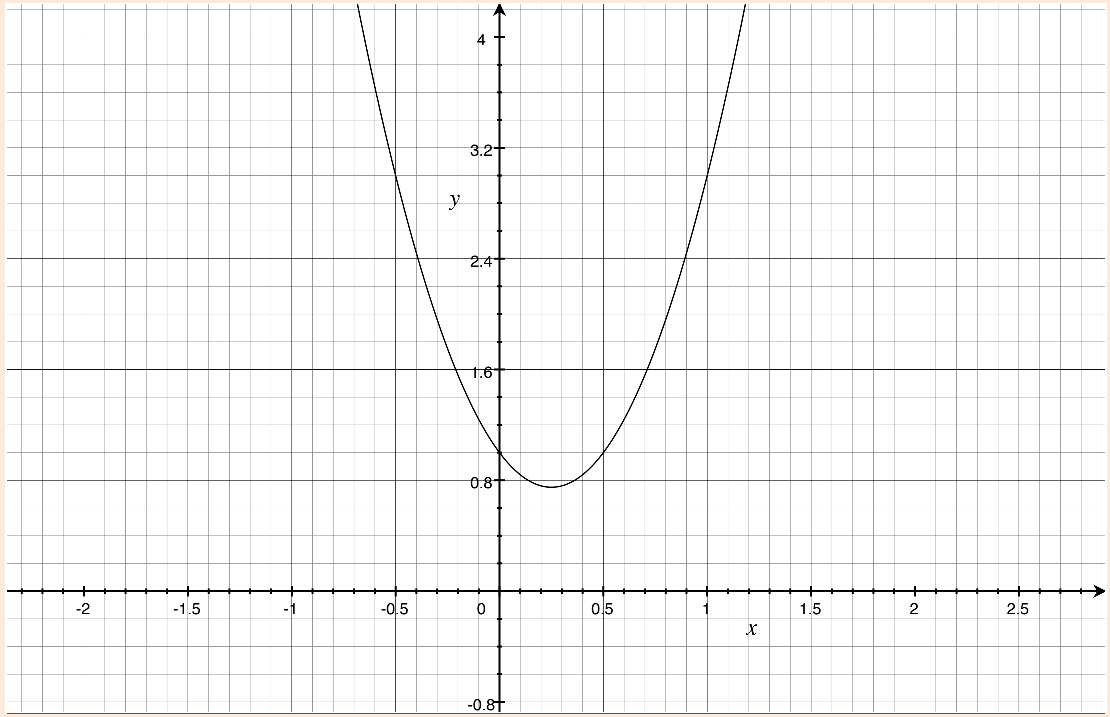
or $w = \dfrac{y^Tx}{\|x\|^2 + \lambda}$

- So as λ gets bigger, 'w' converges to 0.
- However, for all finite λ 'w' will be non-zero unless $y^Tx = 0$.
  – But it's very unlikely that y^Tx will be exactly zero.

Why doesn't L2-Regularization set variables to 0?

- Small λ Big λ





- Solution further from zero

Solution closer to zero (but not exactly 0)

Why does L1-Regularization set things to 0?

- Consider an L1-regularized least squares problem with 1 feature:

$$f(w) = \frac{1}{2}\sum_{i=1}^{n}(wx_i - y_i)^2 + \lambda|w|$$

- If (w = 0), then “left” limit and “right“ limit are given by:

$$f^-(0) = \sum_{i=1}^{n} x_i(0x_i - y_i) - \lambda = \sum_{i=1}^{n} x_i y_i - \lambda$$

$$f^+(0) = \sum_{i=1}^{n} x_i(0x_i - y_i) + \lambda = \sum_{i=1}^{n} x_i y_i + \lambda$$

- So what should gradient descent do if (w=0)?
  - $-f^-(0) = -y^Tx + \lambda$
  - $-f^+(0) = -y^Tx - \lambda$

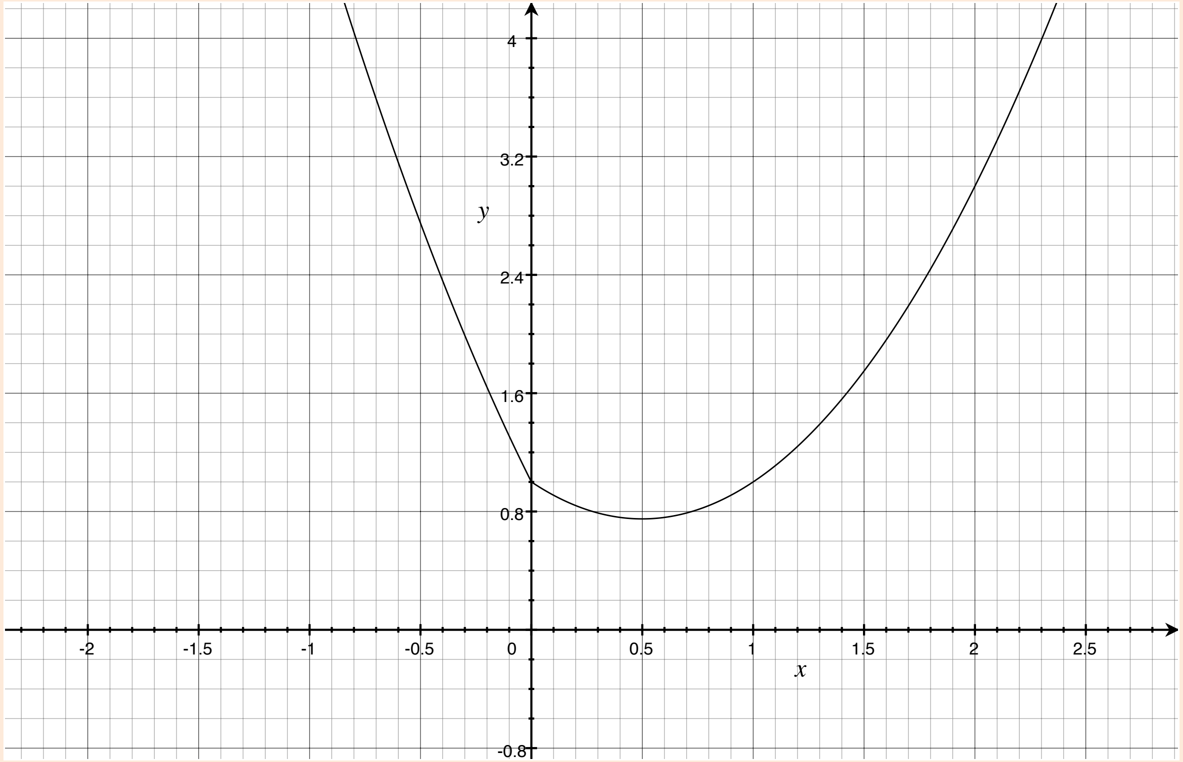
If these are positive $(-y^Tx > \lambda)$, we can improve by increasing 'w'.

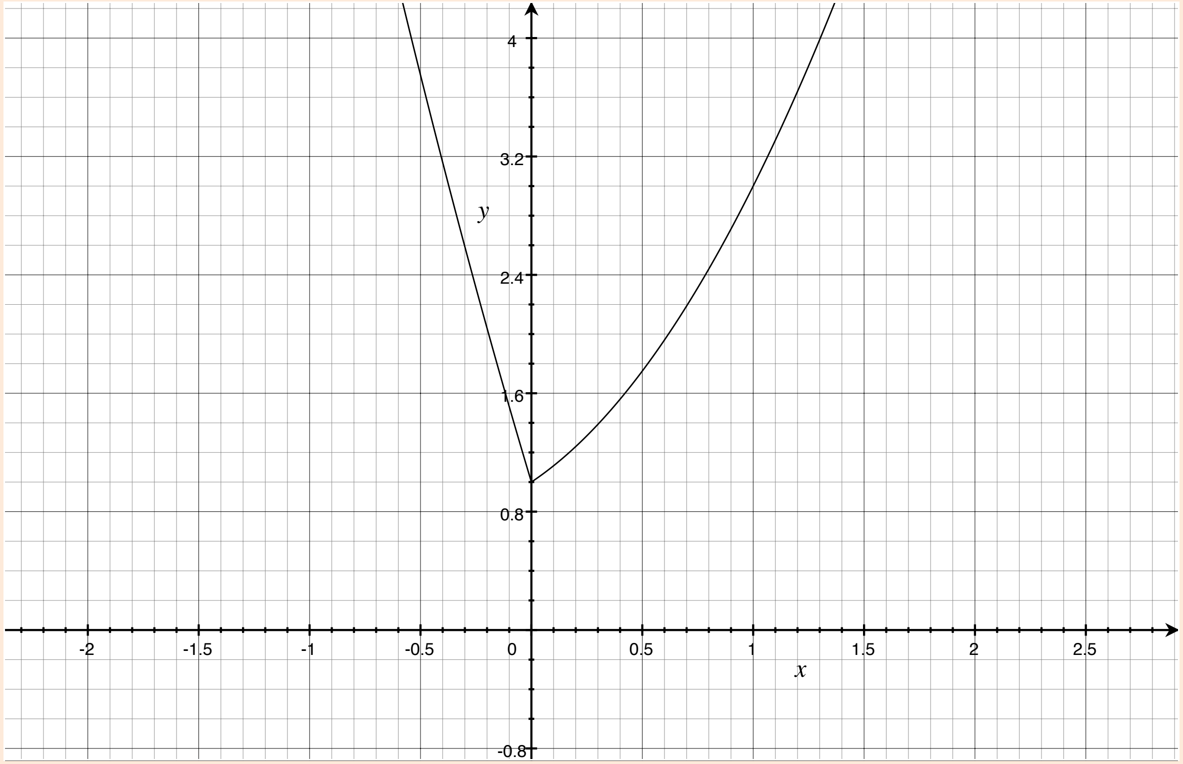
If these are negative $(y^Tx > \lambda)$, we can improve by decreasing 'w'.

But if left and right "gradient descent" directions point in opposite directions $(|y^Tx| \leq \lambda)$, minimum is 0.

Why does L1-Regularization set things to 0?

- Small λ Big λ





- Solution nonzero Solution exactly zero

(minimum of left parabola is past origin, but right parabola is not) (minima of both parabolas are past the origin)

L2-regularization vs. L1-regularization

- So with 1 feature:
  - L2-regularization only sets 'w' to 0 if $y^T x = 0$.
    - There is a only a single possible $y^T x$ value where the variable gets set to zero.
    - And λ has nothing to do with the sparsity.
  - L1-regularization sets 'w' to 0 if $|y^T x| \leq \lambda$.
    - There is a range of possible $y^T x$ values where the variable gets set to zero.
    - And increasing λ increases the sparsity since the range of $y^T x$ grows.
- Note that it's really important that the function is non-differentiable:
  - If we used "Huber regularization", it would select all variables.

L1-Loss vs. Huber Loss

- The same reasoning tells us the difference between the L1 *loss* and the Huber loss. They are very similar in that they both grow linearly far away from 0. So both are both robust but…
  - With the L1 loss the model often passes exactly through some points.
  - With Huber the model doesn't necessarily pass through any points.

- Why? With L1-regularization we were causing the elements of 'w' to be exactly 0. Analogously, with the L1-loss we cause the elements of 'r' (the residual) to be exactly zero. But zero residual for an example means you pass through that example exactly.

Non-Uniqueness of L1-Regularized Solution

- How can L1-regularized least squares solution not be unique?
  - Isn't it convex?
- Convexity implies that minimum value of f(w) is unique (if exists), but there may be multiple 'w' values that achieve the minimum.

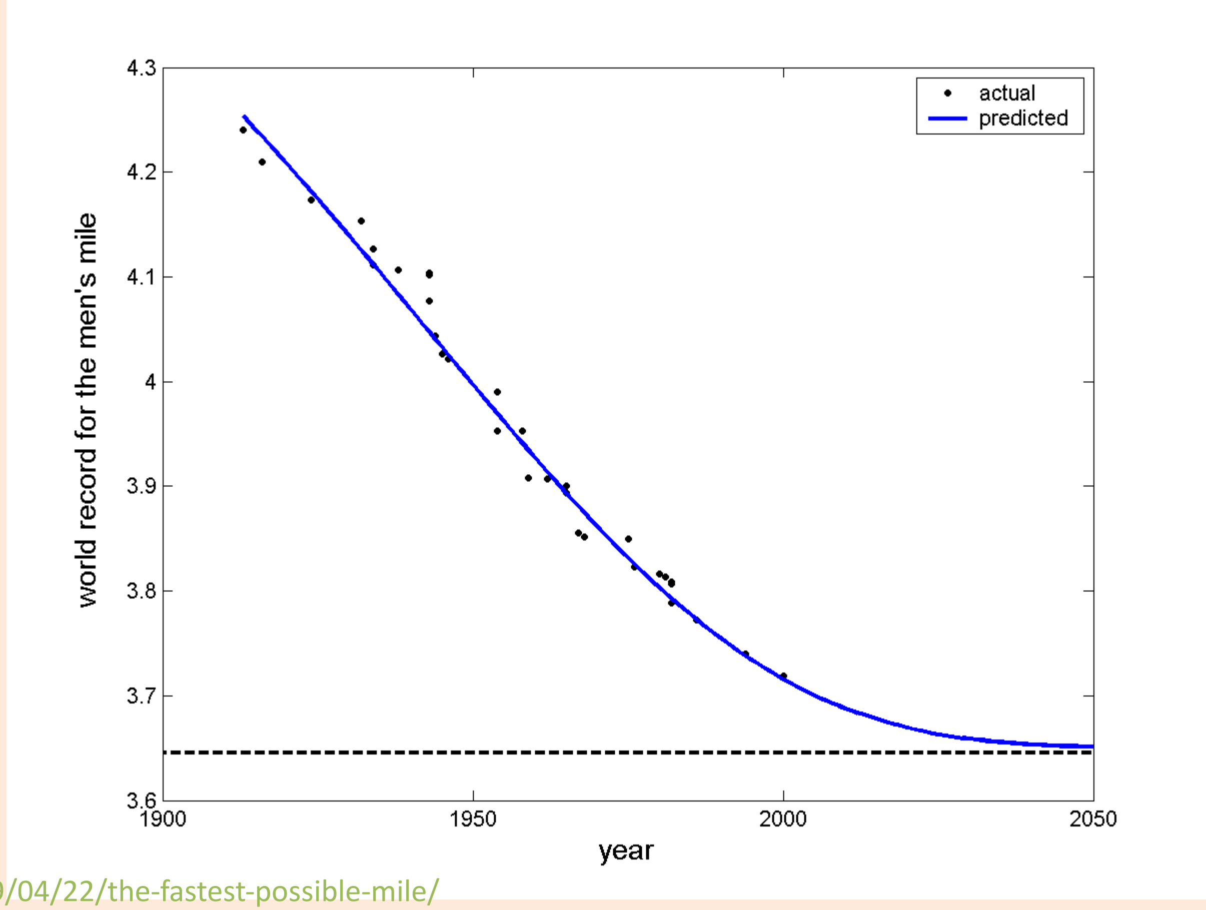
- Consider L1-regularized least squares with d=2, where feature 2 is a copy of a feature 1. For a solution (w_1,w_2) we have:

$$\hat{y}_i = w_1 x_{i1} + w_2 x_{i2} = w_1 x_{i1} + w_2 x_{i1} = (w_1 + w_2) x_{i1}$$

- So we can get the same squared error with different w_1 and w_2 values that have the same sum. Further, if neither w_1 or w_2 changes sign, then $|w_1| + |w_2|$ will be the same so the new w_1 and w_2 will be a solution.

Predicting the Future

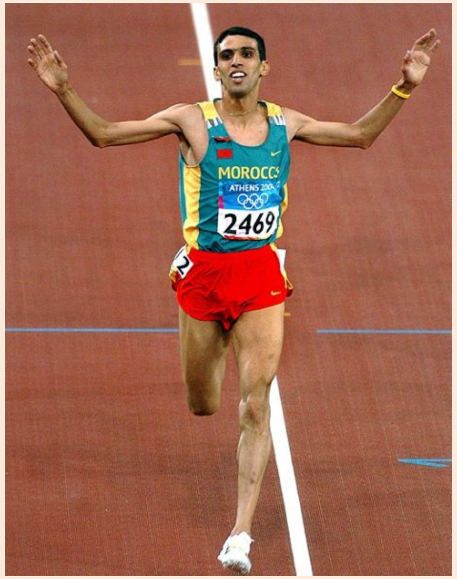
- In principle, we can use any features x_i that we think are relevant.
- This makes it tempting to use time as a feature, and predict future.

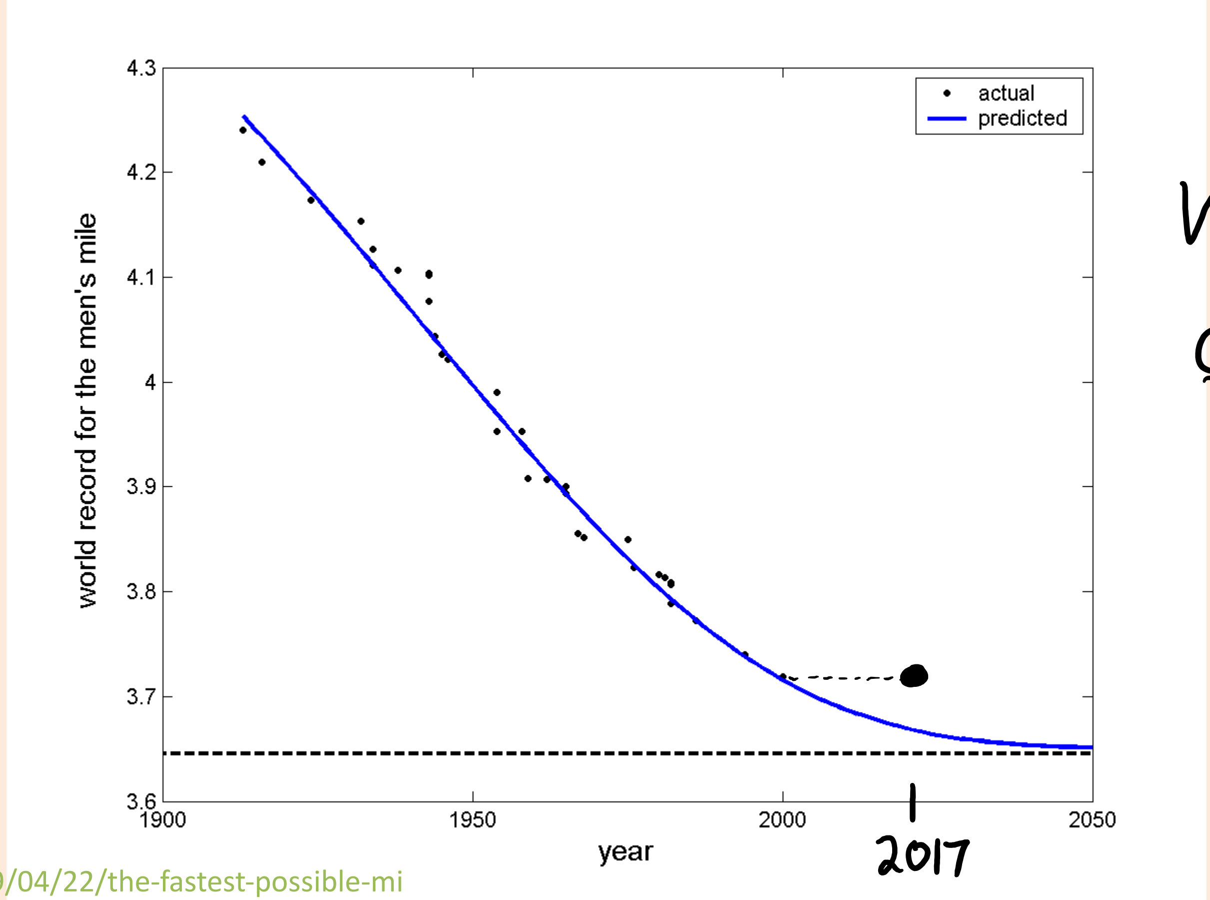


https://gravityandlevity.wordpress.com/2009/04/22/the-fastest-possible-mile/

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.

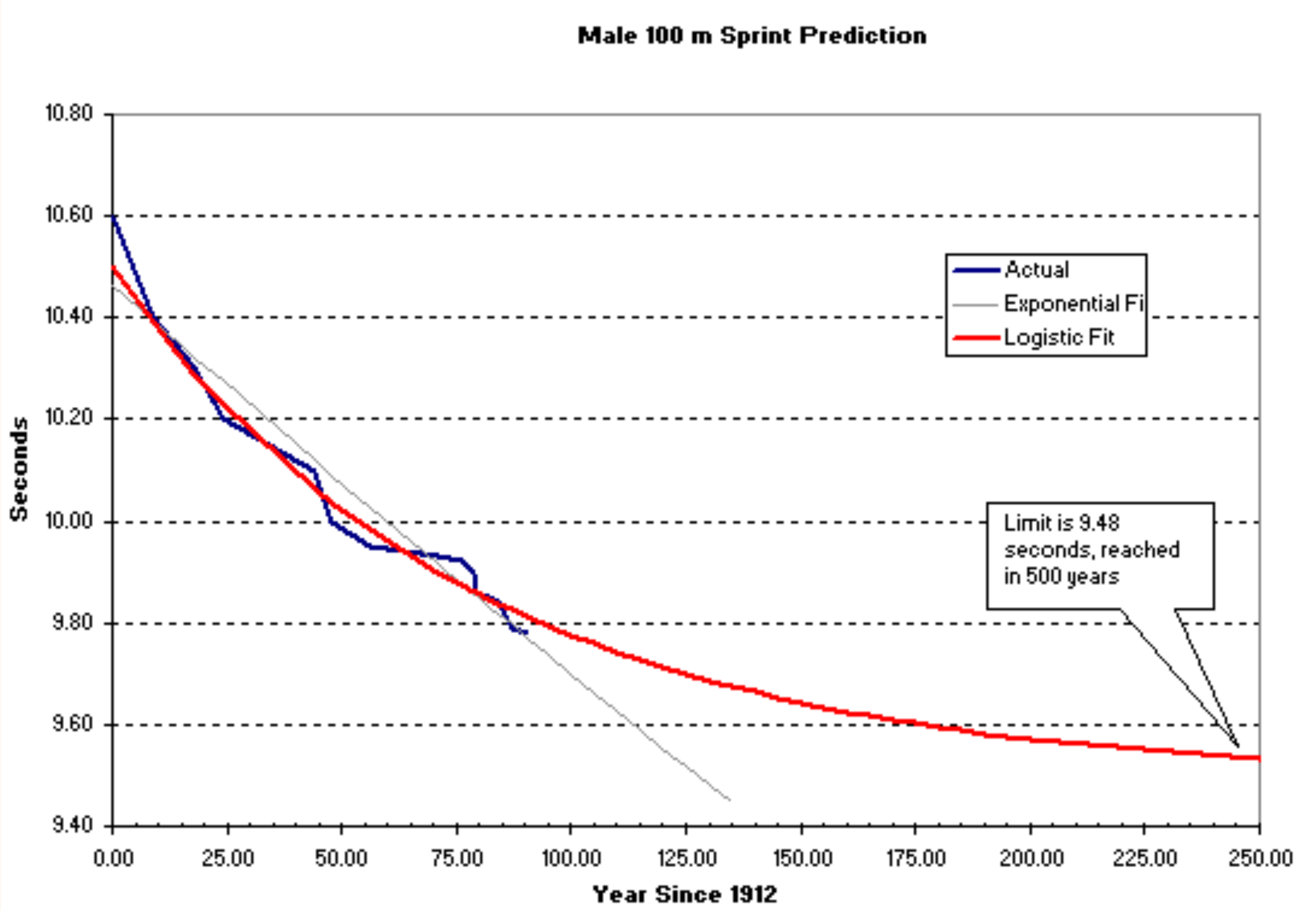




We need to be cautious about doing this.

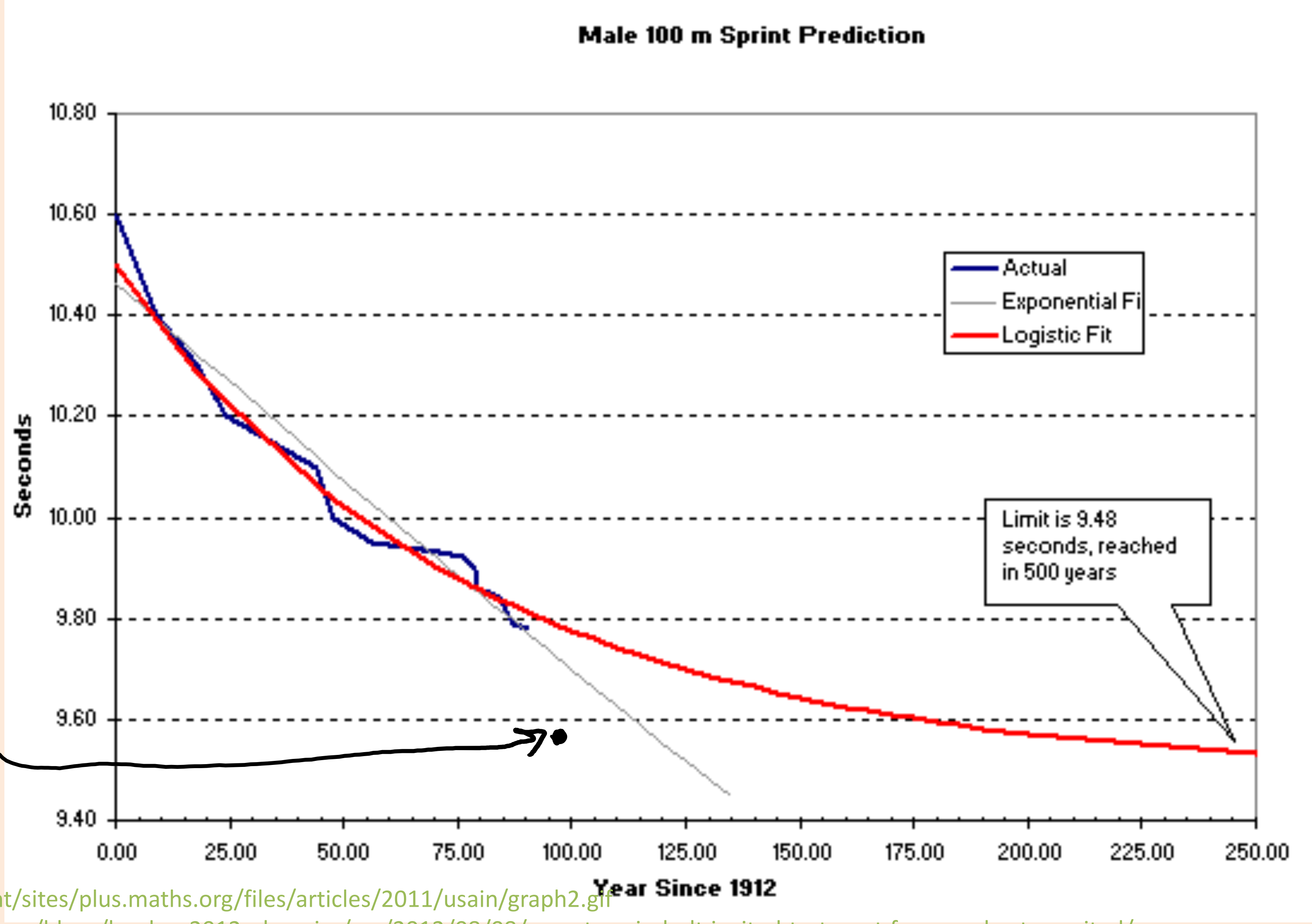
https://gravityandlevity.wordpress.com/2009/04/22/the-fastest-possible-mi
https://overthehillsports.wordpress.com/tag/hicham-el-guerrouj/le/

Predicting 100m times 400 years in the future?



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

Predicting 100m times 400 years in the future?



9.58

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

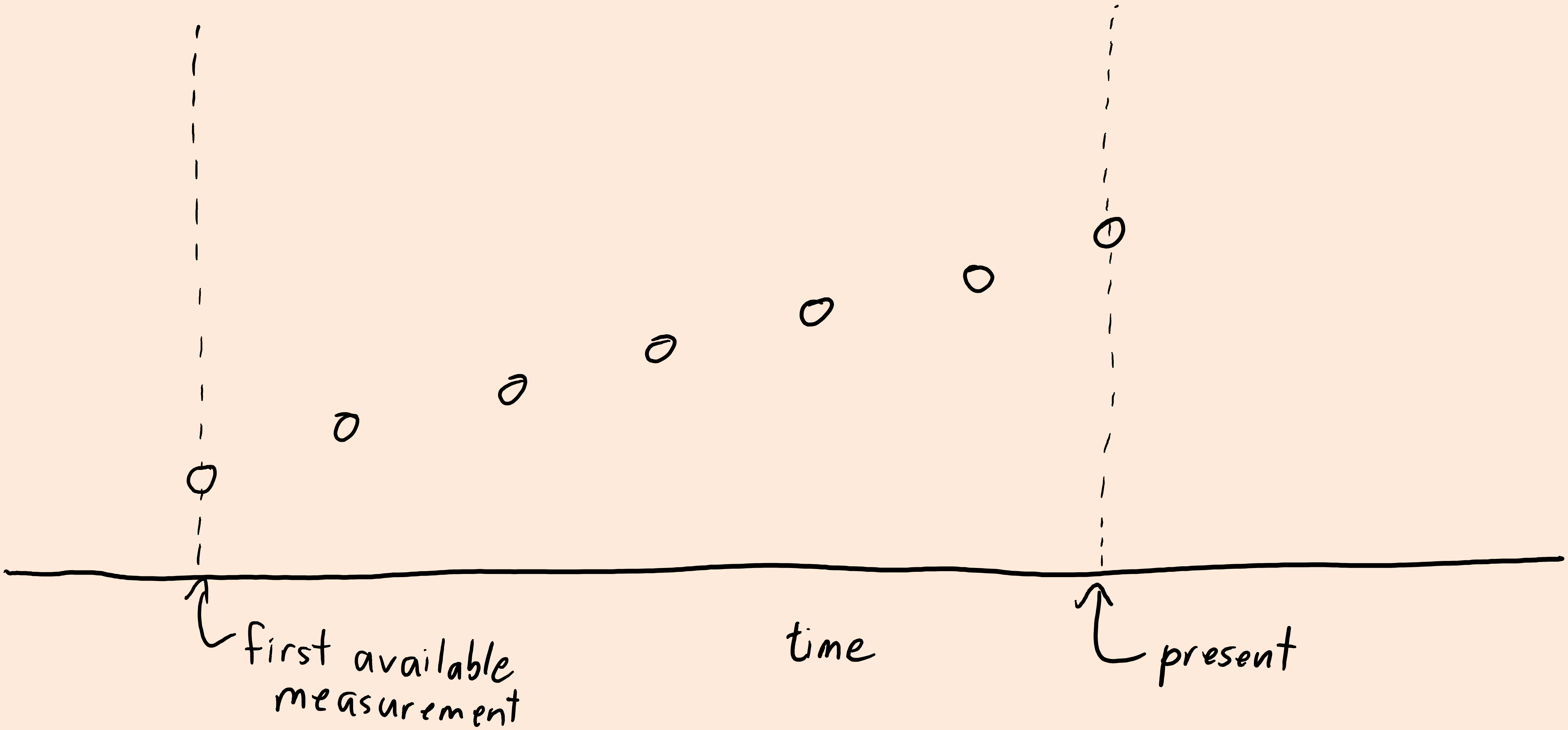
- Interpolation is task of predicting "between the data points".
  - Regression models are good at this if you have enough data and function is smooth.
- Extrapolation is task of prediction outside the range of the data points.
  - Without assumptions, regression models can be embarrassingly-bad at this.

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

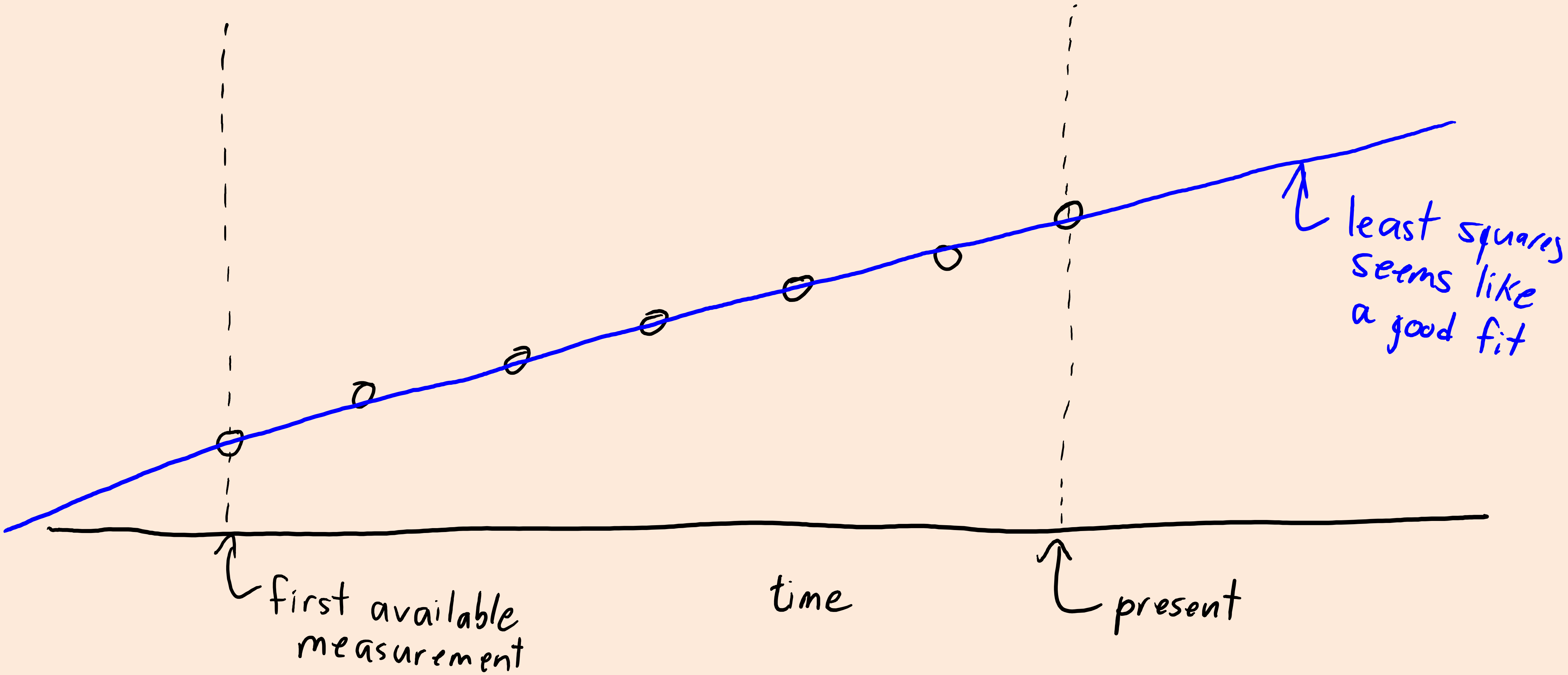
- If you run the 100m regression models forwards in time:
  - They might eventually predict arbitrarily-small 100m times.
  - The linear model actually predicts negative times in the future.
    - These time traveling races in 2060 should be pretty exciting!

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

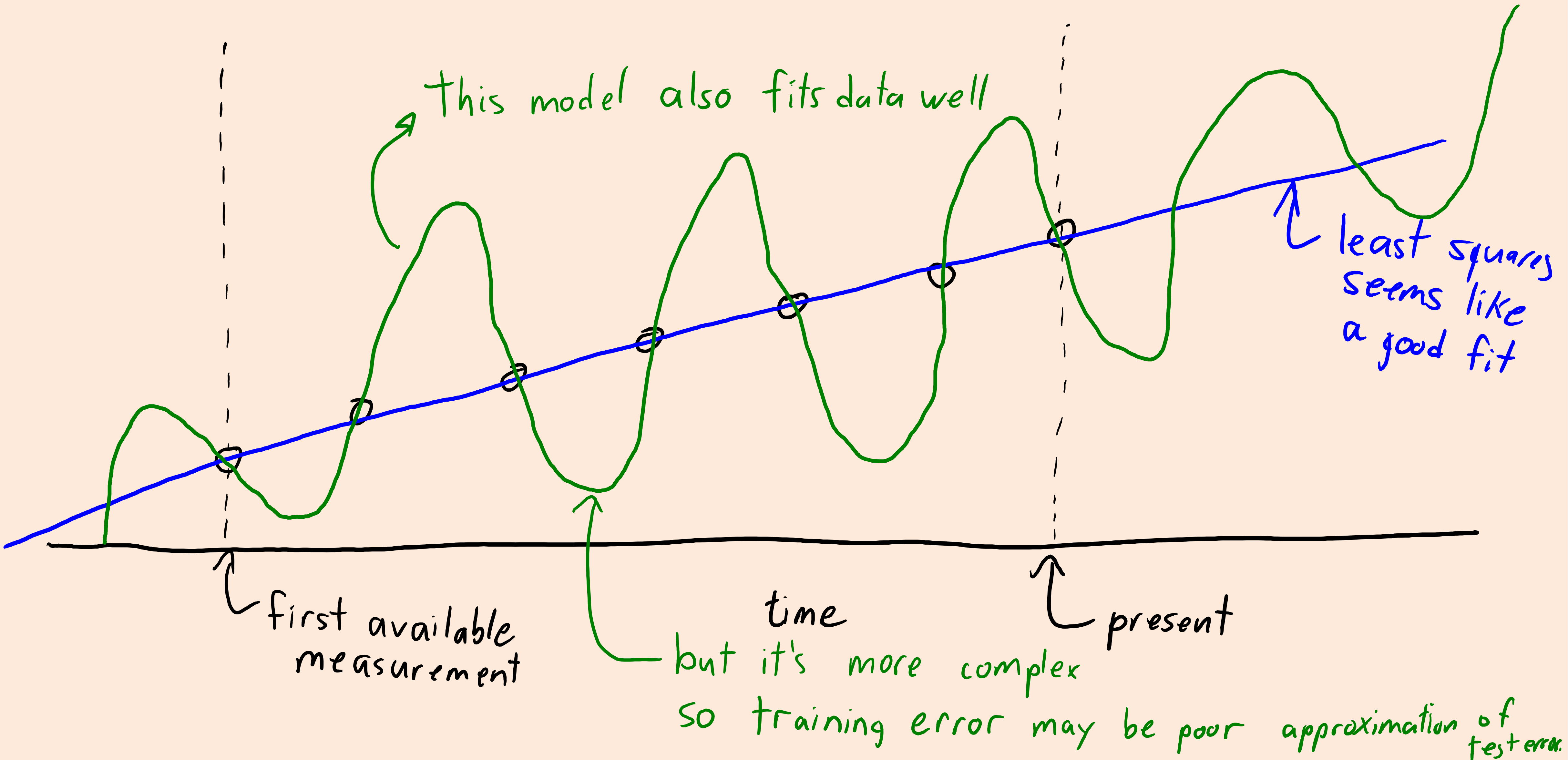
No Free Lunch, Consistency, and the Future



No Free Lunch, Consistency, and the Future

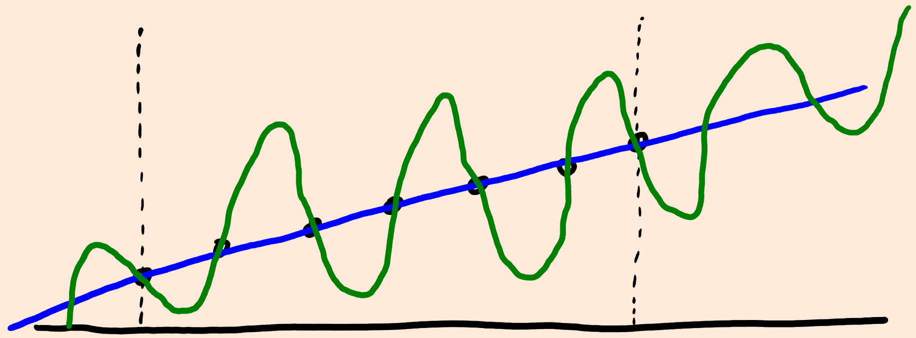


No Free Lunch, Consistency, and the Future

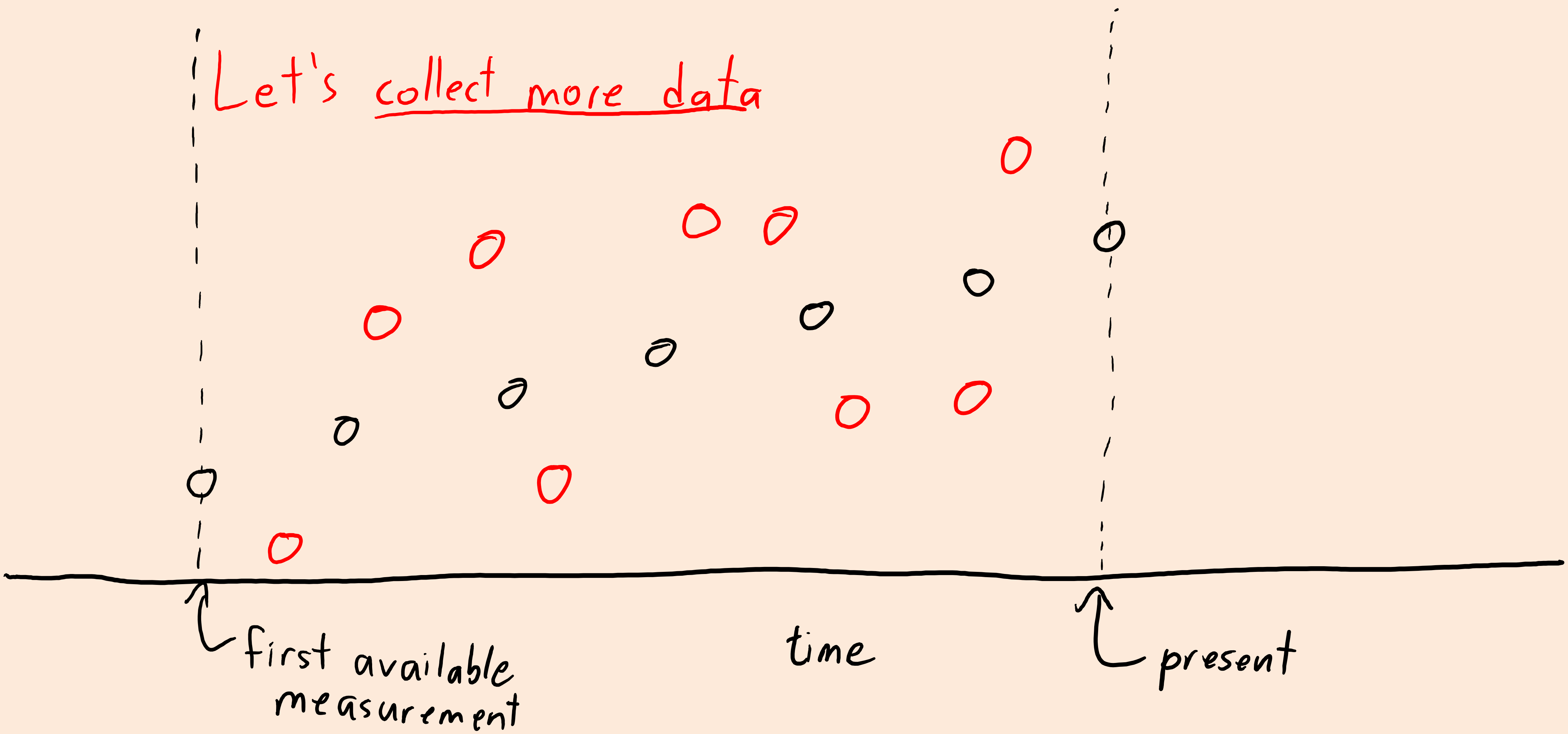


Ockham's Razor vs. No Free Lunch

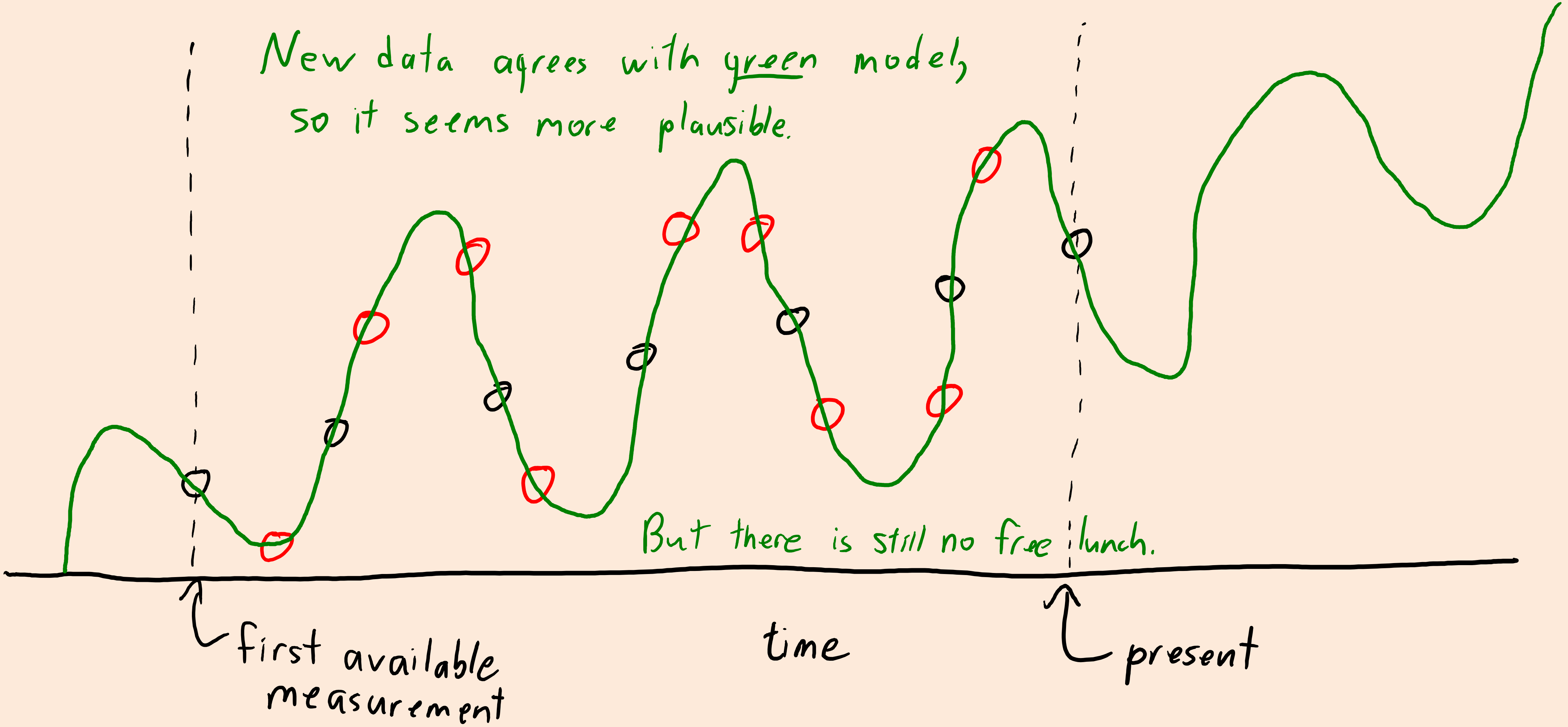
- Ockham's razor is a problem-solving principle:
  - "Among competing hypotheses, the one with the fewest assumptions should be selected."
  - Suggests we should select linear model.
- Fundamental trade-off:
  - If same training error, pick model less likely to overfit.
  - Formal version of Occam's 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.



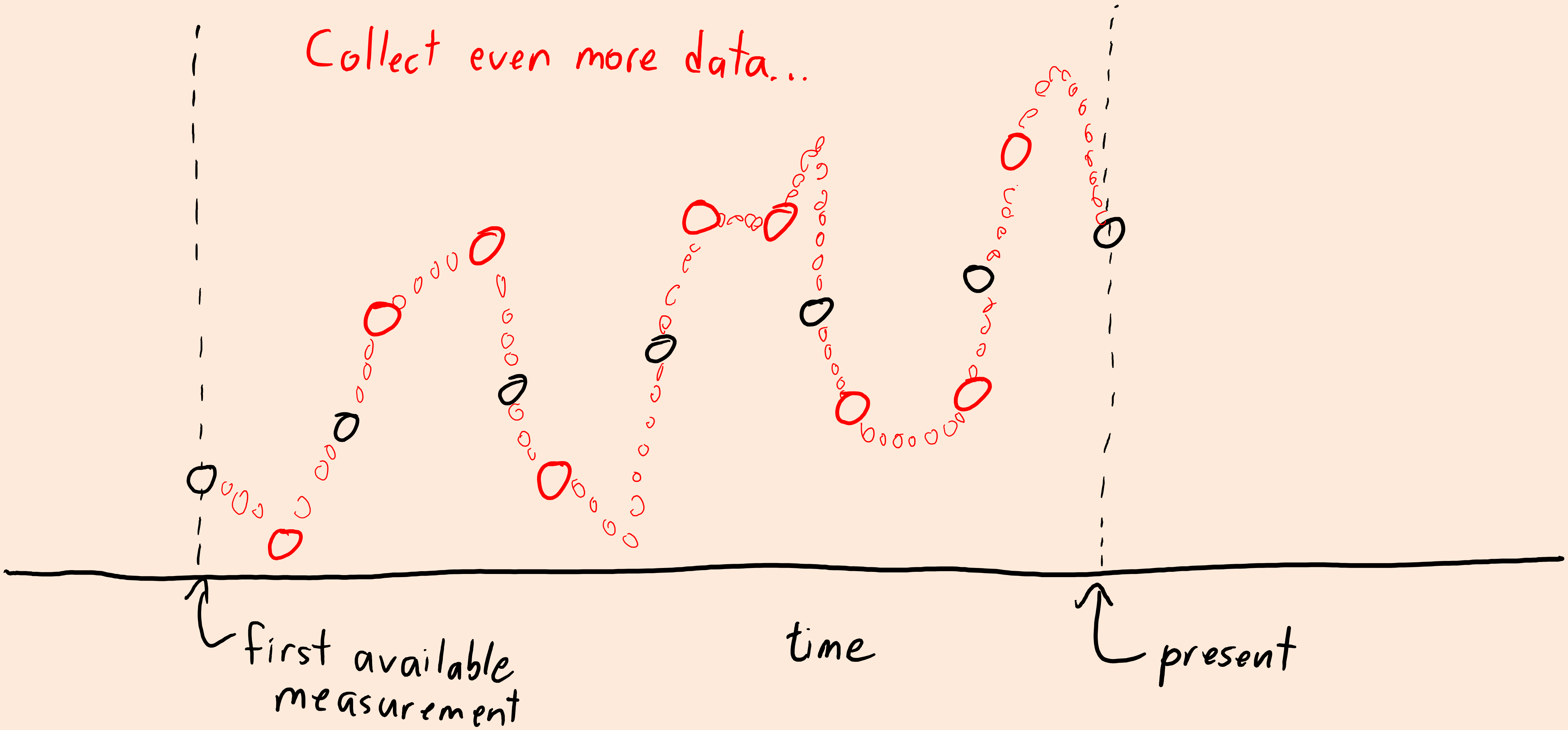
No Free Lunch, Consistency, and the Future



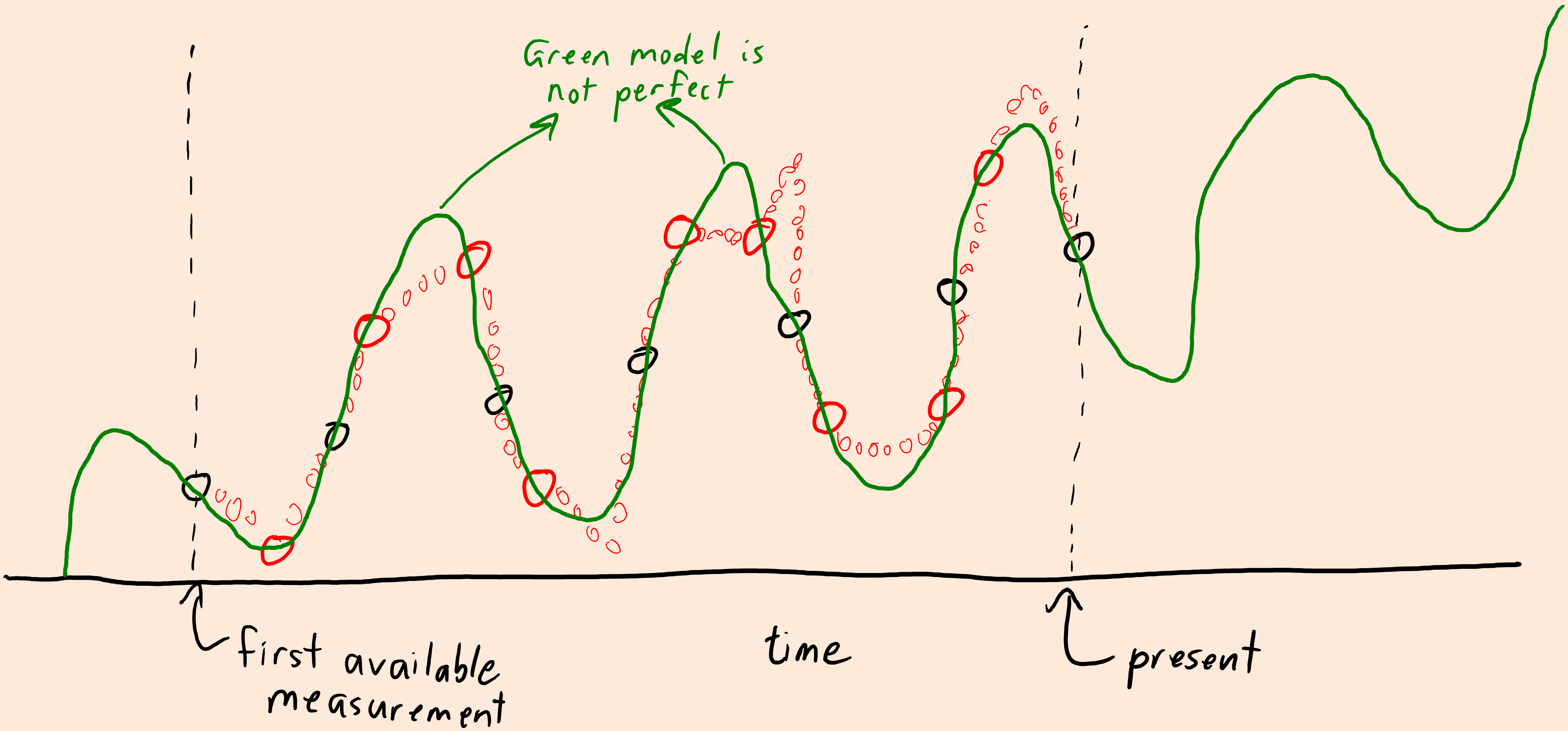
No Free Lunch, Consistency, and the Future



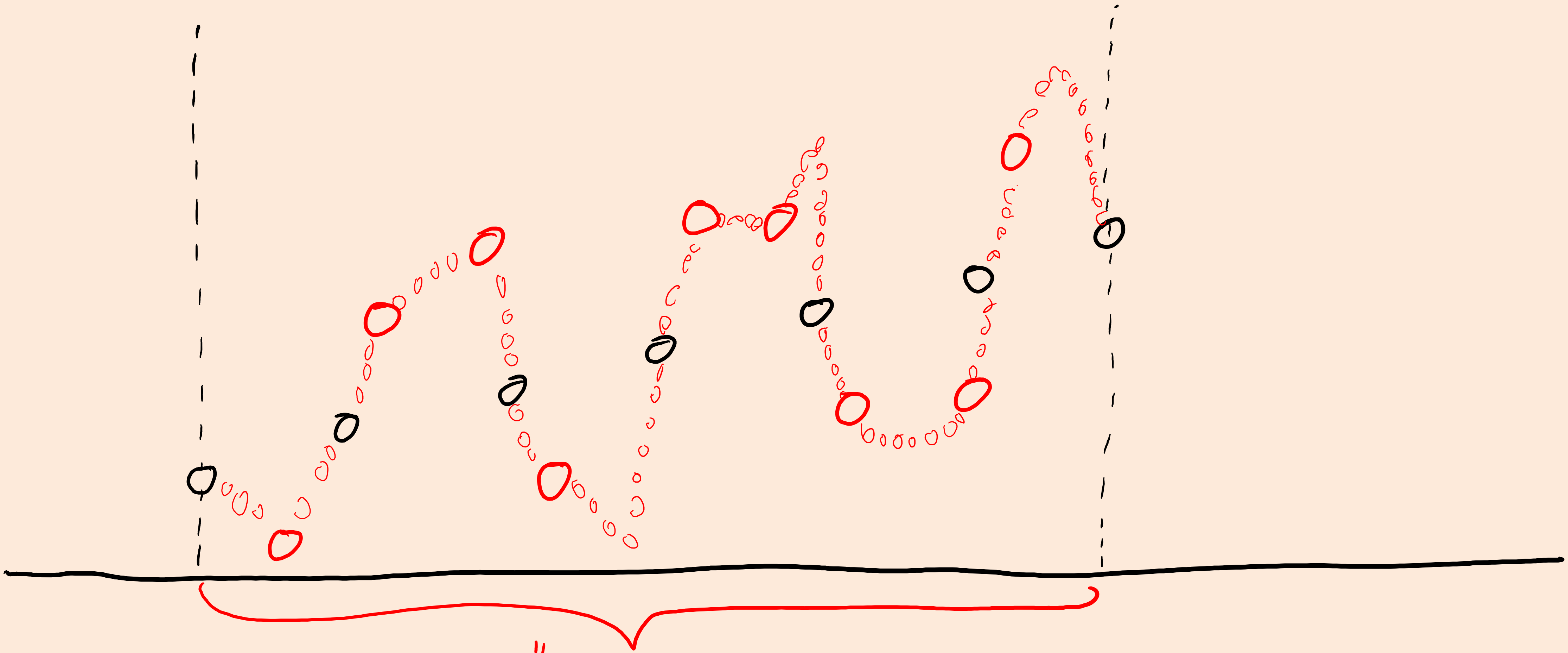
No Free Lunch, Consistency, and the Future



No Free Lunch, Consistency, and the Future



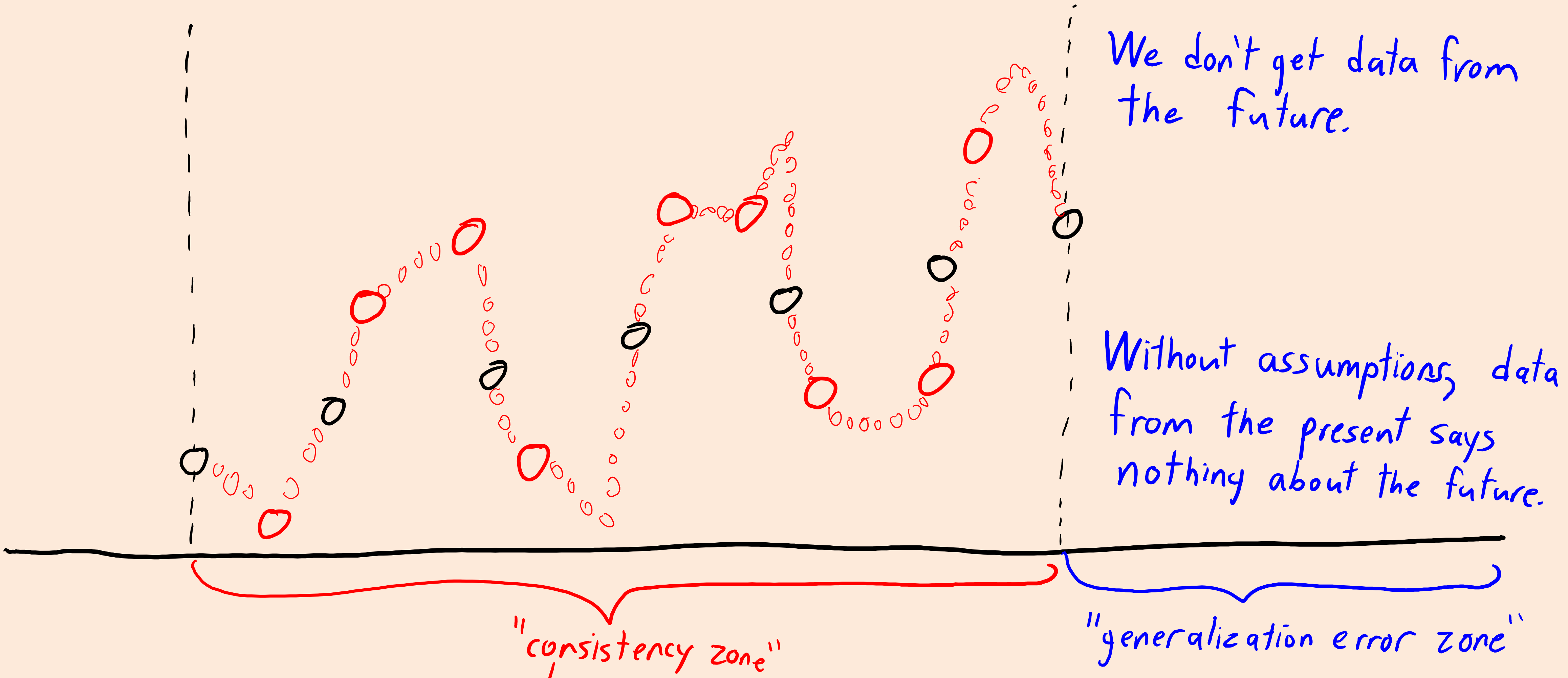
No Free Lunch, Consistency, and the Future



"consistency zone"

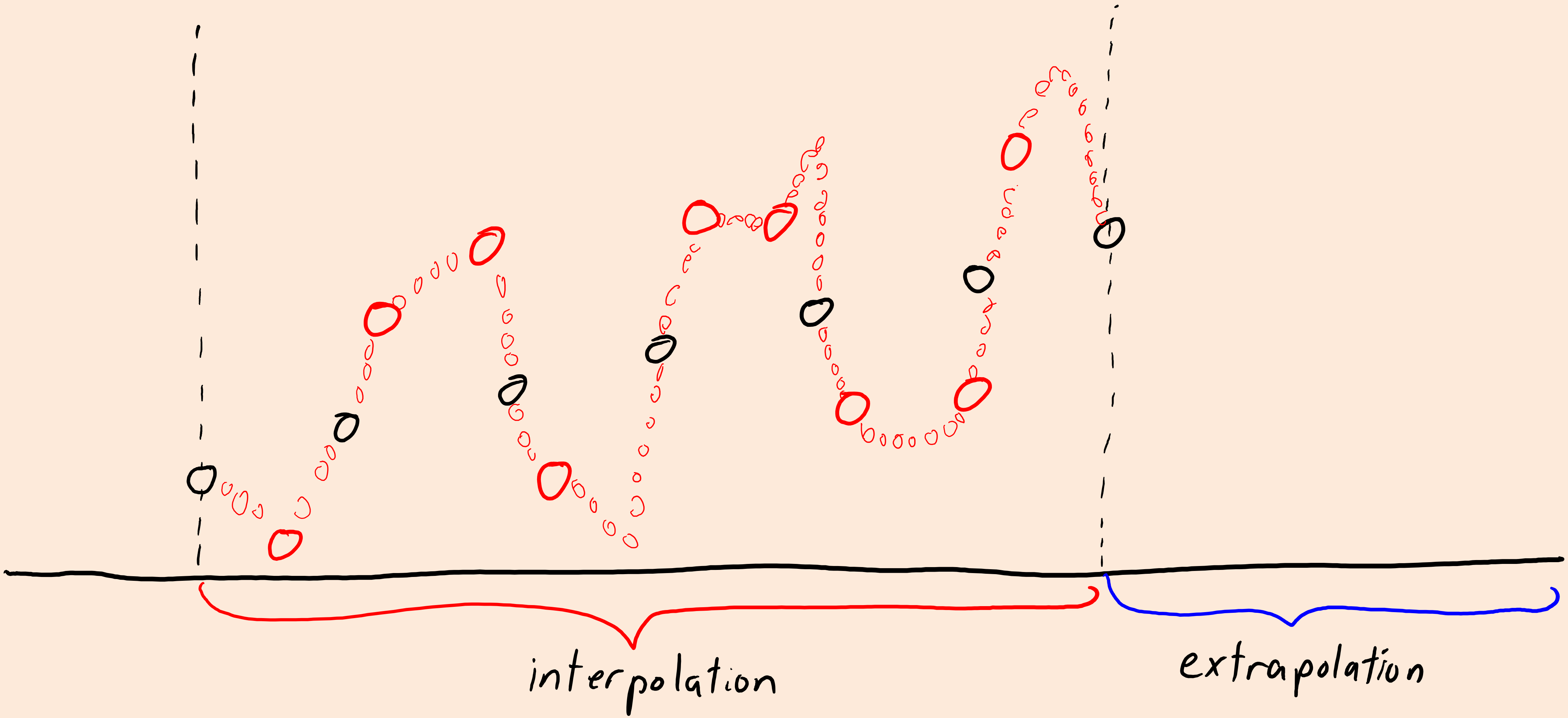
↳ "Universally consistent" methods converge to best model here as $n \to \infty$

No Free Lunch, Consistency, and the Future



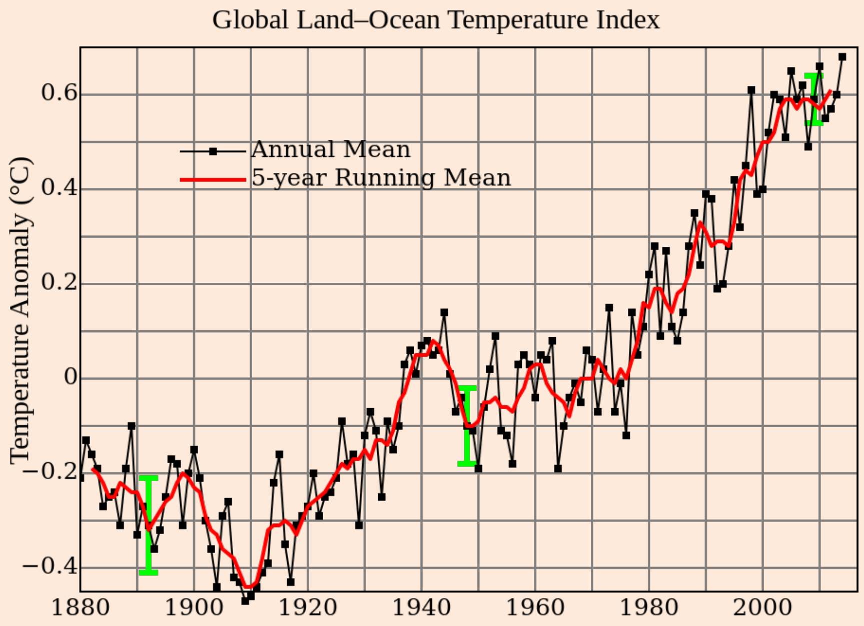
↳ "Universally consistent" methods converge to best model here as $n \to \infty$

No Free Lunch, Consistency, and the Future



Discussion: Climate Models

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

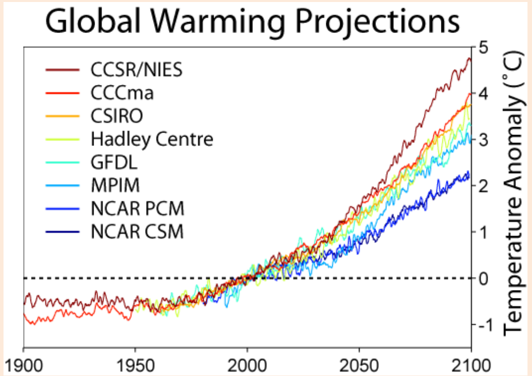


- Will Earth continue to warm over next 100 years? (generalization error)
  – We should be more skeptical about models that predict future events.

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:

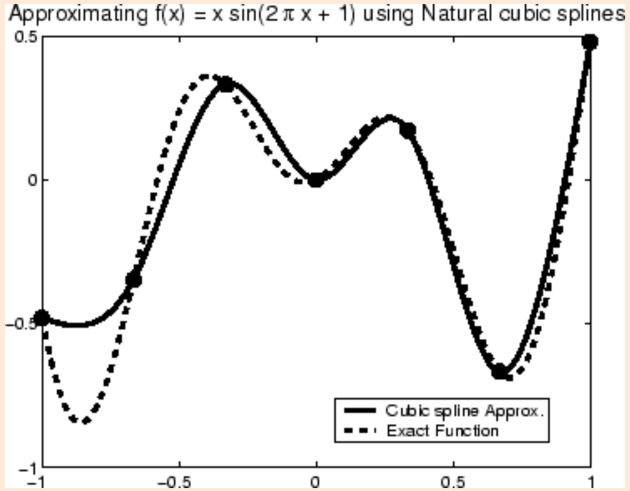


  – We should be skeptical of individual models, but agreeing predictions made by models with different data/assumptions are more likely be true.
- If all near-future predictions agree, they are likely to be accurate.
- As we go further in the future, variance of average will be higher.

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

Splines in 1D

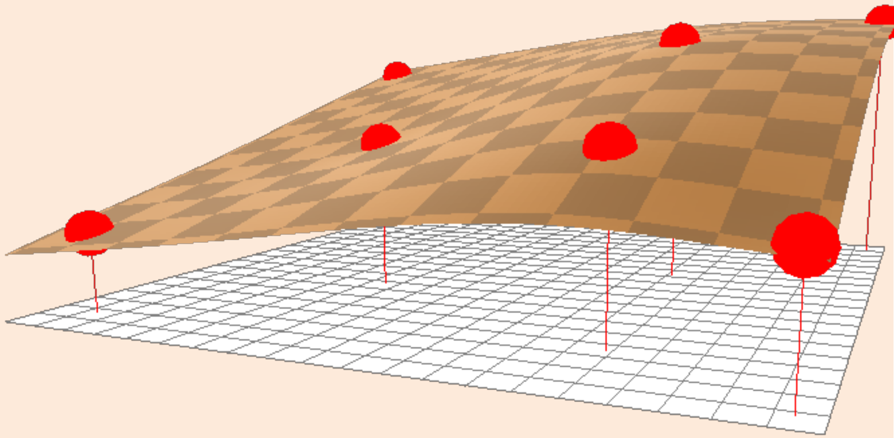
- For 1D interpolation, alternative to polynomials/RBFs are splines:
  - Use a polynomial in the region between each data point.
  - Constrain some derivatives of the polynomials to yield a unique solution.
- Most common example is cubic spline:
  - Use a degree-3 polynomial between each pair of points.
  - Enforce that f'(x) and f''(x) of polynomials agree at all point.
  - "Natural" spline also enforces f''(x) = 0 for smallest and largest x.
- Non-trivial fact: natural cubic splines are sum of:
  - Y-intercept.
  - Linear basis.
  - RBFs with $g(\varepsilon) = \varepsilon^3$.
    - Different than Gaussian RBF because it *increases with distance*.



http://www.physics.arizona.edu/~restrepo/475A/Notes/sourcea-/node35.html

Splines in Higher Dimensions

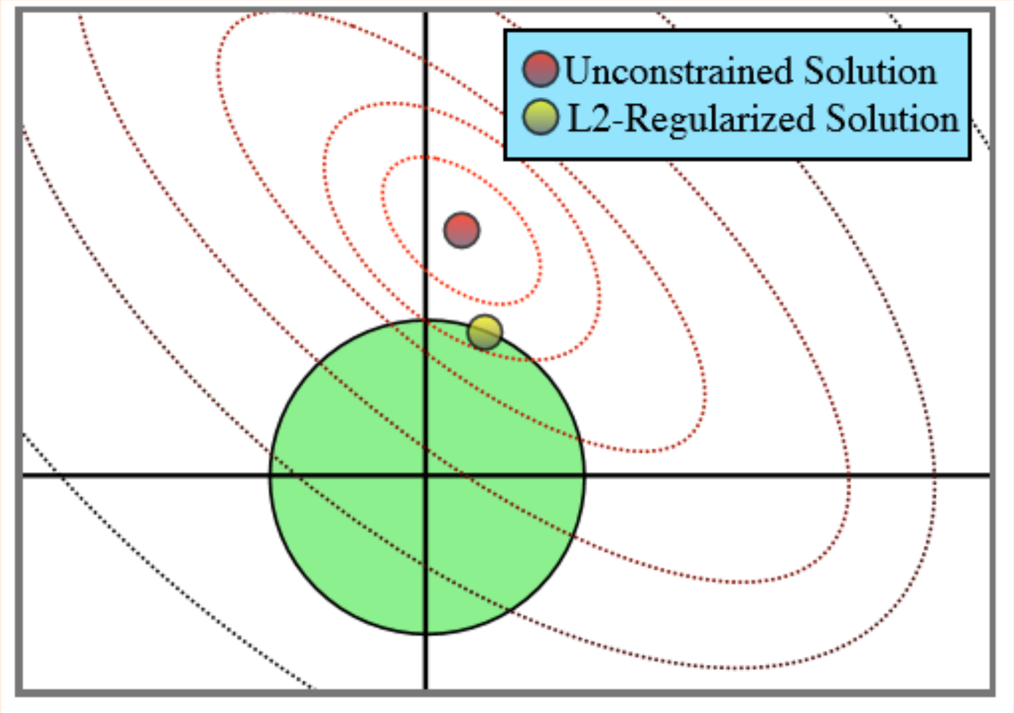
- Splines generalize to higher dimensions if data lies on a grid.
  - For more general ("scattered") data, there isn't a natural generalization.
- Common 2D "scattered" data interpolation is thin-plate splines:
  - Based on curve made when bending sheets of metal.
  - Corresponds to RBFs with $g(\varepsilon) = \varepsilon^2 \log(\varepsilon)$.
- Natural splines and thin-plate splines: special cases of "polyharmonic" splines:
  - Less sensitive to parameters than Gaussian RBF.



http://step.polymtl.ca/~rv101/thinplates/

L2-Regularization vs. L1-Regularization

- L2-regularization conceptually restricts 'w' to a ball.



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

is equivalent to minimizing

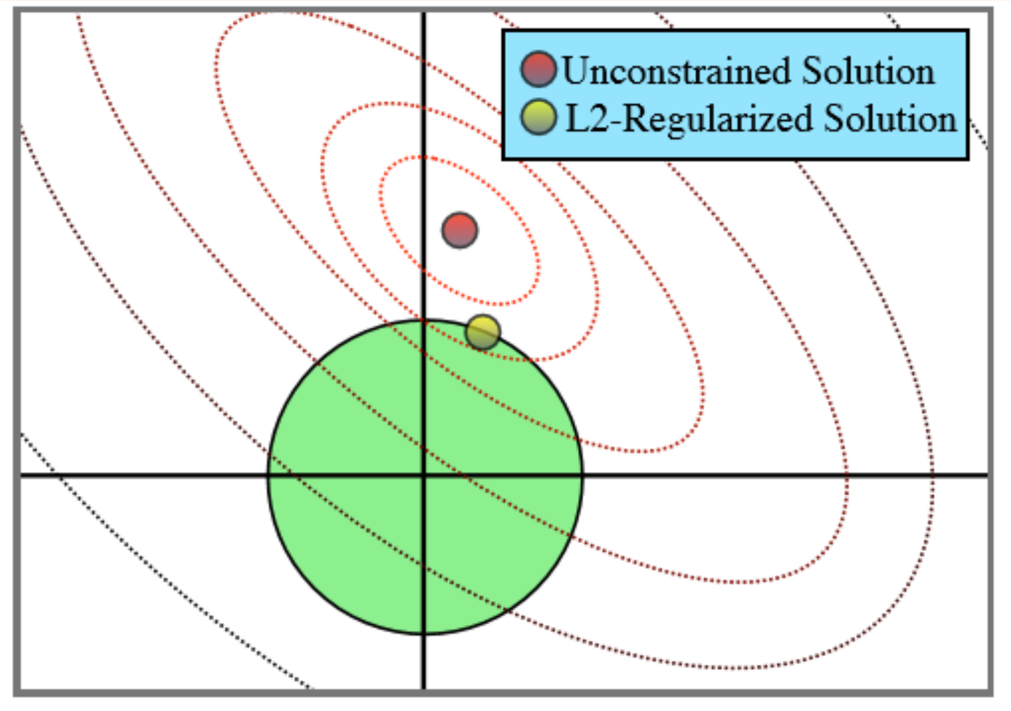
$\frac{1}{2}\|Xw - y\|^2$ subject to

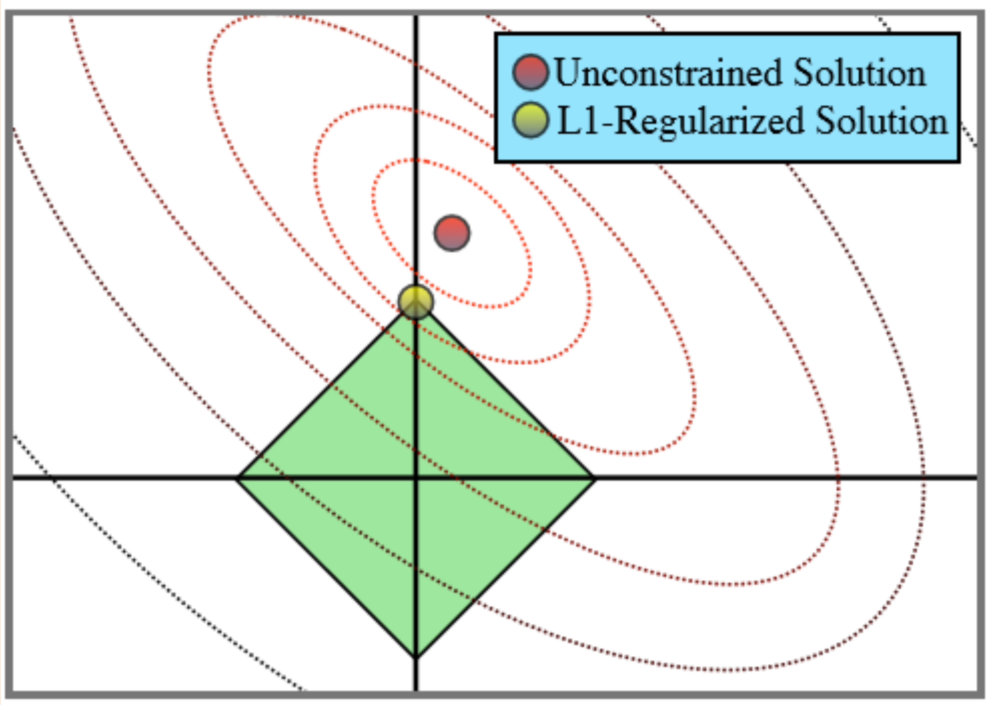
the constraint that $\|w\| \leq \tau$

for some value 'τ'

L2-Regularization vs. L1-Regularization

- L2-regularization conceptually restricts 'w' to a ball.





- L1-regularization restricts to the L1 "ball":
  - Solutions tend to be at corners where w_j are zero.

[Related Infinite Series video]

- L2-regularization
  - Can learn with *linear* number of irrelevant features.
    - E.g., only O(d) relevant features.

- L1-regularization
  - Can learn with **exponential** number of irrelevant features.
    - E.g., only O(log(d)) relevant features.
    - Paper on this result by Andrew Ng:
      - http://www.andrewng.org/portfolio/feature-selection-l1-vs-l2-regularization-and-rotational-invariance/

Some hyperparameter optimization software

- Hyperparameter tuning with scikit-learn:
  - https://github.com/hyperopt/hyperopt-sklearn
  - https://github.com/automl/auto-sklearn
  - https://sigopt.com/docs/overview/scikit_learn
- Other software (not scikit-learn specific):
  - https://github.com/rhiever/tpot
  - https://github.com/hyperopt/hyperopt
  - https://github.com/zygmuntz/hyperband
  - http://www.cs.ubc.ca/labs/beta/Projects/SMAC/
  - https://github.com/Yelp/MOE
  - https://github.com/mwhoffman/pybo
  - https://github.com/HIPS/Spearmint
  - https://github.com/rmcantin/bayesopt
  - https://github.com/PythonOptimizers/opal
- Note: this list is biased towards Bayesian optimization, since that's what I (Mike) know best. This list isn't meant to be exhaustive.
- The recently announced Amazon SageMaker also does hyperparameter optimization for you.