CPSC 340: Machine Learning and Data Mining

Over-Parameterized Models

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University of British Columbia, Fall 2022

https://www.students.cs.ubc.ca/~cs-340

Last Time: Neural Networks

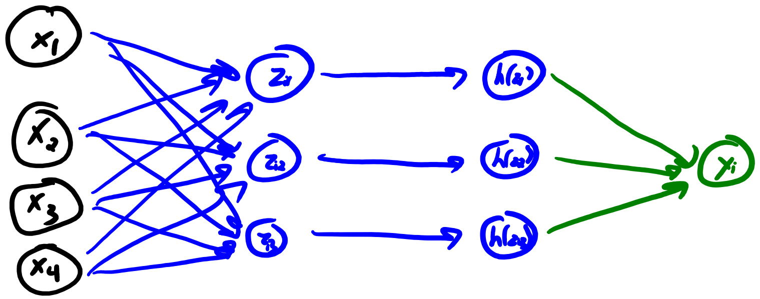
- Neural networks with one hidden layer:
  - Learn features and classifier at the same time.
  - Two linear transformations (W,v), separated by non-linearity (h):

$$\hat{y}_i = v^T h(W \underbrace{x_i}_{\text{input}})$$

Linear combination of "activations"

Non-linear transformation of each z_{ic}

"z_i": linear combination of input



  - Linear classification/regression using non-linearly transformed latent features z_i.
  - Optimize logistic/softmax loss (classification) or squared error loss (regression) using SGD:

$$\frac{1}{2}\sum_{i=1}^{n}\left(v^T h(Wx_i) - y_i\right)^2$$

(regression)

$$\sum_{i=1}^{n}\log\left(1+\exp(-y_i v^T h(Wx_i))\right)$$

(binary classification)

Is Training Neural Networks Scary?

- Learning:
  - For binary classification, the NLL under the sigmoid likelihood is:

$$f(W,v) = \sum_{i=1}^{n} \underbrace{\log(1+\exp(-y_i v^T h(Wx_i)))}_{f_i}$$

loss function on example 'i'

    - With 'W' fixed this is convex, but with both 'W' and 'v' as variables it is non-convex.
    - And finding the global optimum is NP-hard in general.
  - Nearly-always trained with variations on stochastic gradient descent (SGD).

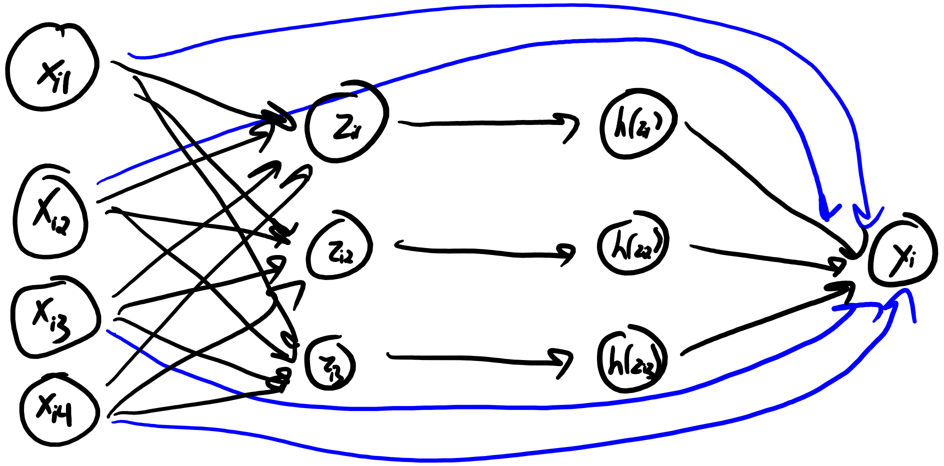
$$W^{k+1} = W^k - \alpha^k \nabla_W f_{i_k}(W^k, v^k)$$
$$v^{k+1} = v^k - \alpha^k \nabla_v f_{i_k}(W^k, v^k)$$

i_k is a training example chosen uniformly at random

    - Many variations exist (adding "momentum", AdaGrad, Adam, and so on).
    - But SGD is not guaranteed to reach a global minimum for non-convex problems.
- Is non-convexity a big drawback compared to logistic regression?
  - And if 'k' is large, is this likely to overfit?

Neural Networks ≥ Logistic Regression

- Consider a neural network with one hidden layer and connections from input to output layer.
  - The extra connections are called “skip” connections.



$$\hat{y}_i = \underbrace{w^T x_i}_{\text{linear model}} + \underbrace{v^T h(W x_i)}_{\text{neural network}}$$

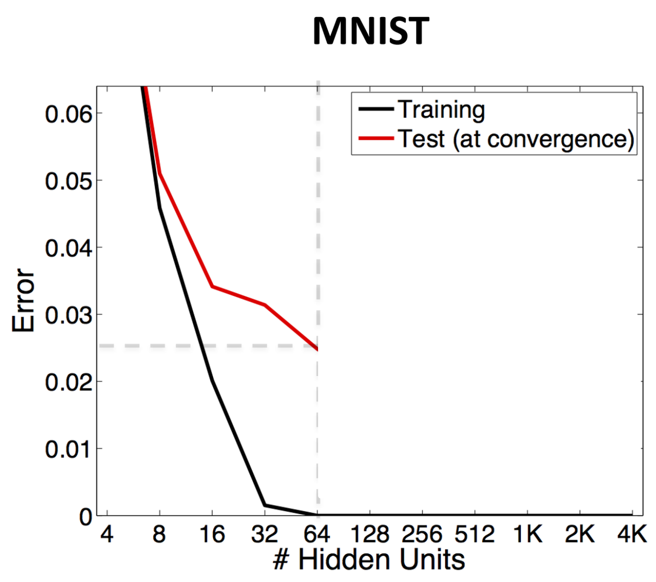
- You could first set v=0, then optimize ‘w’ using logistic regression.
  - This is a convex optimization problem that gives you the logistic regression model.
- You could then set ‘W’ and ‘v’ to small random values, and start SGD from the logistic regression model.
  - And if you are worried about overfitting, you could use early stopping based on validation set.
  - Even though this is non-convex, the neural network can only improve on logistic regression.

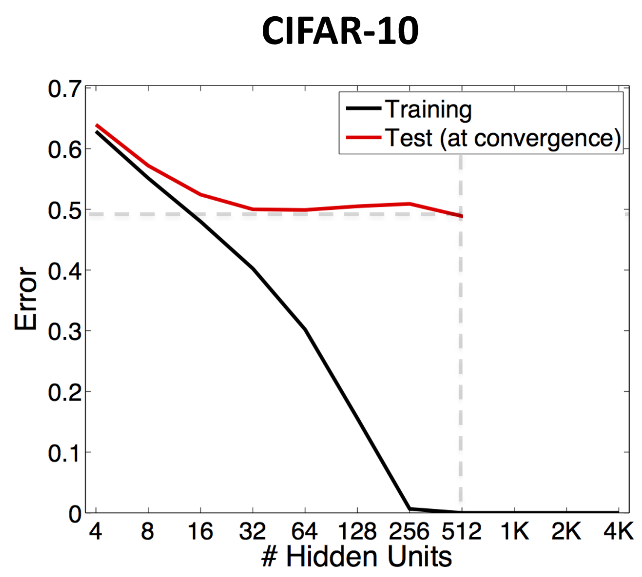
- In practice, we typically optimize everything at once (which usually works better than the above).

Next Topic: Over-Parameterized Models

“Hidden” Regularization in Neural Networks

- Fitting neural network with one hidden layer (SGD, no regularization):



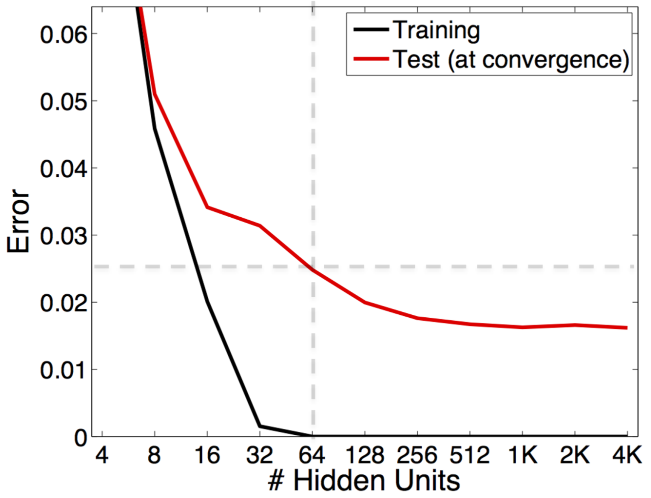


- On each step of the x-axis, the network is re-trained from scratch.
- Training error goes to 0 with enough units: we’re finding a global min.
- What should happen to test error as we increase size of hidden layer?

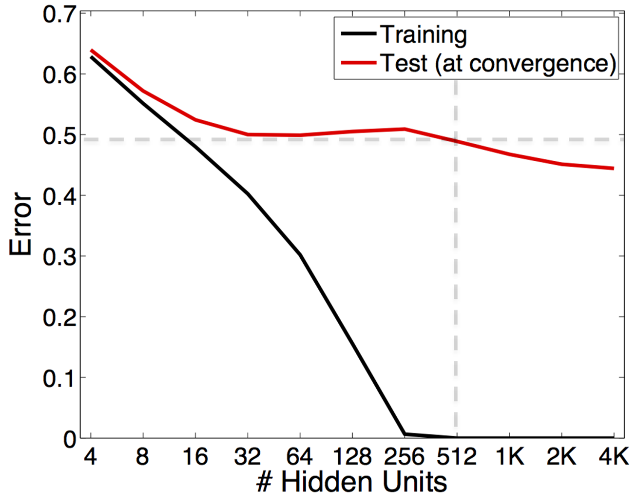
“Hidden” Regularization in Neural Networks

- Fitting neural network with one hidden layer (SGD, no regularization):

MNIST



CIFAR-10

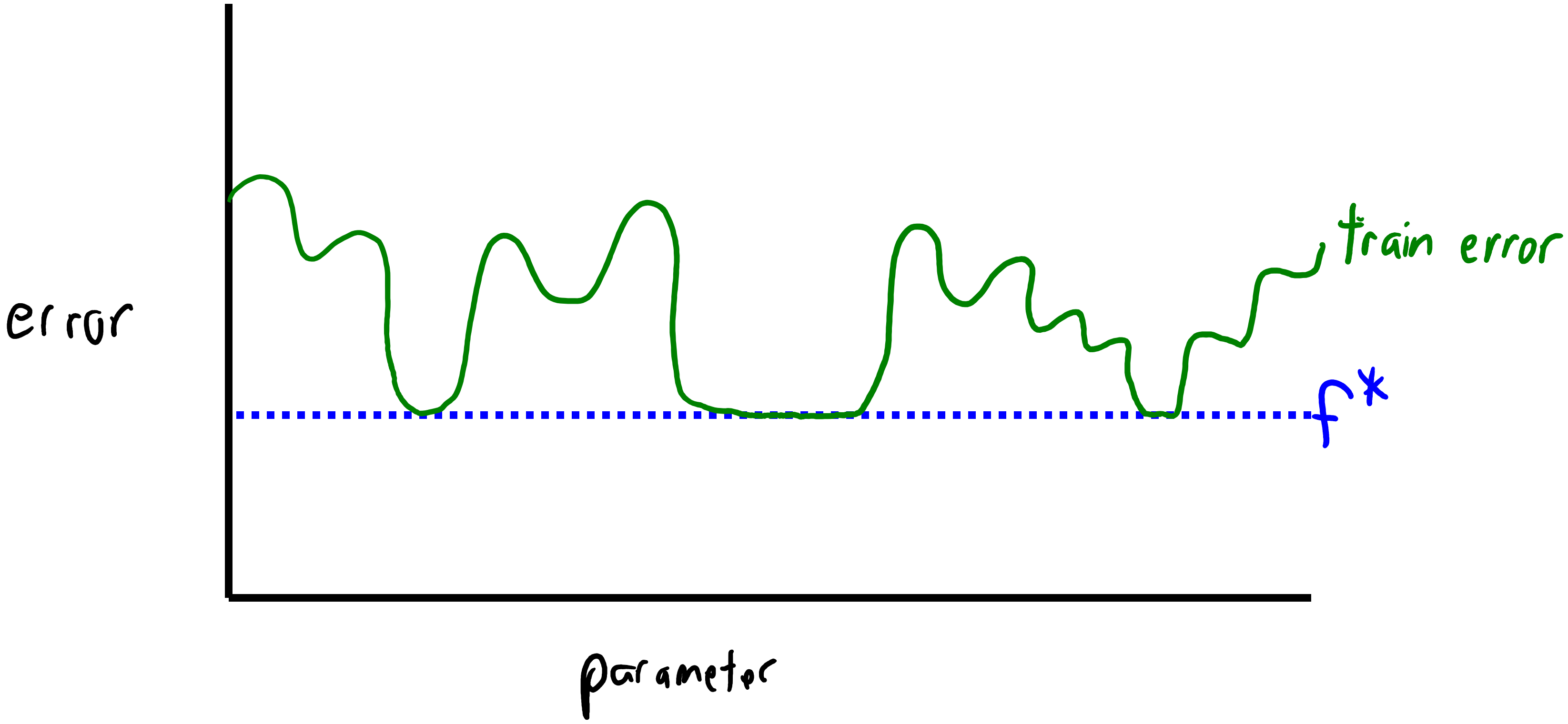


- Test error continues to go down!?! Where is fundamental trade-off??
  - Is it is still fundamental, but trade-off focuses on the “worst” global minimum.
- There do exist global mins with large #hidden units have test error = 1.
  - But among the global minima, SGD is somehow converging to “good” ones.

https://www.neyshabur.net/papers/inductive_bias_poster.pdf

Multiple Global Minima?

- For standard objectives, there is a global min function value f*:



Multiple Global Minima?

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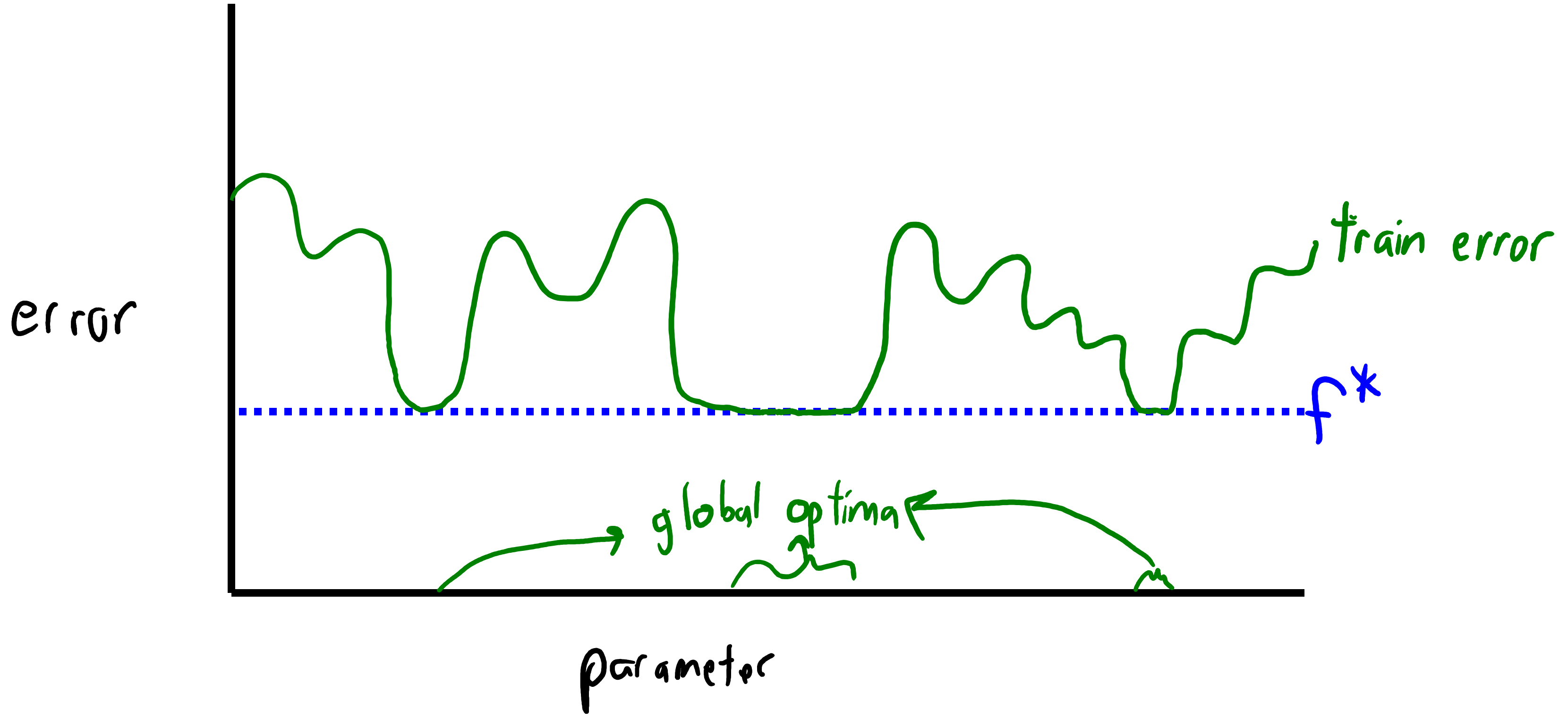
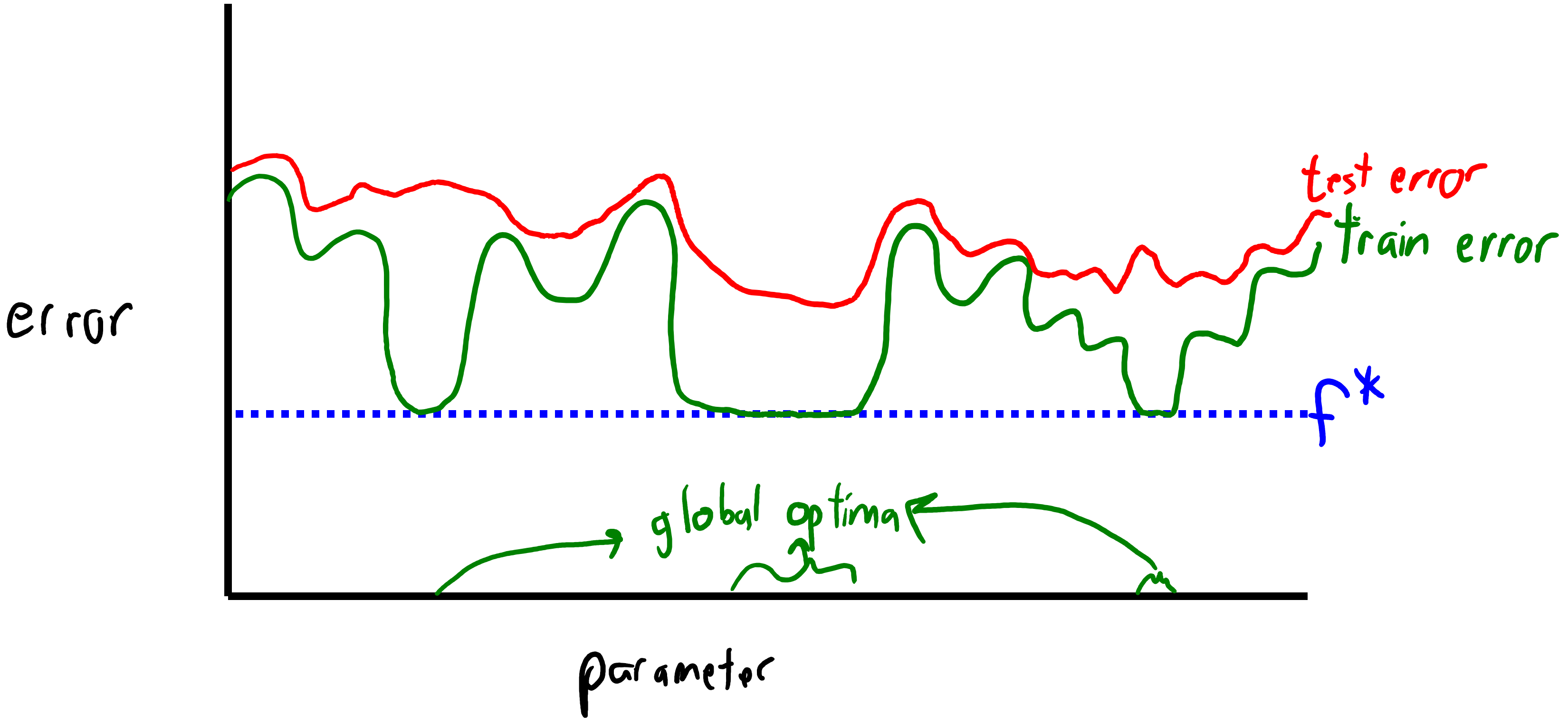


- But this may be achieved by many different parameter values.

Multiple Global Minima?



- These training error "global minima" may have very-different test errors.
- Some of these global minima may be more "regularized" than others.

Implicit Regularization of SGD

- There is empirical evidence SGD finds regularized parameters.
  - We call this the "implicit regularization" of the optimization algorithm.

- Beyond empirical evidence, we know this happens in simpler cases.

- An example of provable implicit regularization:
  - Consider a least squares problem where there exists a 'w' where Xw=y.
    - Residuals are all zero and we fit the data exactly for some 'w'.
  - You run gradient descent or SGD starting from w=0.
  - Converges to solution Xw=y that has the minimum L2-norm.
    - So using SGD is like using L2-regularization, but regularization is "implicit".
    - In this case, using w=X\y in Julia also gives you this regularized solution.

Implicit Regularization of SGD

- Another example of provable implicit regularization:
  - Consider a logistic regression problem where data is linearly separable.
    - A linear model can perfectly separate the data.
  - You run gradient descent from any starting point.
  - Converges to max-margin solution of the problem (minimum L2-norm solution).
    - So using gradient descent is equivalent to encouraging large margin.

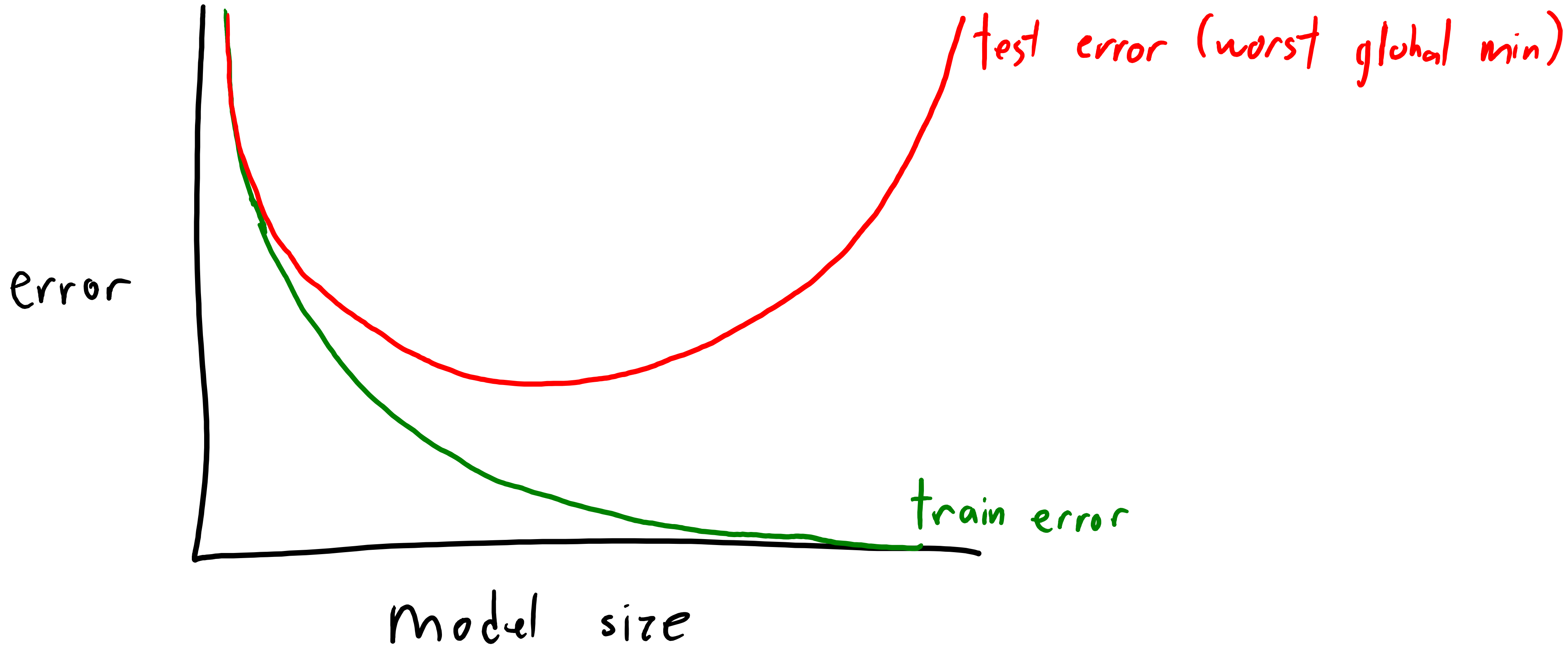
- Related implicit regularization results are known for boosting, matrix factorization, and linear neural networks.

Double Descent Curves

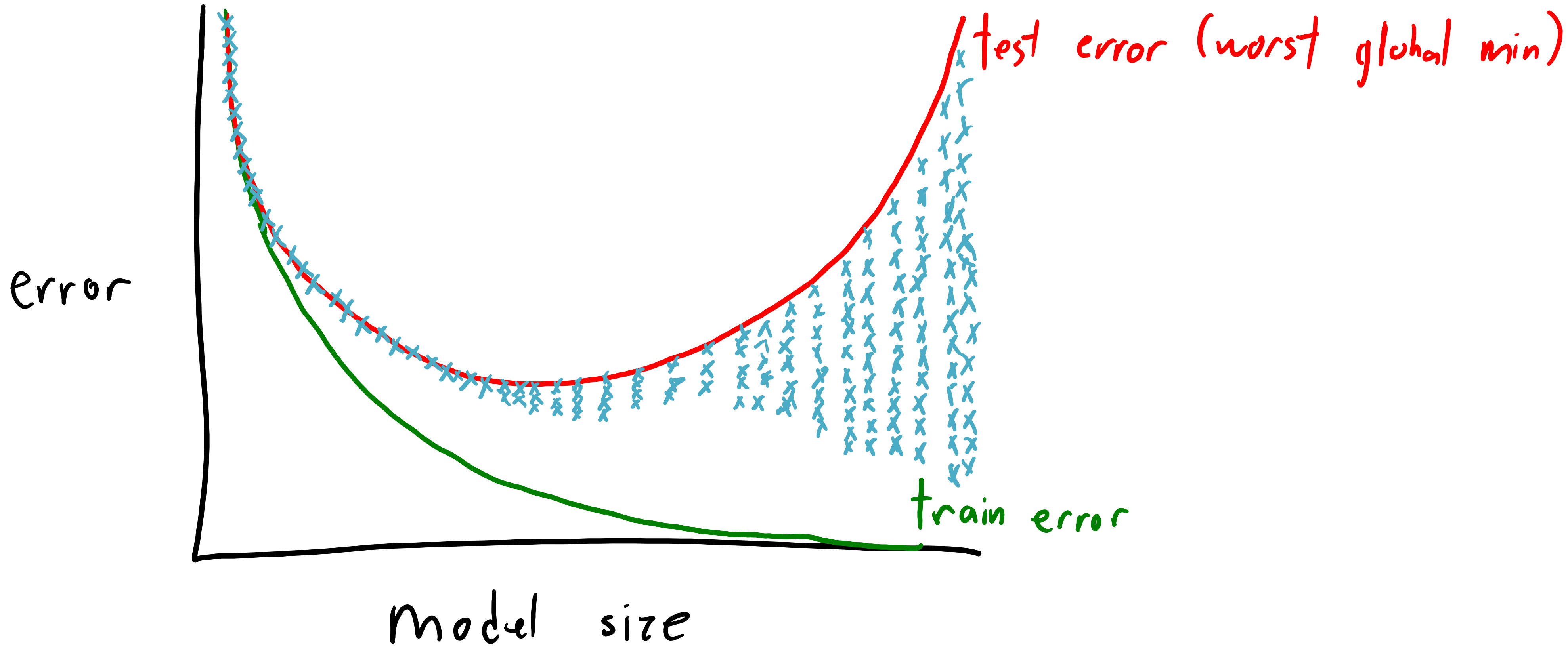
- What is going on???

https://openai.com/blog/deep-double-descent/

Worst vs. Best "Global Minimum"

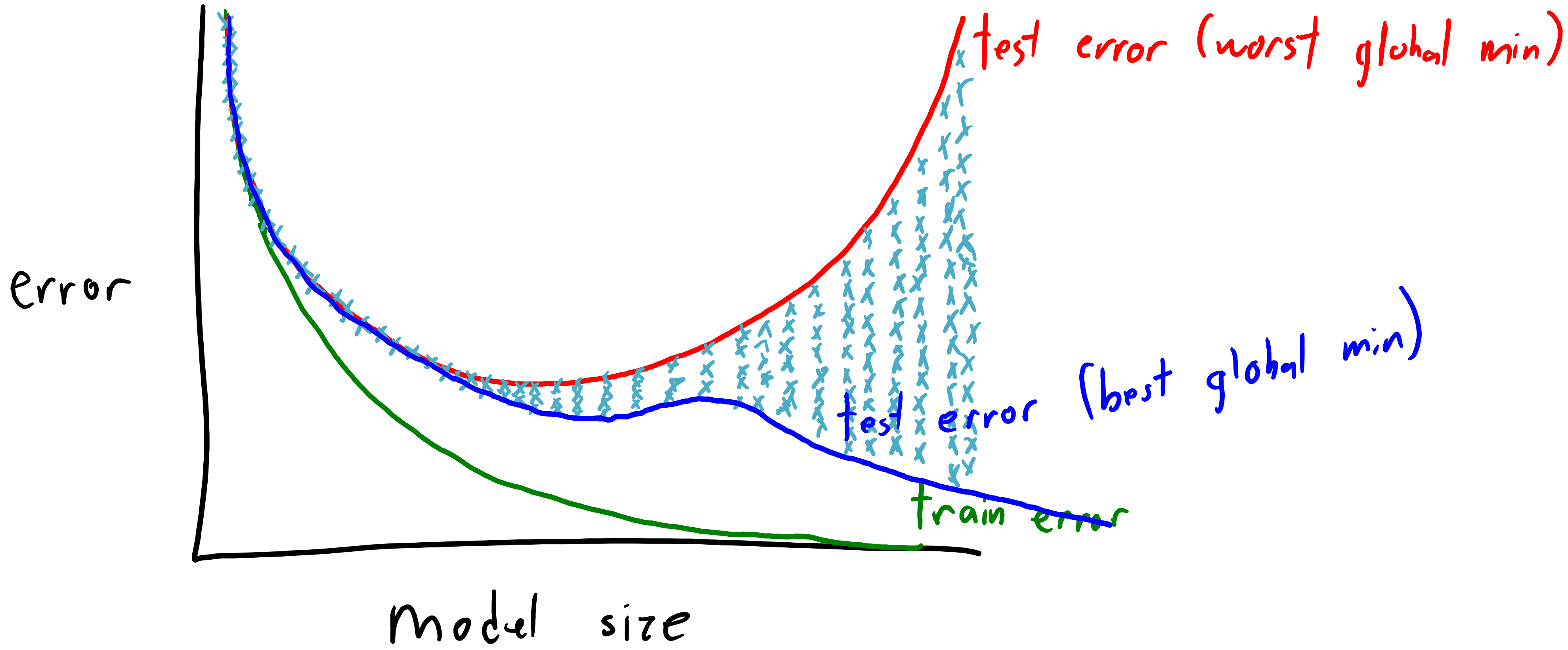


Worst vs. Best "Global Minimum"



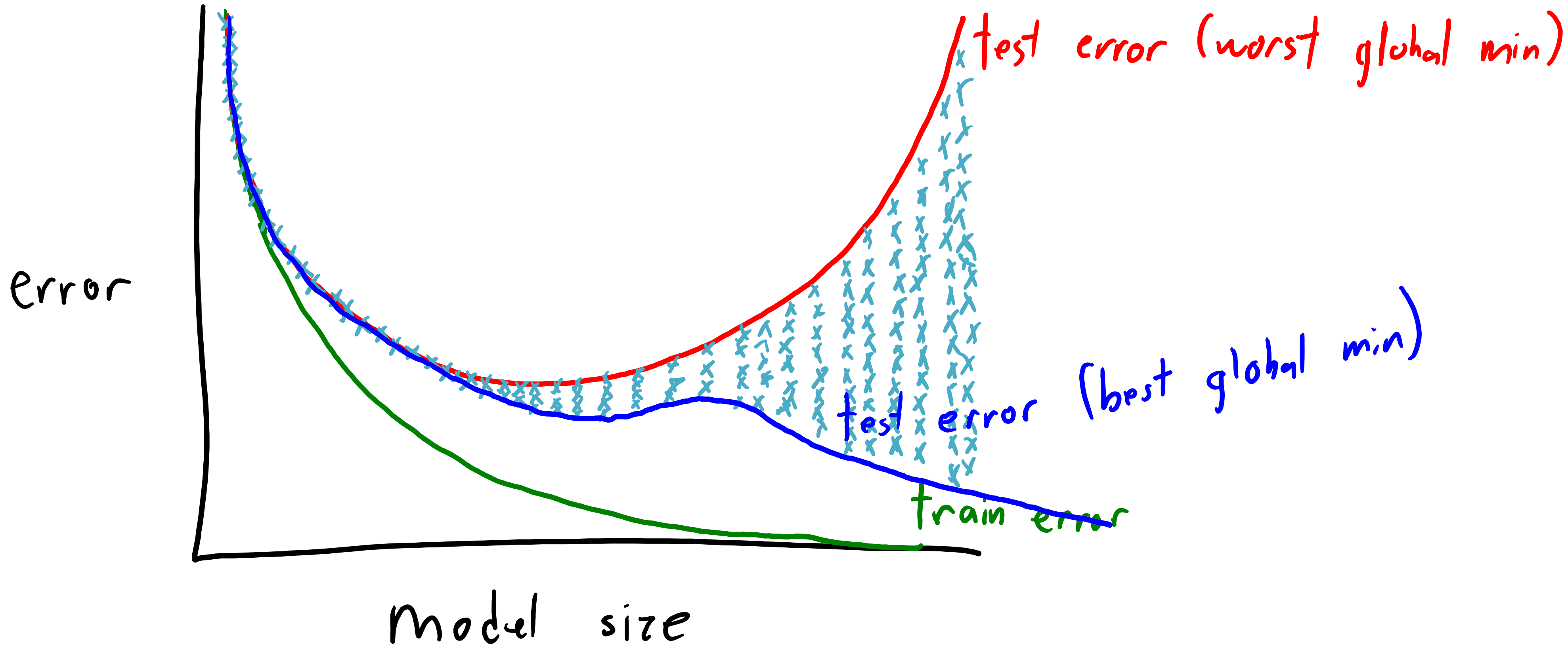
- Learning theory (trade-off) results analyze global min with worst test error.
  - Actual test error for different global minima will be better than worst case bound.
  - Theory is correct, but maybe "worst overfitting possible" is too pessimistic?

Worst vs. Best "Global Minimum"



- Consider instead the global min with best test error.
  - With small models, "minimize training error" leads to unique (or similar) global mins.
  - With larger models, there is a lot of flexibility in the space of global mins (gap between best/worst).
- Gap between "worst" and "best" global min can grow with model complexity.

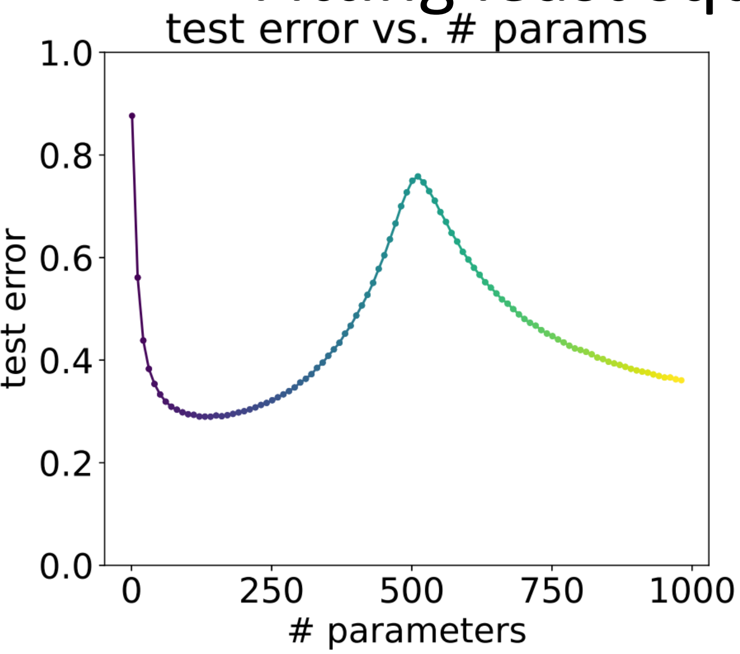
Worst vs. Best "Global Minimum"



- Can get "double descent" curve in practice if parameters roughly track "best" global min shape.
  - One way to do this: increase regularization as you increase model size.
- Maybe "neural network trained with SGD" has "more implicit regularization for bigger models"?
  - But "double descent" is not specific to implicit regularization of SGD and not specific to neural networks.

Double Descent on a Linear Least Squares Problem

- Fitting least squares with gradient descent (n=500):



https://cs229.stanford.edu/lectures-spring2022/main_notes.pdf

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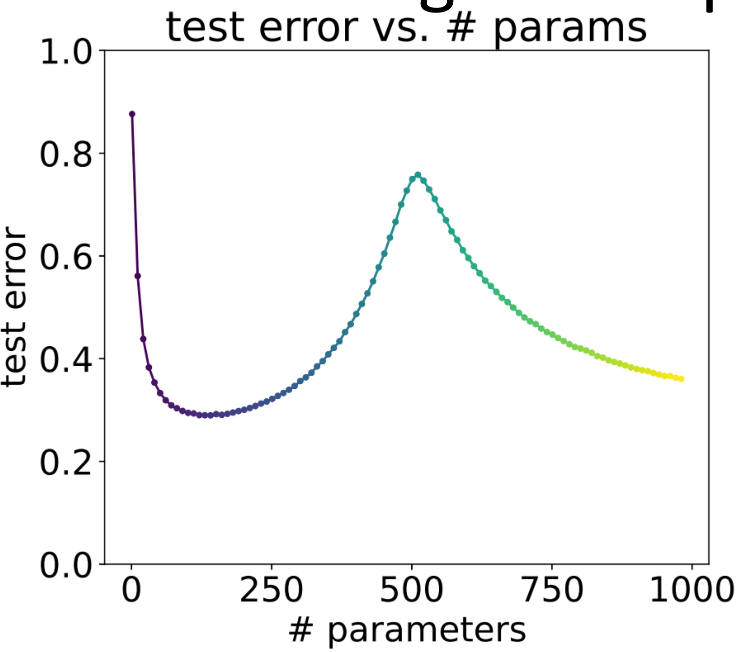

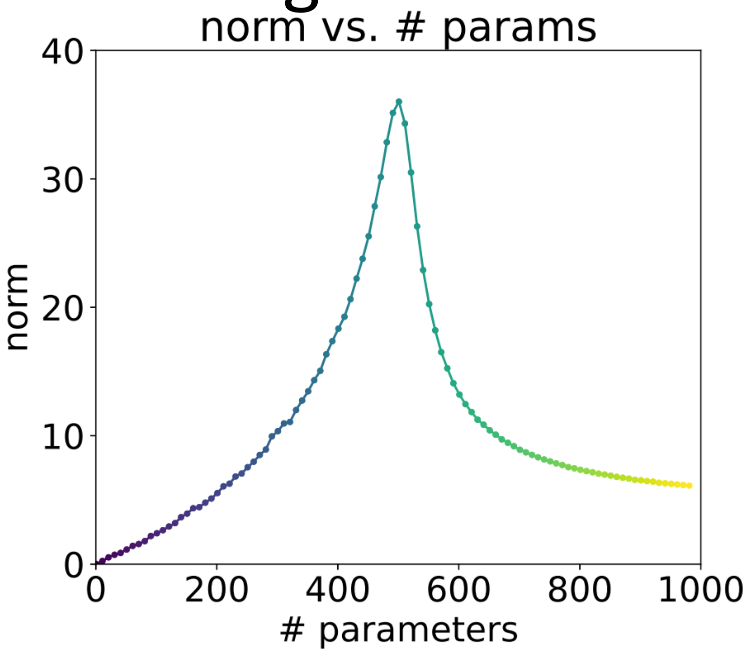

- ||w|| increases until you fit data exactly (only one ‘w’ fits exactly).
- Then norm of parameters starts decreasing (many ‘w’ can fit exactly).
  - So implicit regularization of gradient descent gives lower norm ‘w’ values.

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Double Descent on a Linear Least Squares Problem

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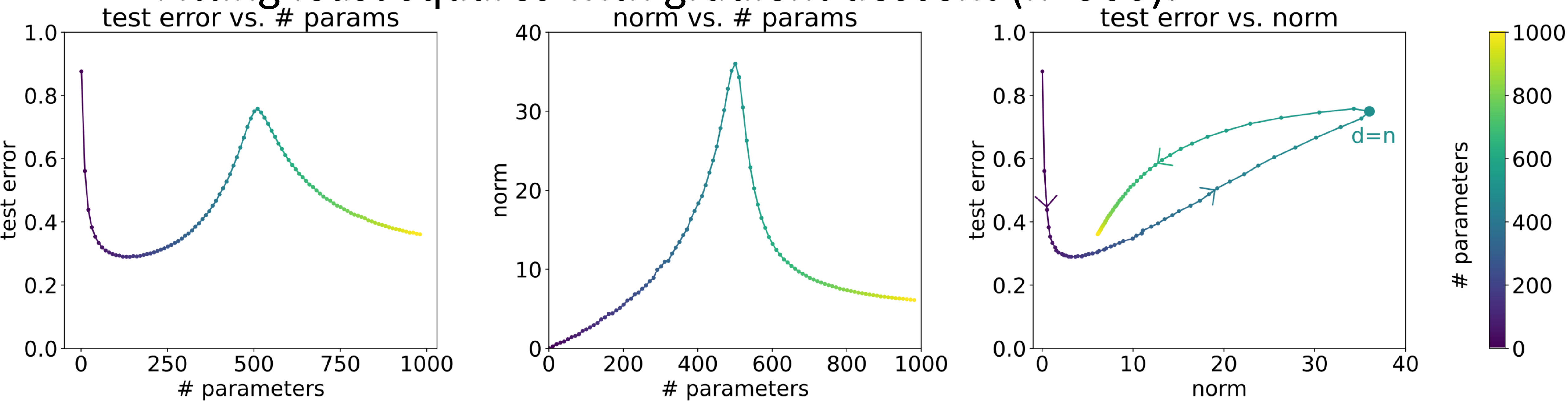
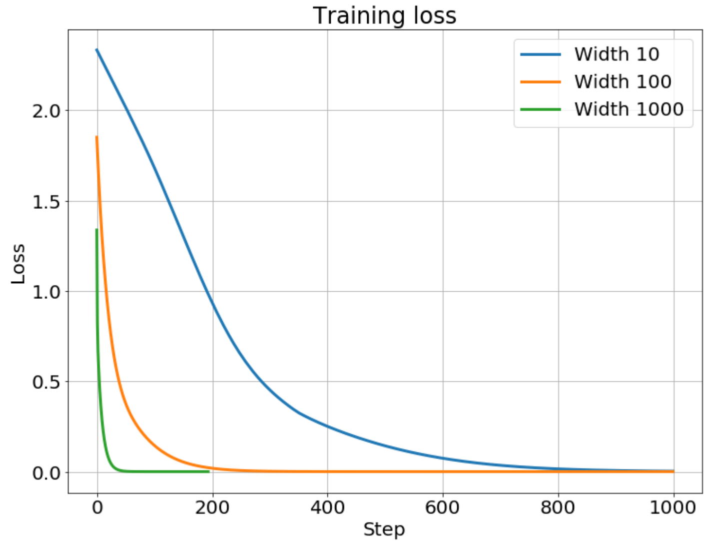


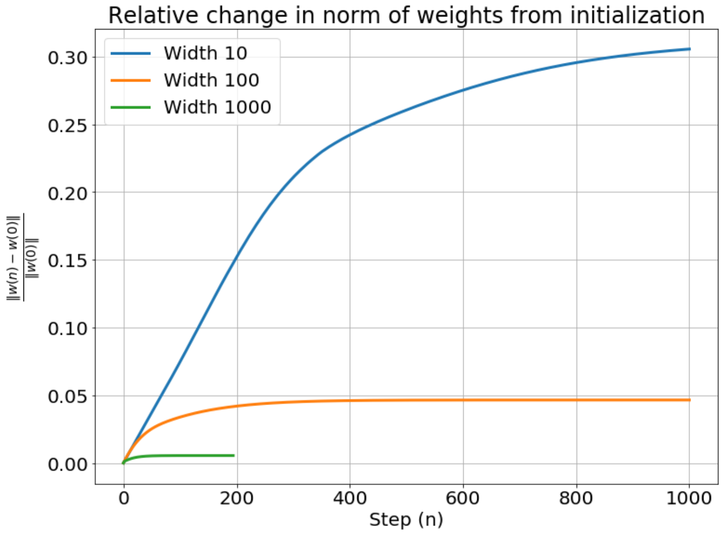
- We see fundamental trade-off if we plot error vs. norm.
  - After we have fit data exactly, models are less “complicated” as we add more parameters.
- Can also make double descent curves by increasing explicit regularization.
- Under right conditions, can see double descent in other models like random forests.

https://cs229.stanford.edu/lectures-spring2022/main_notes.pdf

Implicit Regularization of SGD for Neural Networks

- For neural networks, why would
  SGD implicit regularization increase with number of hidden units?
  - Similar to least squares, maybe SGD finds low-norm solutions?
    - In higher-dimensions, there is flexibility in global mins to have a low norm?
  - Maybe SGD stays closer to starting point as we increase dimension?
    - This would be more like a regularizer of the form $||w - w^0||$.





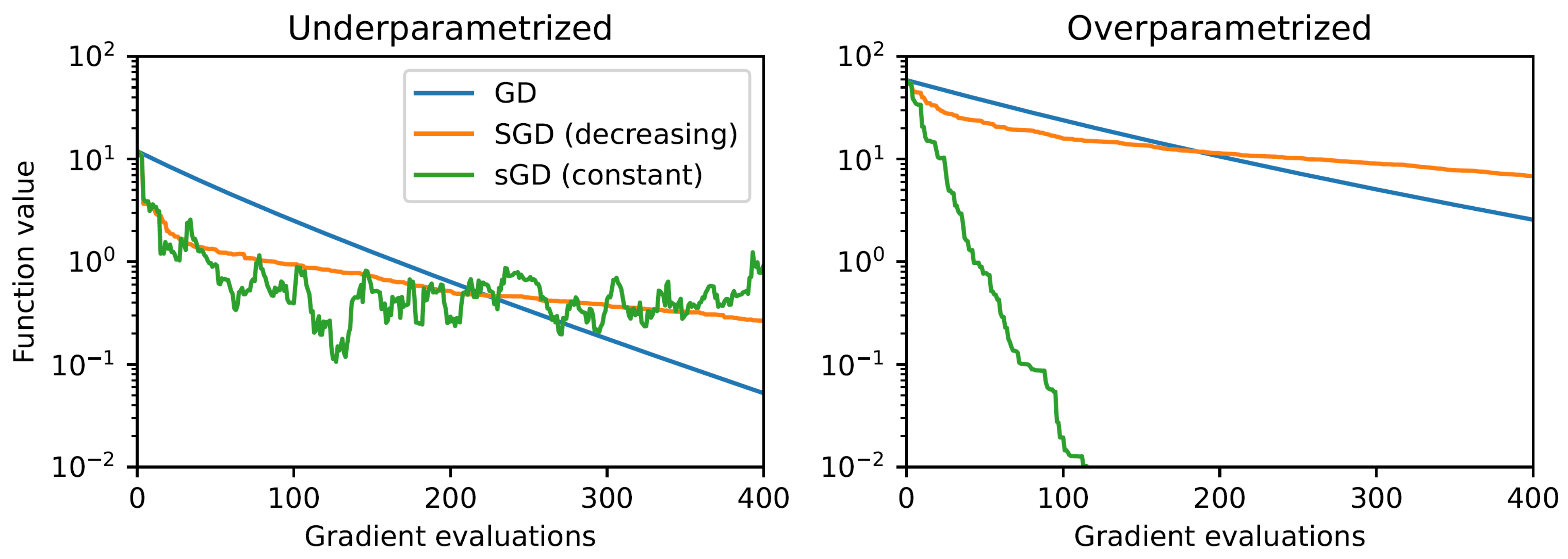
Over-Parameterization and SGD

- Over-parameterized model:
  - A model that has more parameters than needed to fit data exactly.
- Amazing properties of SGD for many over-parameterized models:
  - SGD tends to find a global minimum of training error.
  - SGD tends to have implicit regularization.
  - SGD converges with a constant step size.
    - At nearly the speed of gradient descent.

- Why can SGD converge with a constant step size?
  - Variation in gradients is 0 at solutions that fit all training examples.
    - No “region of confusion”.

Over-Parameterization and SGD

- Gradient descent vs. SGD for under/over-parameterized least squares:

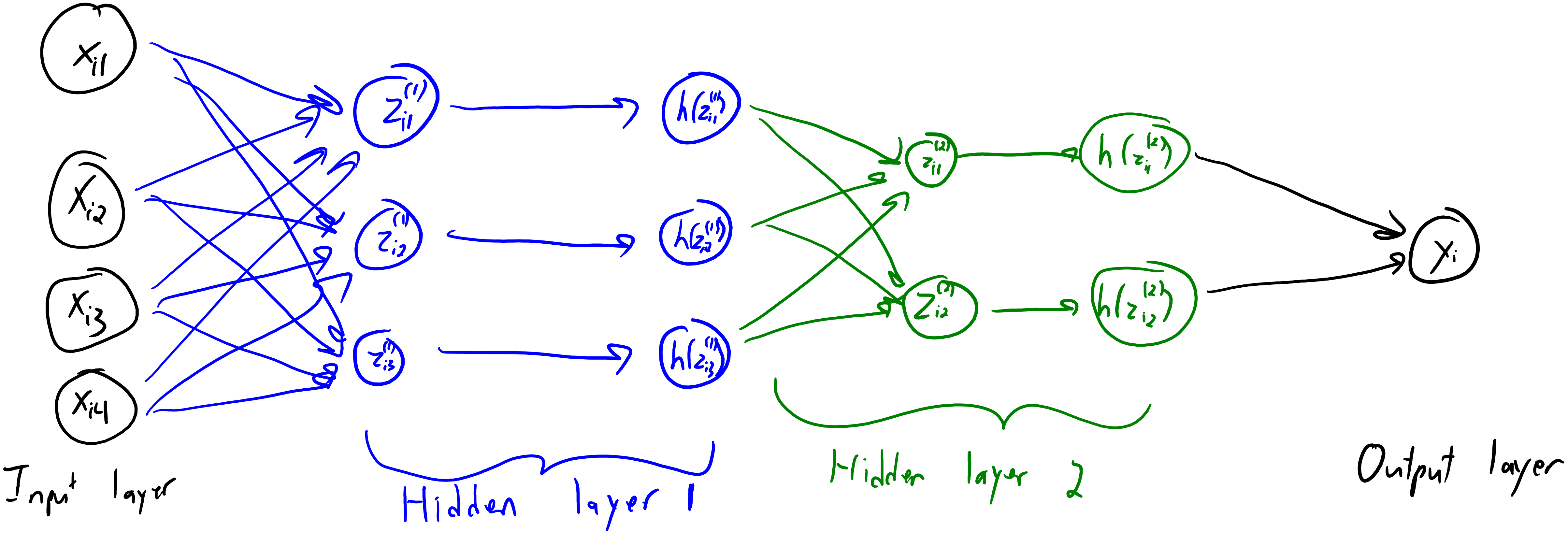


  - No need to decrease step sizes or increase batch sizes for over-parameterized.
    - And nice ways to set the step size as you go (“painless SGD”, “Polyak step size”).
  - Still expect good performance if you are close to being over-parameterized.

Next Topic: Deep Learning

Deep Learning (As a Picture)

- Deep learning models have more than one hidden layer:



- We apply linear transformation and activation function at each "layer".

Deep Learning (As a Function)

Linear model:

$$\hat{y}_i = w^T x_i$$

Neural network with 1 hidden layer:

$$\hat{y}_i = v^T h(\underbrace{W x_i}_{z_i})$$

Neural network with 2 hidden layers:

$$\hat{y}_i = v^T h(\underbrace{W^{(2)} h(\underbrace{W^{(1)} x_i}_{z_i^{(1)}})}_{z_i^{(2)}})$$

Neural network with 3 hidden layers

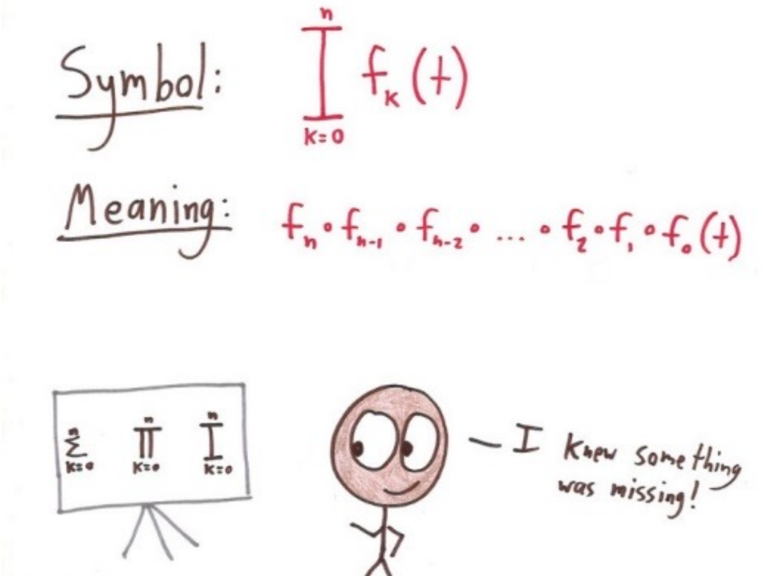
$$\hat{y}_i = v^T h(\underbrace{W^{(3)} h(\underbrace{W^{(2)} h(\underbrace{W^{(1)} x_i}_{z_i^{(1)}})}_{z_i^{(2)}})}_{z_i^{(3)}})$$

Neural network with 4 hidden layers:

$$\hat{y}_i = v^T h(W^{(4)} h(W^{(3)} h(W^{(2)} h(W^{(1)} x_i))))$$

With 'm' layers we could use:

$$\hat{y}_i = v^T \left(\mathop{\mathrm{I}}\limits_{\ell=1}^{m} h(W^{(\ell)} x_i) \right)$$



Prediction with Deep Neural Networks

- The "textbook" choice for deep neural networks:
  - Alternate between doing linear transformations and non-linear transforms.

$$\hat{y}_i = v^T h(W^4 h(W^3 h(W^2 h(W^1 x_i))))$$

  - Each "layer" might have a different size.
    - W^1 is $k^1 \times d$.
    - W^2 is $k^2 \times k^1$.
    - W^3 is $k^3 \times k^2$.
    - W^4 is $k^4 \times k^3$.
    - v is $k^4 \times 1$.

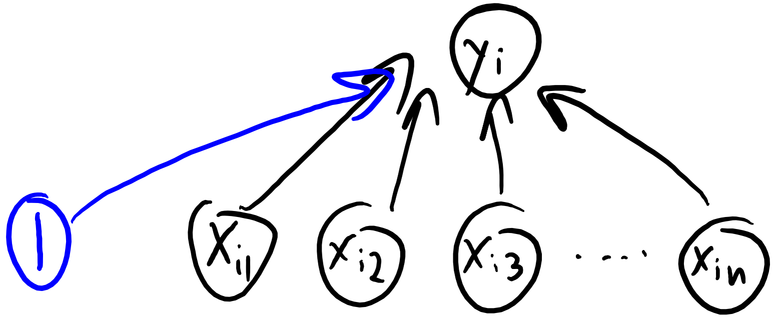
```
z[1] = W1*x
for layer in 2:nLayers
    z[layer] = Wm[layer-1]*h(z[layer-1])
end
yhat = v'*h(z[end])
```

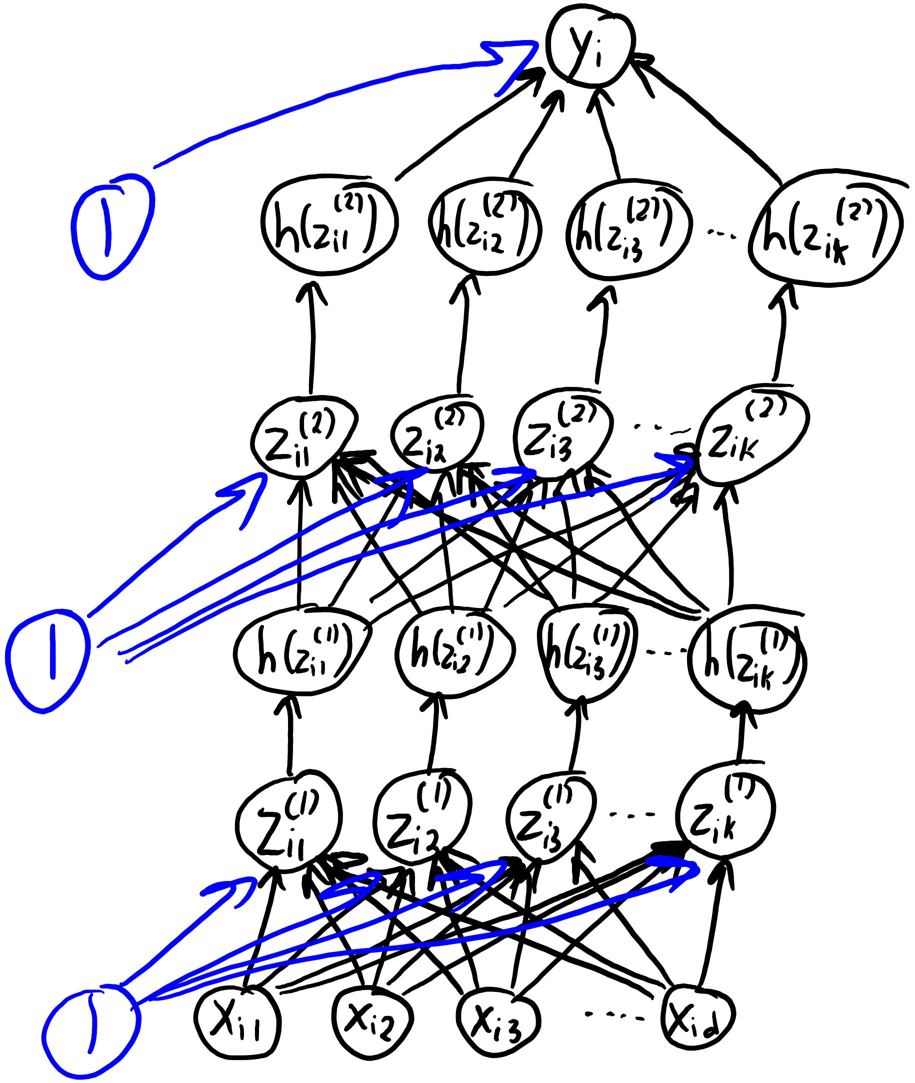
  - We often use the same non-linear transform, such as sigmoid, at each layer.
  - Cost for prediction, which is called "forward propagation":
    - Cost of the matrix multiplies: $O(k^1 d + k^2 k^1 + k^3 k^2 + k^4 k^3)$
    - Cost of the non-linear transforms is $O(k^1 + k^2 + k^3 + k^4)$, so does not change cost.
  - Only need to change last layer based on task (like regression or classification).
    - Squared error, logistic, softmax, and so on.

Adding Bias Variables

- We typically add a bias to each layer:

Linear model with bias:





Summary

- Empirical "good news" for training neural networks with SGD:
  - With enough hidden units, SGD often finds a global minimum.
- Implicit regularization and double descent curves.
  - Possible explanations for why neural networks often generalize well.
- Over-parameterized models, that can fit data exactly.
  - SGD converges fast with a constant step size for these models.
- Deep learning:
  - Neural networks with multiple hidden layers.

- Next time: "Where is my gradient?"