

Deep Learning for Data Science

DS 542

<https://dl4ds.github.io/fa2025/>

Measuring Performance and Generalization



Plan for Today

- MNIST1D dataset model and performance
- Noise, bias, and variance
- Reducing variance
- Reducing bias & bias-variance trade-off
- Double descent
- Choosing hyperparameters

MNIST1D

Scaling down Deep Learning

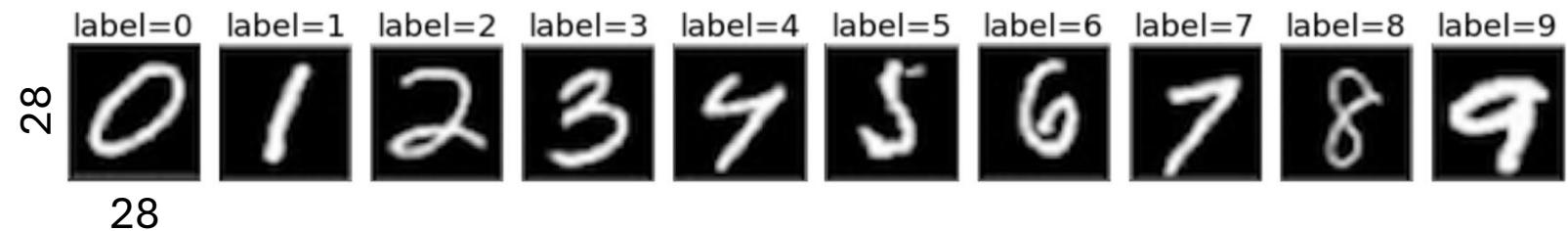
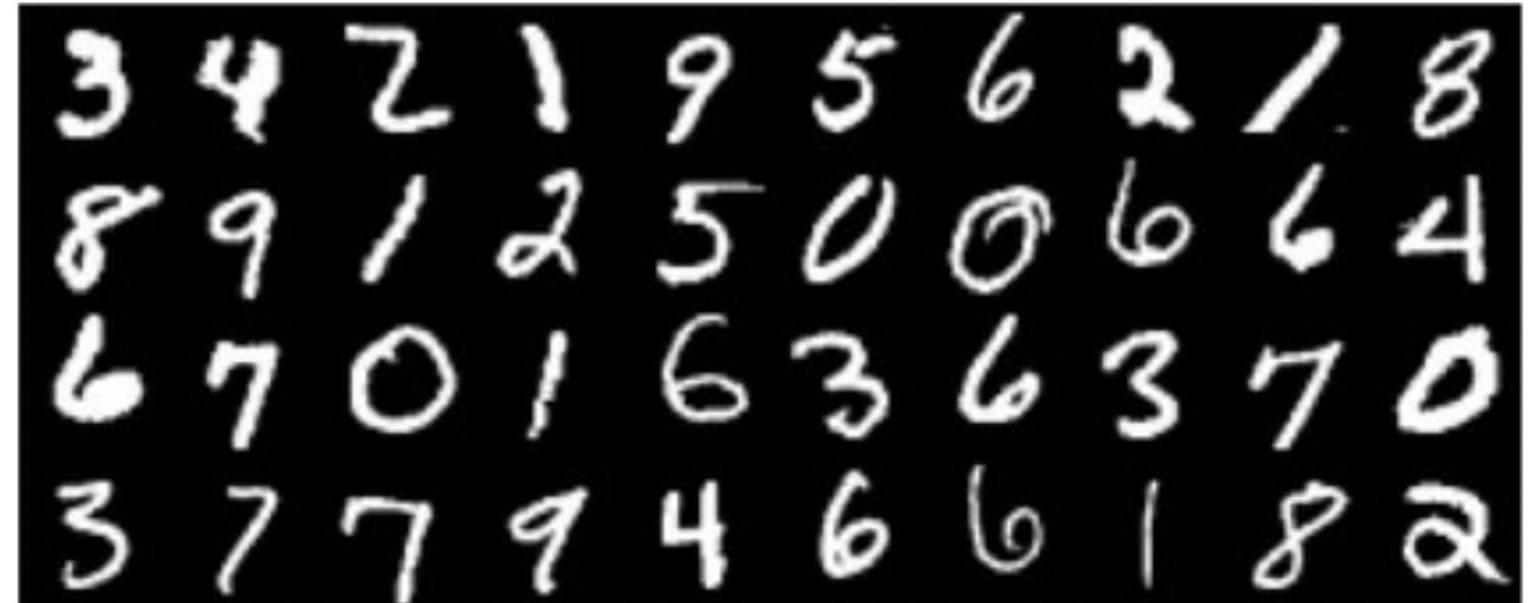
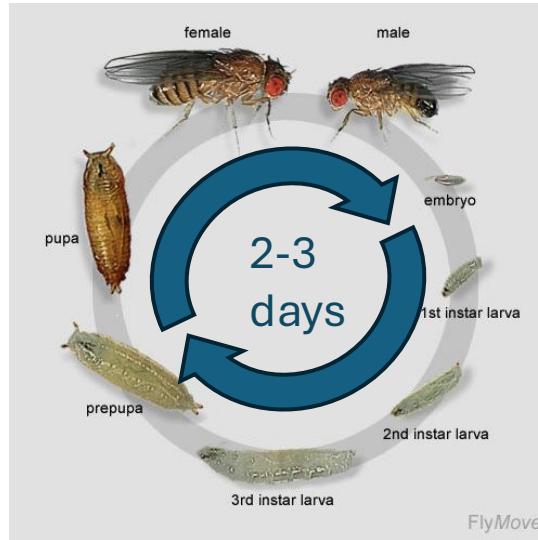
Sam Greydanus¹

“A large number of deep learning innovations including [dropout](#), [Adam](#), [convolutional networks](#), [generative adversarial networks](#), and [variational autoencoders](#) began life as MNIST experiments. Once these innovations proved themselves on small-scale experiments, scientists found ways to scale them to larger and more impactful applications.”

S. Greydanus, “Scaling down Deep Learning.” arXiv, Dec. 04, 2020. doi:
[10.48550/arXiv.2011.14439](https://doi.org/10.48550/arXiv.2011.14439)
<https://github.com/greydanus/mnist1d>

MNIST Dataset

- 28x28x1 grayscale images
- 60K Training, 10K Test
- “Is to Deep Learning what fruit flies are to genetics research”



But poorly differentiates model performance:

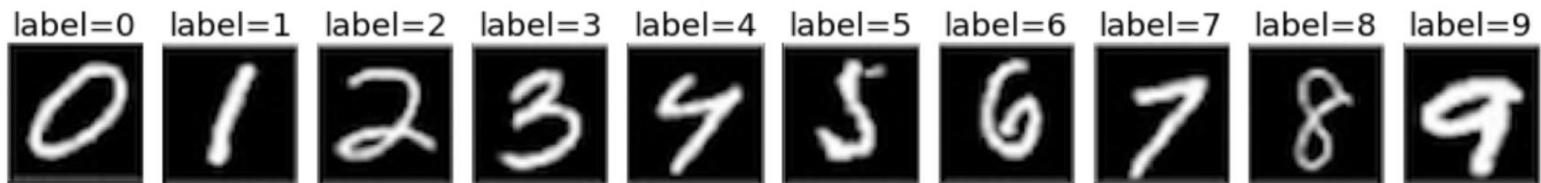
Model Type	Accuracy
Logistic Regression	94%
MLP	99+%
CNN	99+%

MNIST 1D Dataset

Fixed, 1-D, length-12
templates for each of 10
digit classes

Generate dataset by
programmatically applying
6 parametric
transformations.

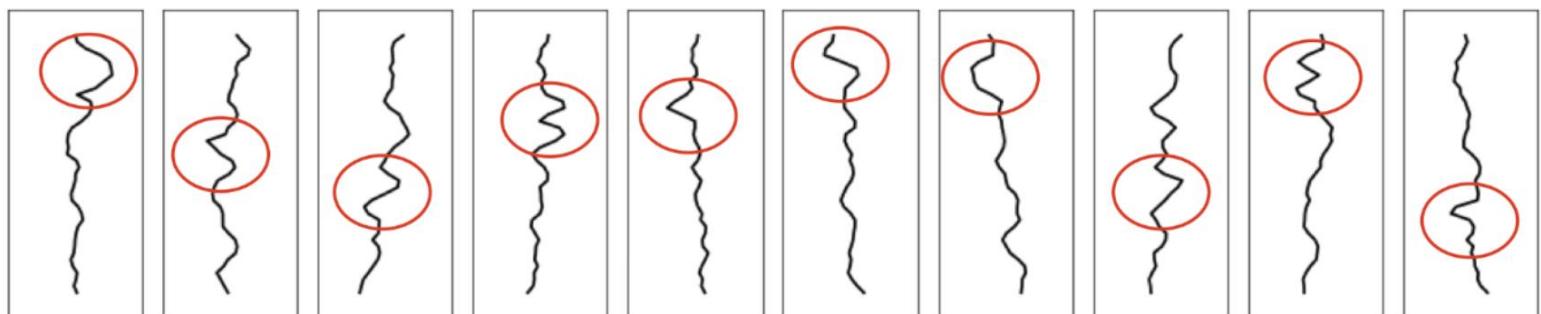
Original MNIST examples



Represent digits as 1D patterns



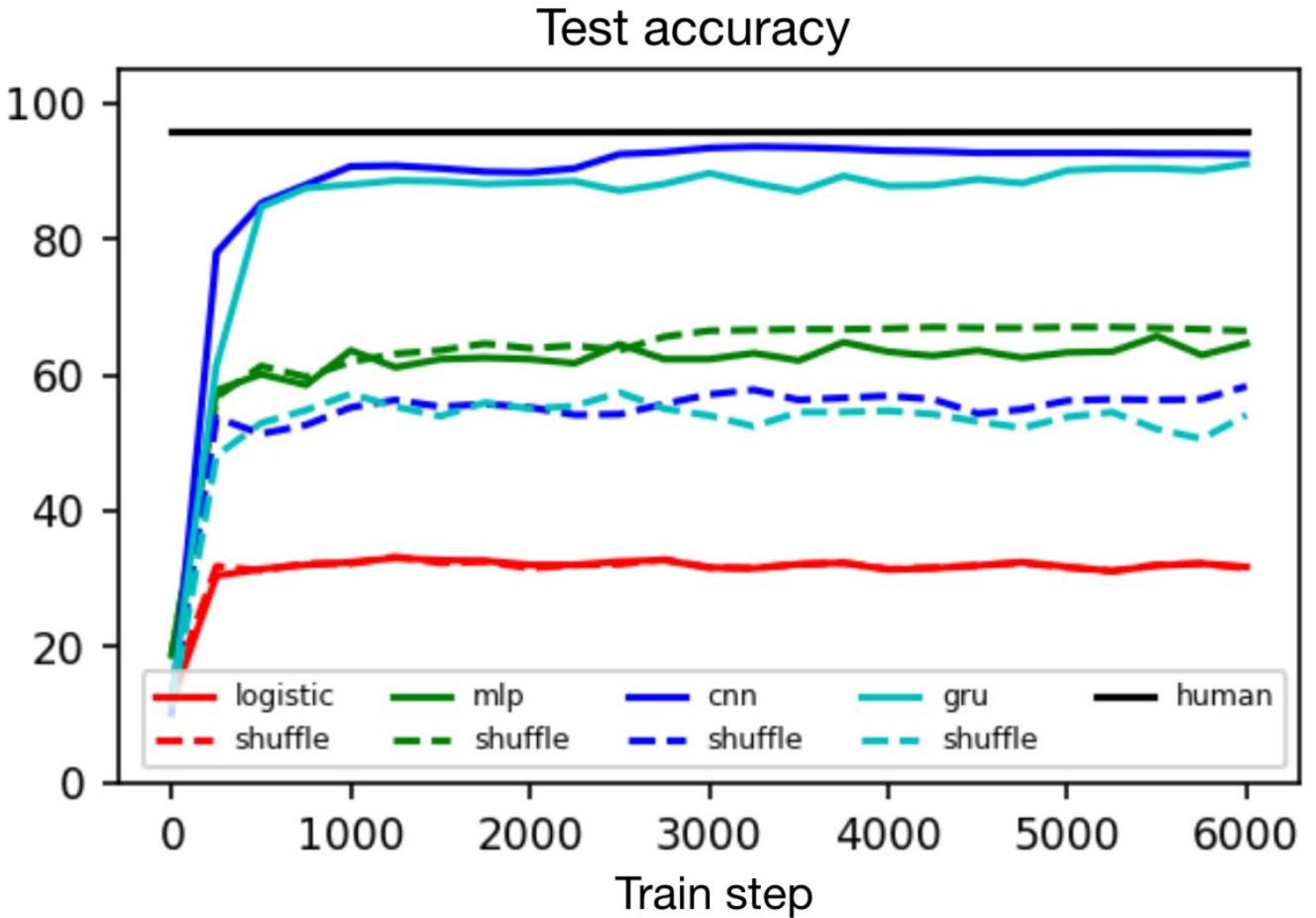
Pad, translate & transform



E.g. pad, shear, translate, correlated noise, i.i.d. noise, interpolation.

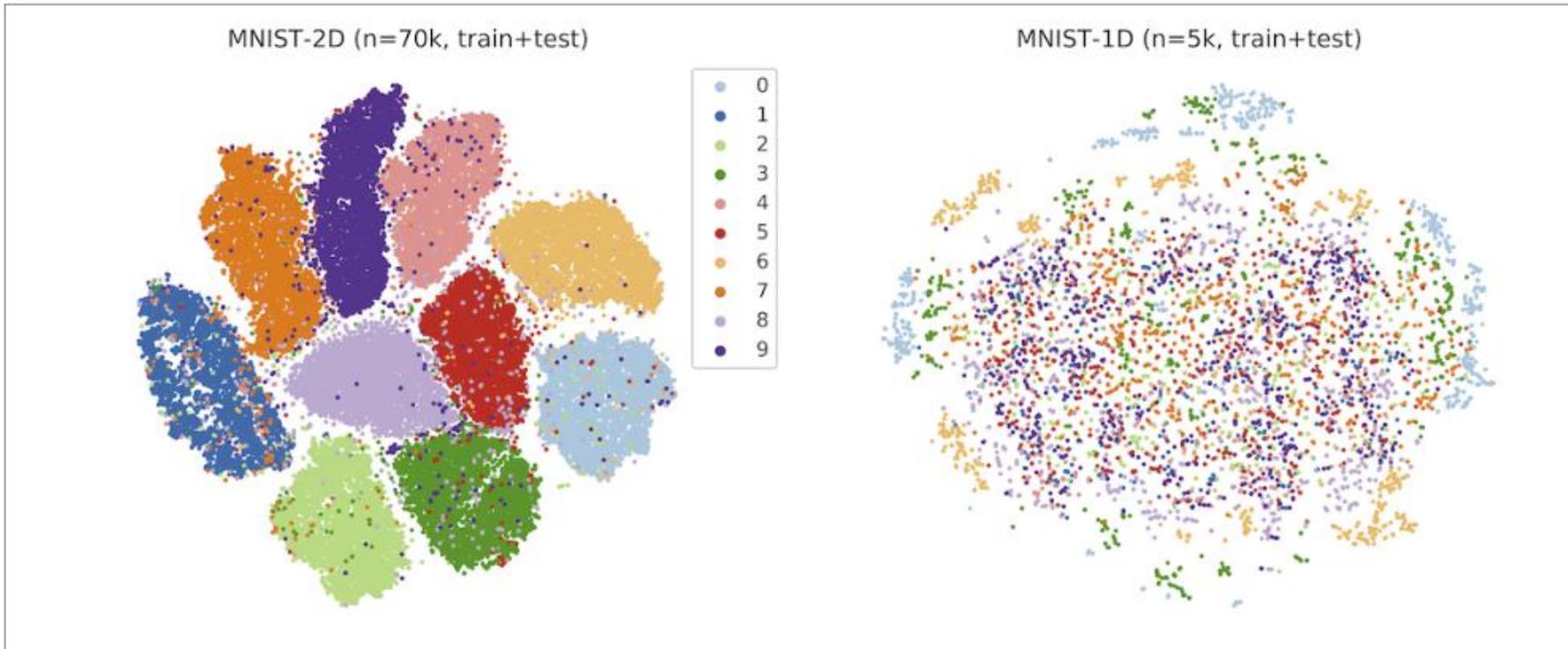
MNIST 1D

Differentiates performance of different model types much more than MNIST



Dataset	Logistic regression	Fully connected model	Convolutional model	GRU model	Human expert
MNIST	94 ± 0.5	> 99	> 99	> 99	> 99
MNIST-1D	32 ± 1	68 ± 2	94 ± 2	91 ± 2	96 ± 1
MNIST-1D (shuffled)	32 ± 1	68 ± 2	56 ± 2	57 ± 2	$\approx 30 \pm 10$

Visualizing MNIST and MNIST-1D with tSNE



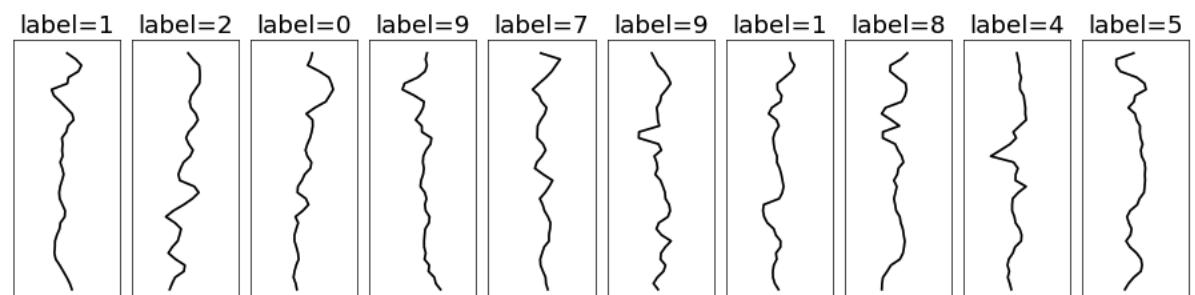
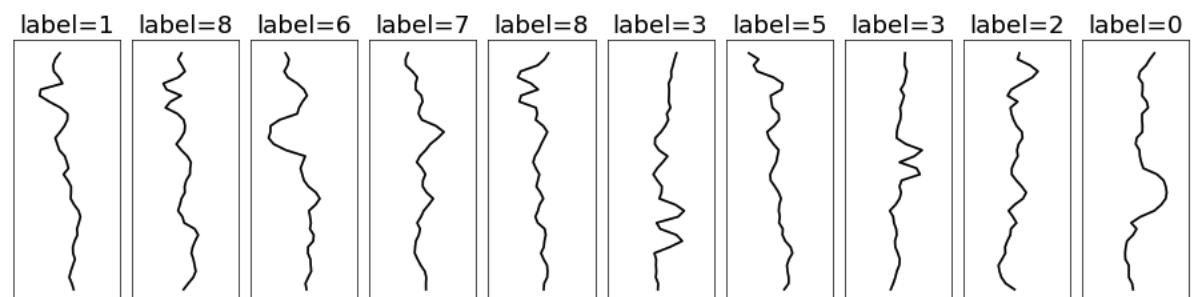
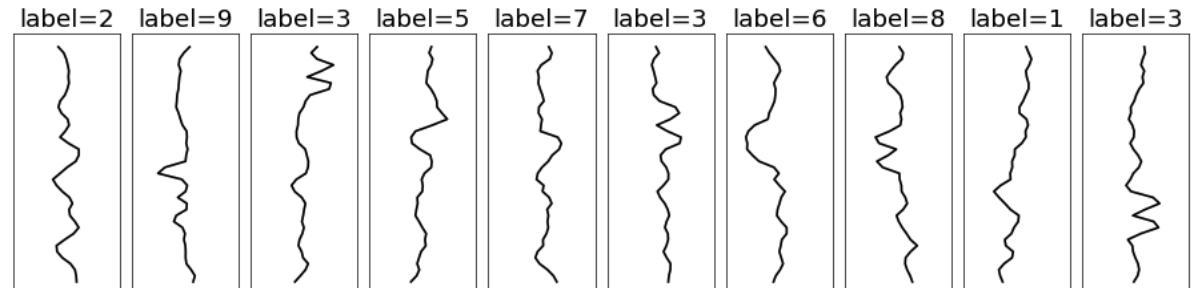
Visualizing the MNIST and MNIST-1D datasets with tSNE. The well-defined clusters in the MNIST plot indicate that the majority of the examples are separable via a kNN classifier in pixel space. The MNIST-1D plot, meanwhile, reveals a lack of well-defined clusters which suggests that learning a nonlinear representation of the data is much more important to achieve successful classification. Thanks to [Dmitry Kobak](#) for making this plot.

<https://twitter.com/hippopedoid>

MNIST1D Train and Test Set

- 1D, Length 40 samples
- 4,000 training samples
- 1,000 test samples (80/20 split)

Dataset Samples



Network

- 40 inputs
- 10 outputs
- Two hidden layers
 - 100 hidden units each
- SGD with batch size 100, learning rate 0.1
- 6000 steps (?? Epochs)

```
# choose cross entropy loss function
loss_function = torch.nn.CrossEntropyLoss()

# construct SGD optimizer and initialize learning rate and momentum
optimizer = torch.optim.SGD(model.parameters(), lr = 0.1)

# object that decreases learning rate by half every 10 epochs
scheduler = StepLR(optimizer, step_size=10, gamma=0.5)

# load the data into a class that creates the batches
data_loader = DataLoader(TensorDataset(x_train,y_train), batch_size=100, shuffle=True)
```

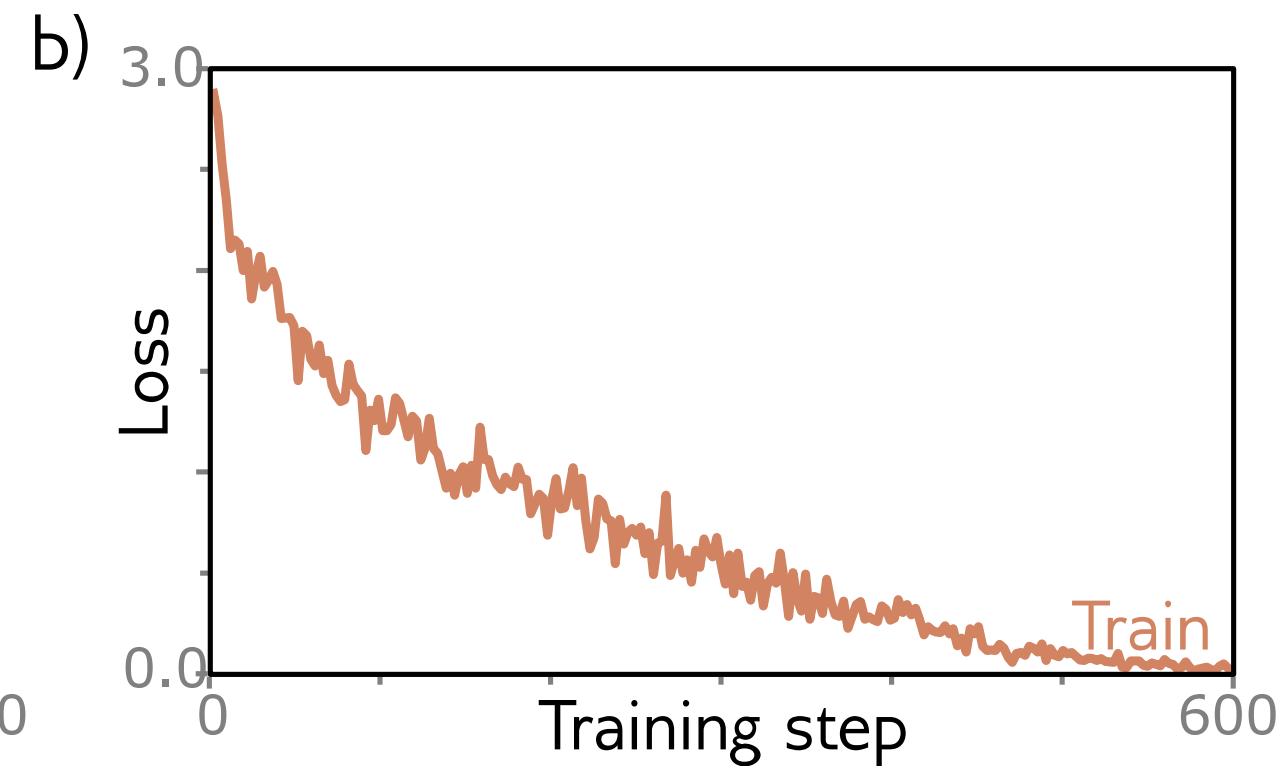
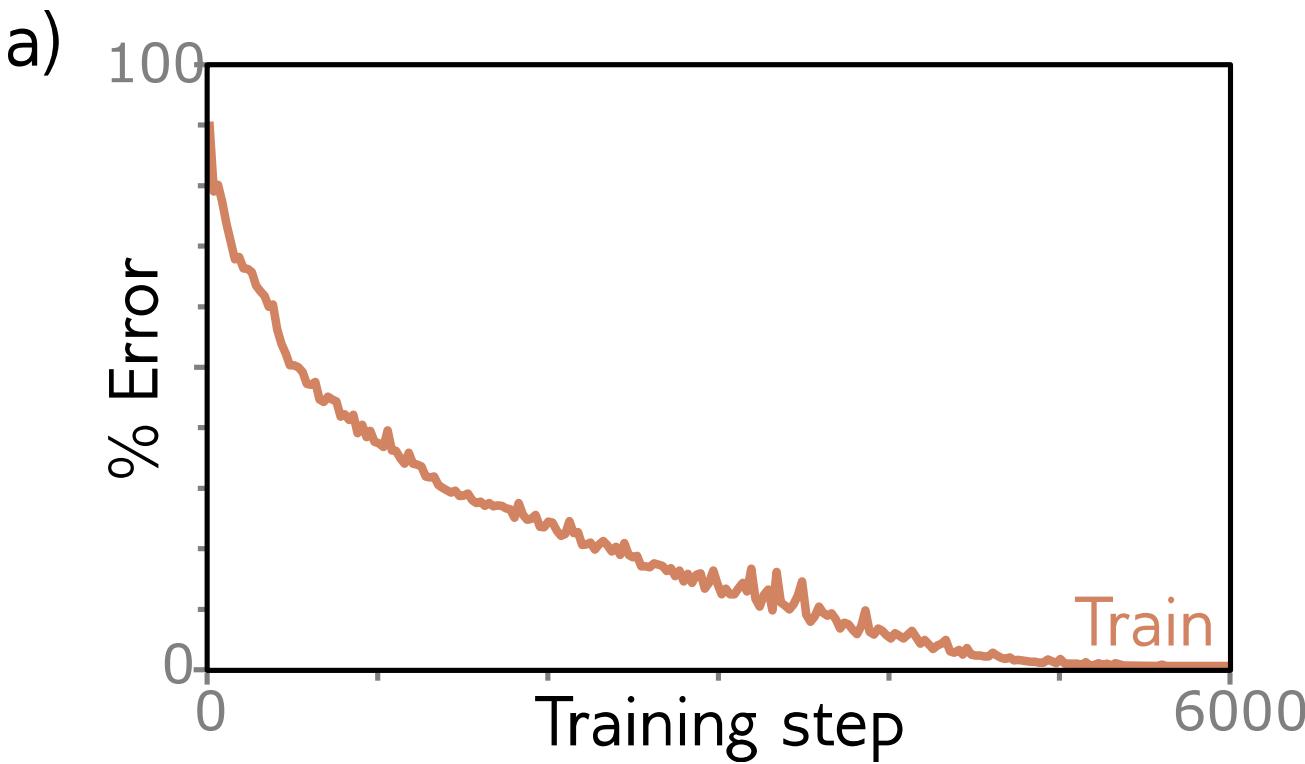
• • •

```
# inference – just choose the max
pred_train = model(x_train)
pred_test = model(x_test)
_, predicted_train_class = torch.max(pred_train.data, 1)
_, predicted_test_class = torch.max(pred_test.data, 1)
```

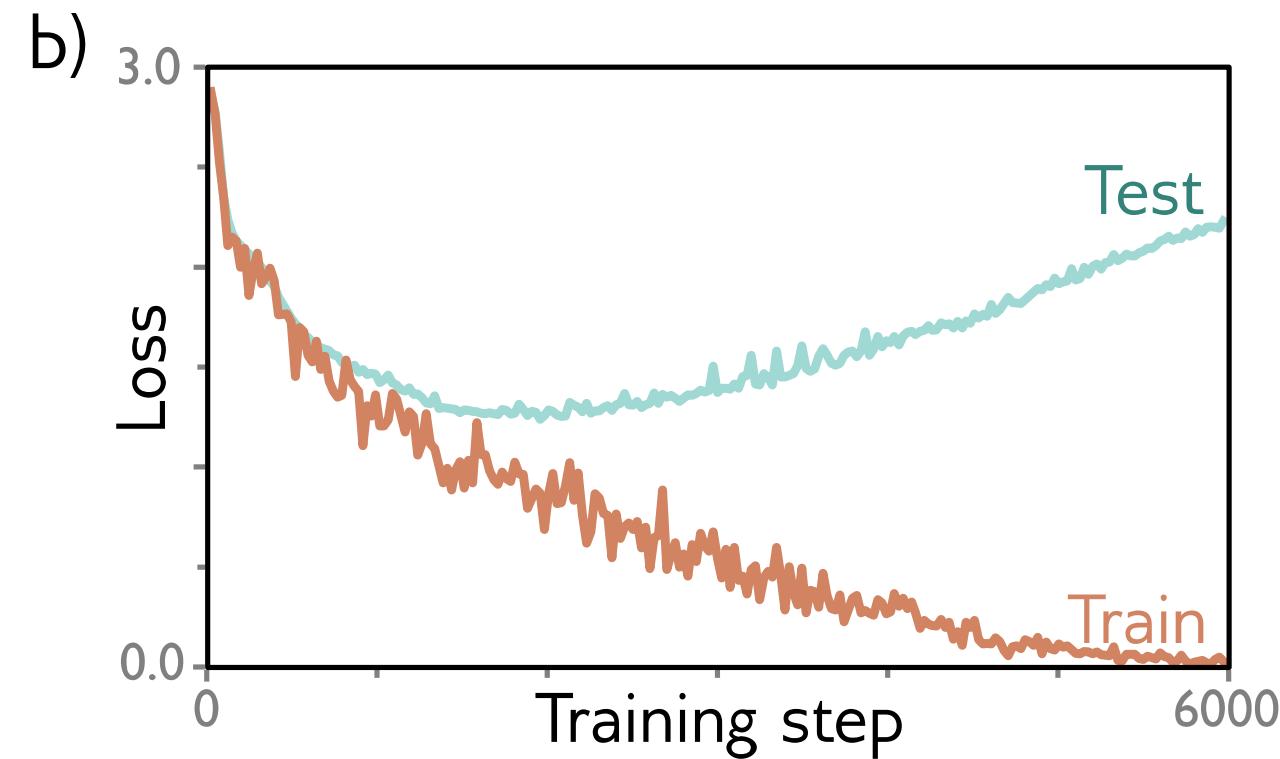
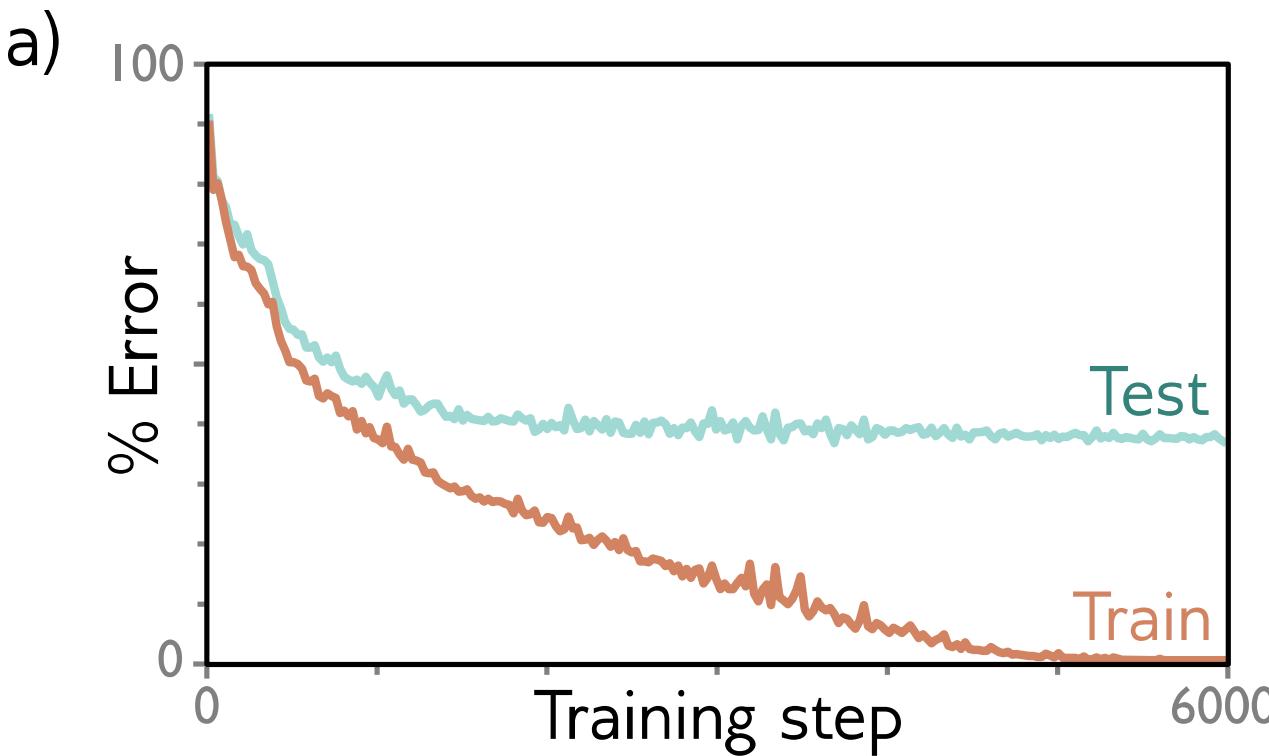
```
model = torch.nn.Sequential(
    torch.nn.Linear(40, 100),
    torch.nn.ReLU(),
    torch.nn.Linear(100, 100),
    torch.nn.ReLU(),
    torch.nn.Linear(100, 10))
```

Layer (type:depth-idx)	Output Shape	Param #
Sequential	[1, 10]	-
--Linear: 1-1	[1, 100]	4,100
--ReLU: 1-2	[1, 100]	-
--Linear: 1-3	[1, 100]	10,100
--ReLU: 1-4	[1, 100]	-
--Linear: 1-5	[1, 10]	1,010
Total params:	15,210	
Trainable params:	15,210	
Non-trainable params:	0	
Total mult-adds (Units.MEGABYTES):	0.02	
Input size (MB):	0.00	
Forward/backward pass size (MB):	0.00	
Params size (MB):	0.06	
Estimated Total Size (MB):	0.06	

Results



Need to use separate test data



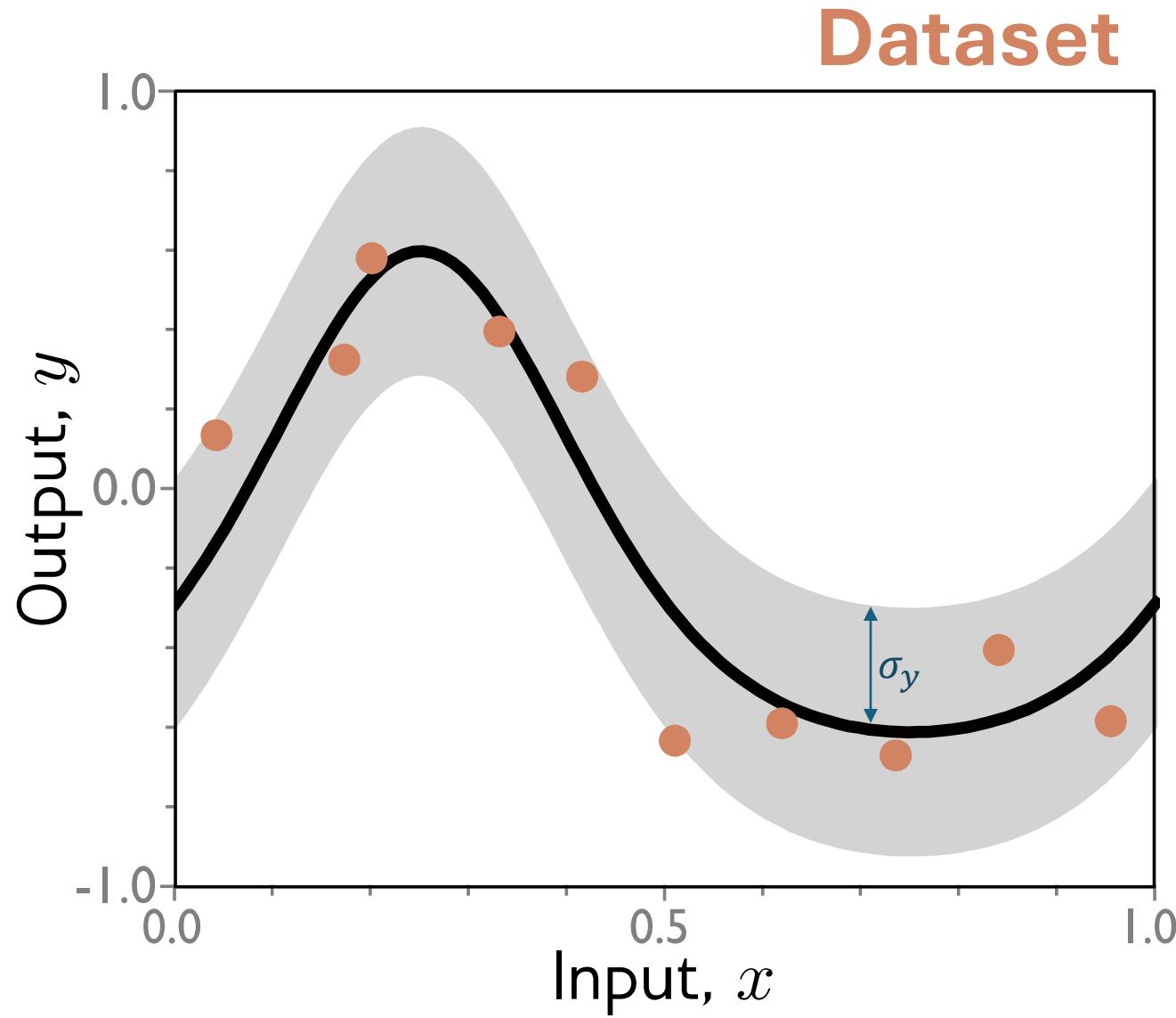
The model has not generalized well to the new data

Any Questions?

???

- MNIST1D dataset model and performance
- Noise, bias, and variance
- Reducing variance
- Reducing bias & bias-variance trade-off
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Regression example with Toy Model



"True" function:

$$y = e^{\sin(2\pi x)}$$

Add small uniform noise to x:

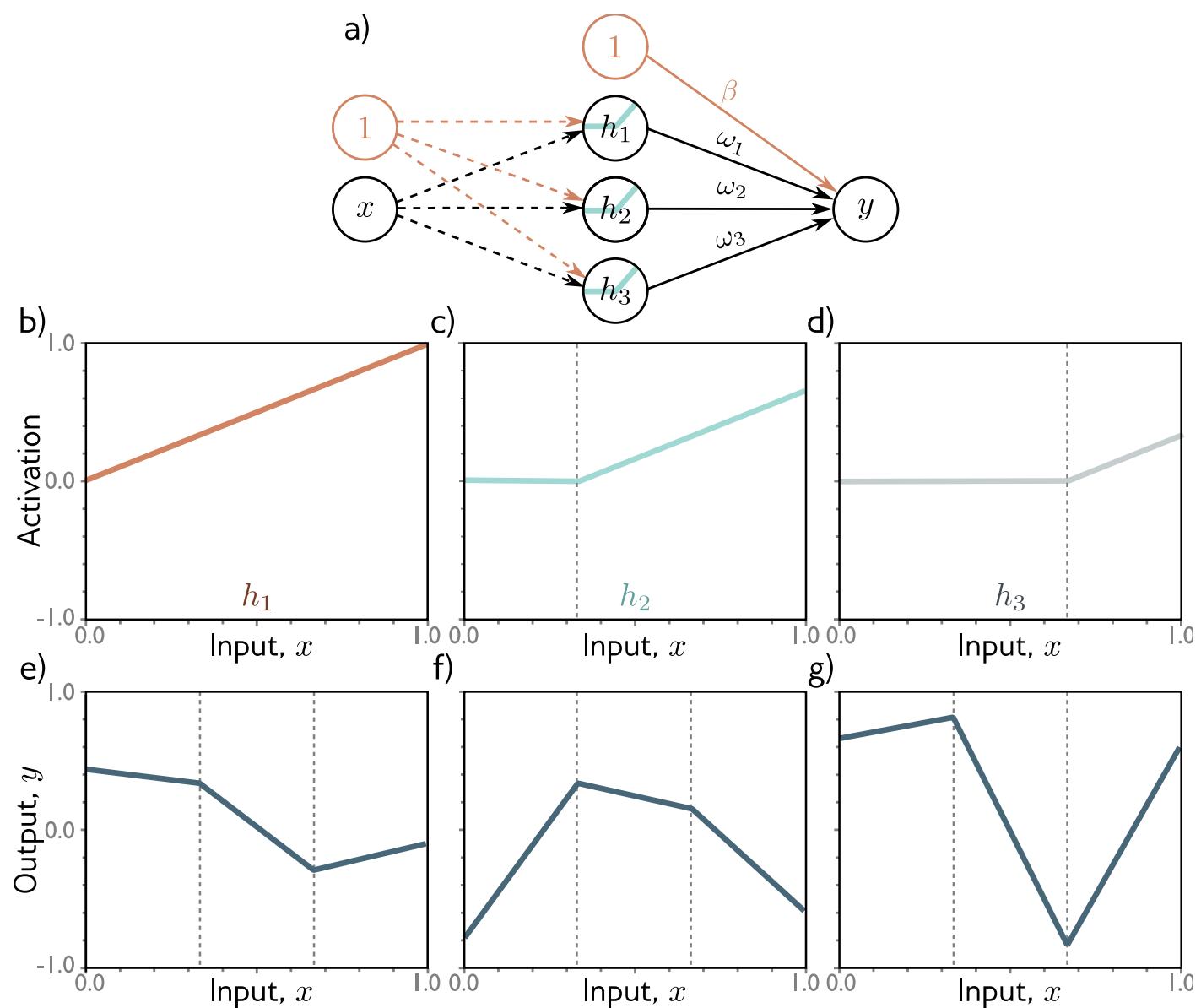
$$x = x + \mathcal{U}(\pm 1/\text{num_data})$$

Add small Gaussian noise to y:

$$y = y + \mathcal{N}(0, \sigma_y)$$

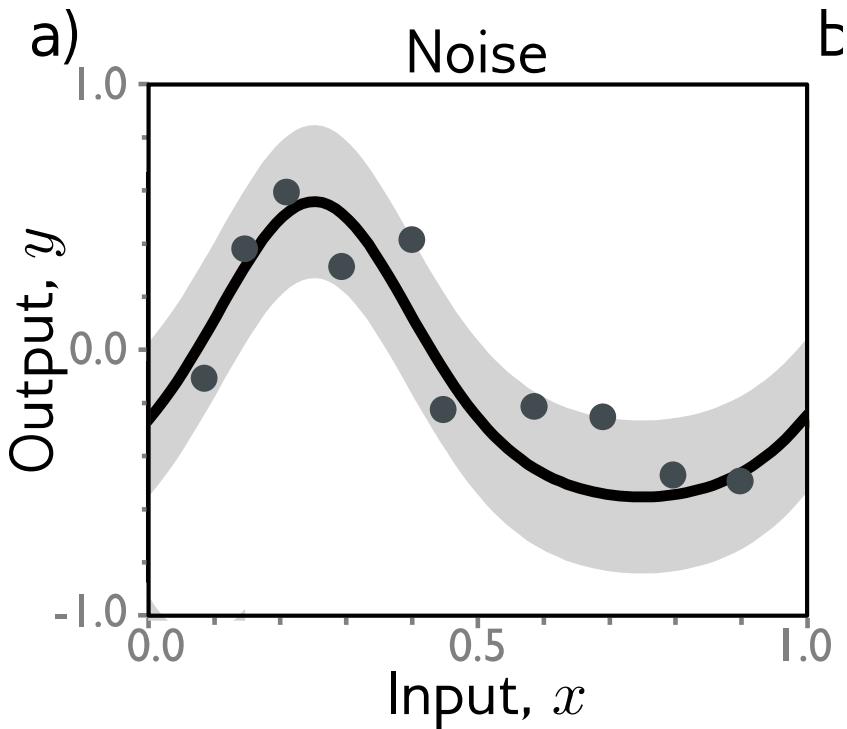
Toy model

- D hidden units
- First layer fixed so “joints” divide interval evenly, e.g. $0, 1/D, 2/D, \dots, (D-1)/D$
- Second layer trained
- But... now linear in \mathbf{h}
 - so convex cost function
 - can find best soln in closed-form
- A piecewise linear model with D regions.

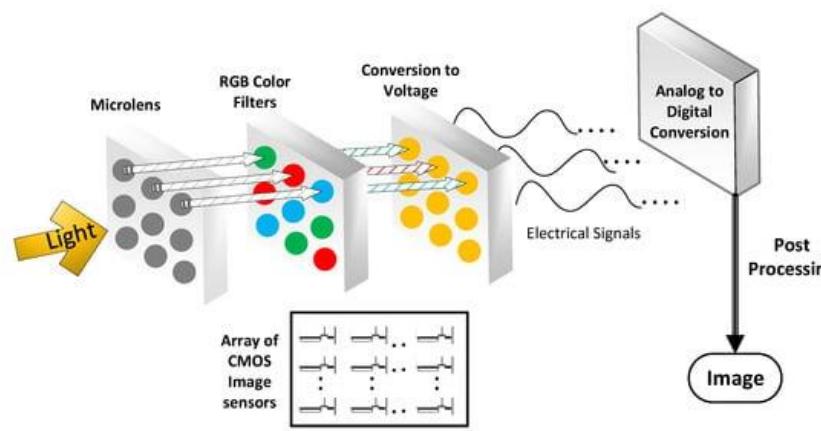


Three possible sources of error:
noise, *bias* and *variance*

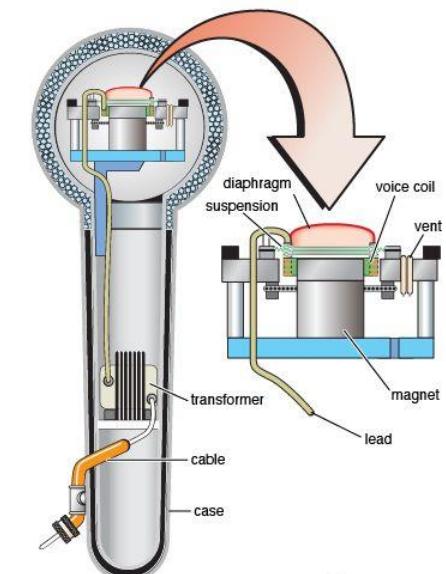
Noise, bias, and variance



- Genuine stochastic nature of the underlying model
- Noise in measurements, e.g. from sensors
- Some variables not observed
- Data mislabeled



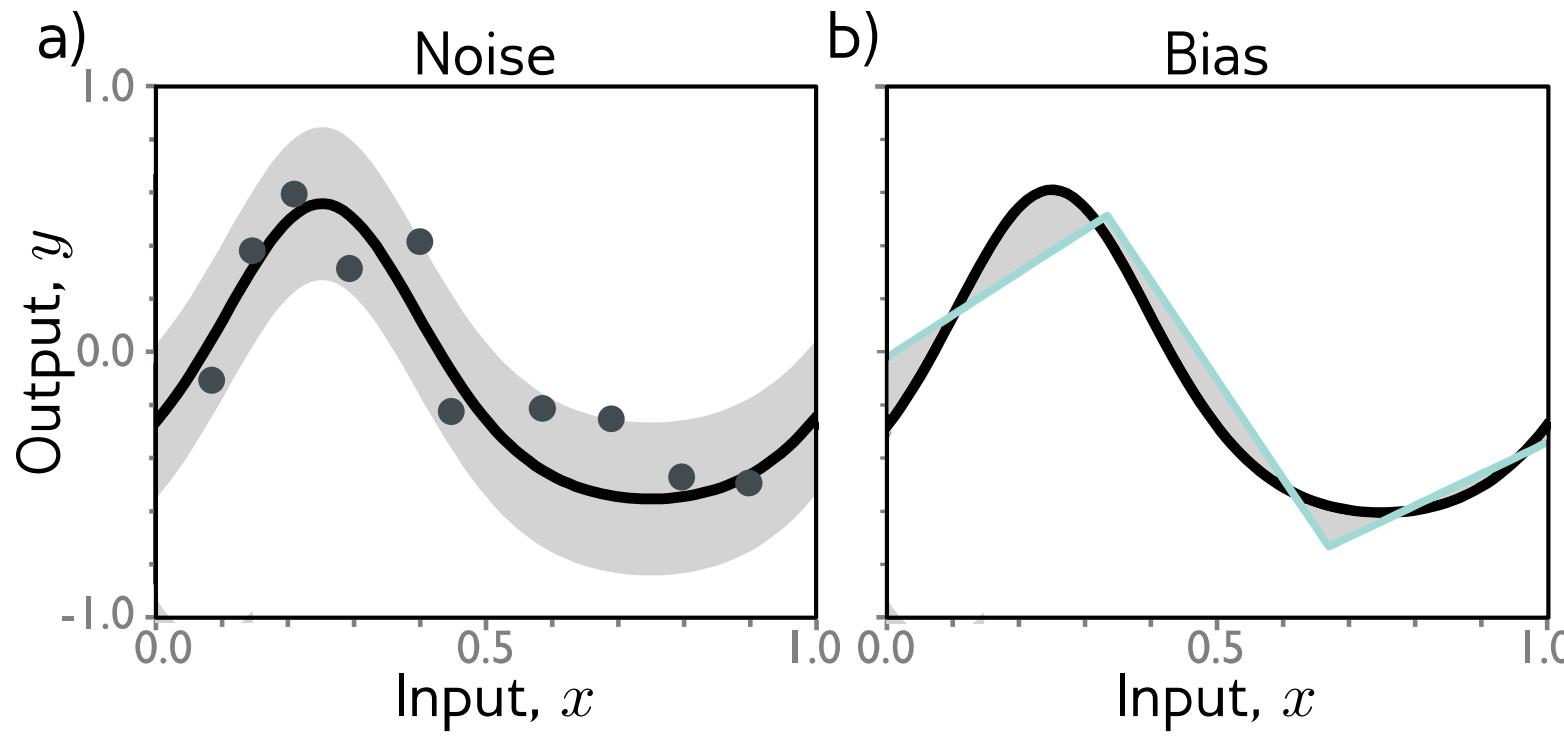
<https://images.app.goo.gl/2PuBhaFpfL9Pyjb8>



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<https://images.app.goo.gl/CMDaXSCdX4pqN8YxZ>

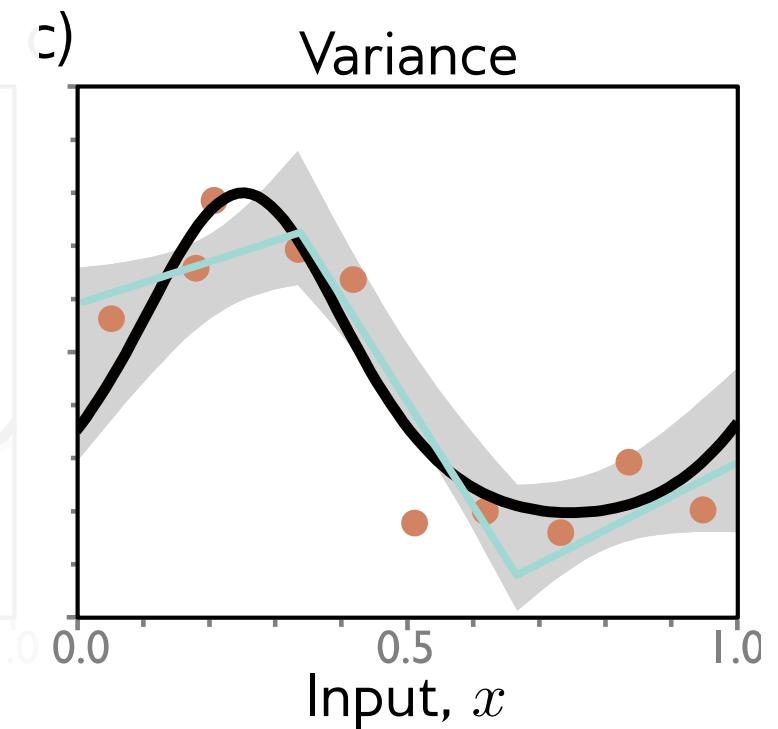
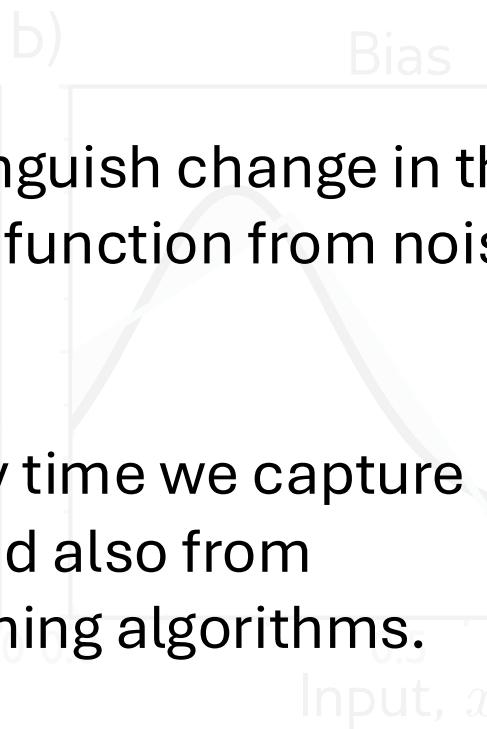
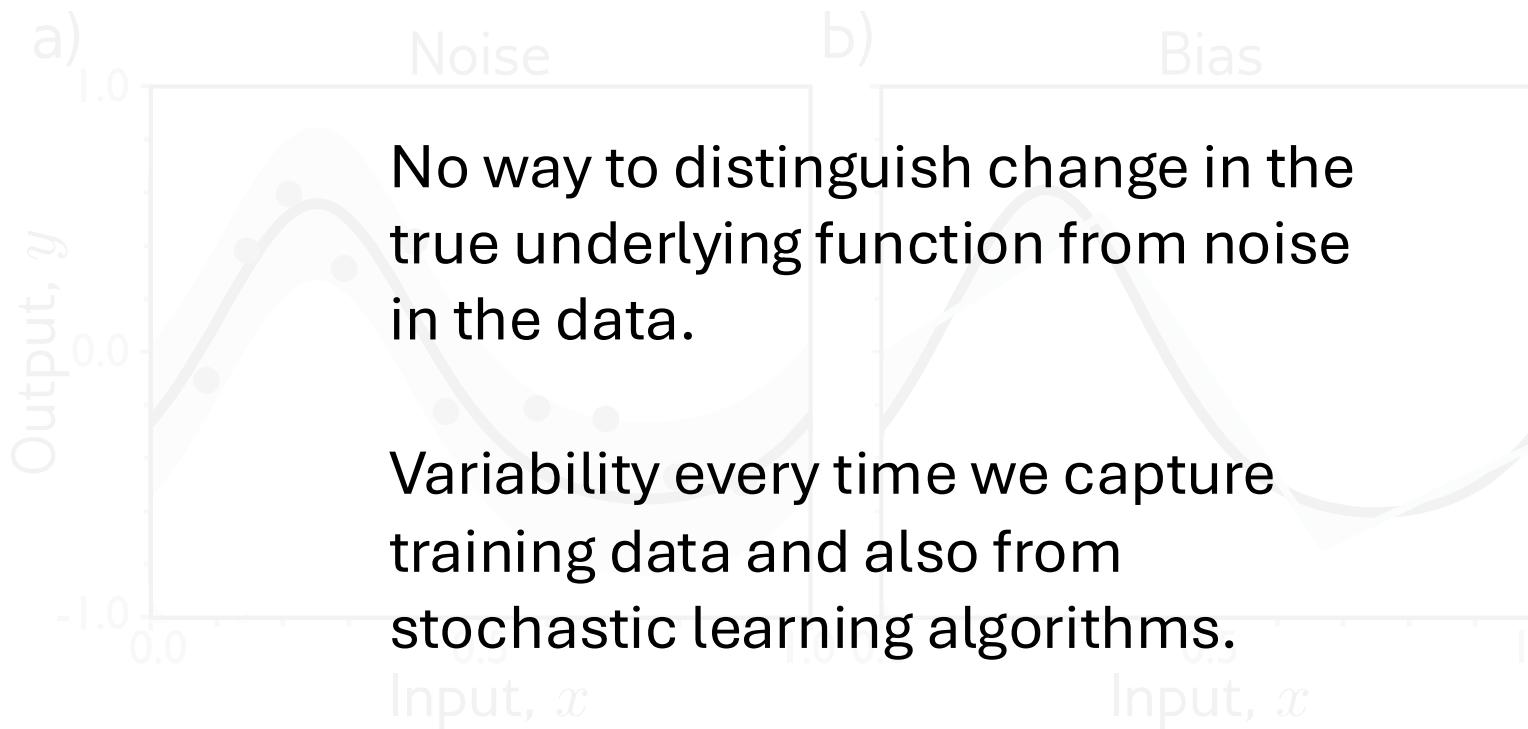
Noise, **bias**, and variance



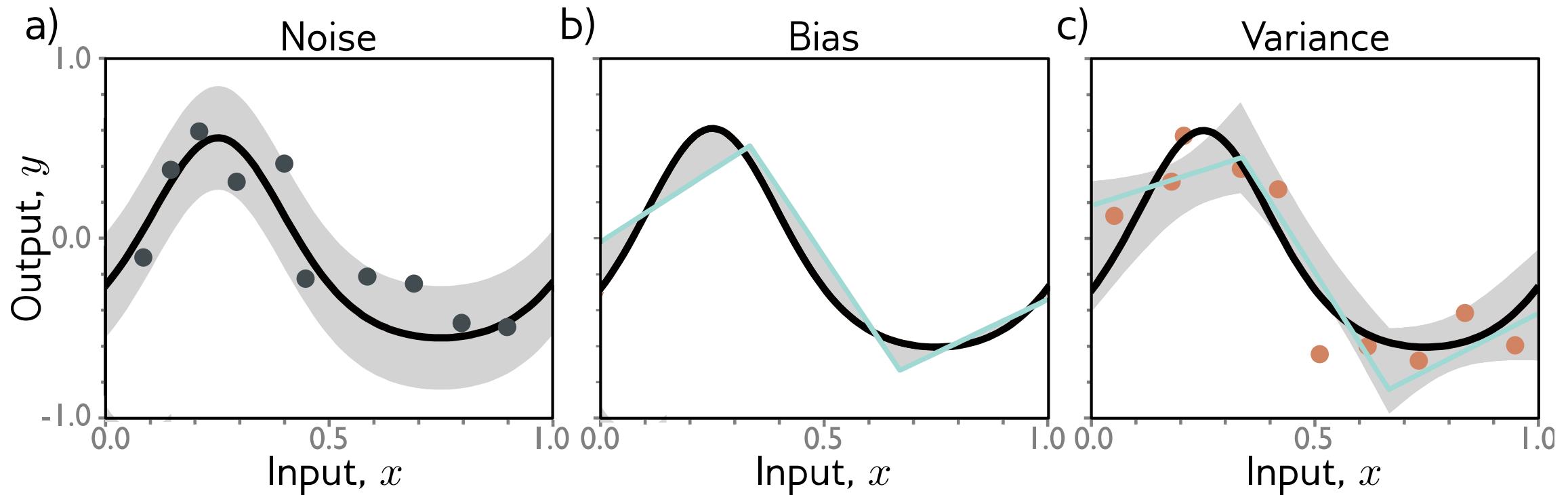
Bias occurs because the model lacks precision or capacity to accurately match the underlying function.

E.g. optimal fit with 3 hidden units and 3 line segments

Noise, bias, and variance



Noise, bias, and variance



Least squares regression only

For derivation see Section 8.2.2 in UDL.

$$L[x] = (f[x, \phi] - y[x])^2$$

- We can show that:

$$\mathbb{E}_y[L[x]] = (f[x, \phi] - \mu[x])^2 + \sigma^2$$

- And then:

$$\mathbb{E}_{\mathcal{D}}[\mathbb{E}_y[L[x]]] = \underbrace{\mathbb{E}_{\mathcal{D}}[(f[x, \phi|\mathcal{D}] - f_{\mu}[x])^2]}_{\text{variance}} + \underbrace{(f_{\mu}[x] - \mu[x])^2}_{\text{bias}} + \underbrace{\sigma^2}_{\text{noise}}$$

Expectation over noise in training data Expectation over noise in test data Actual model Best possible model if we had infinite data True function

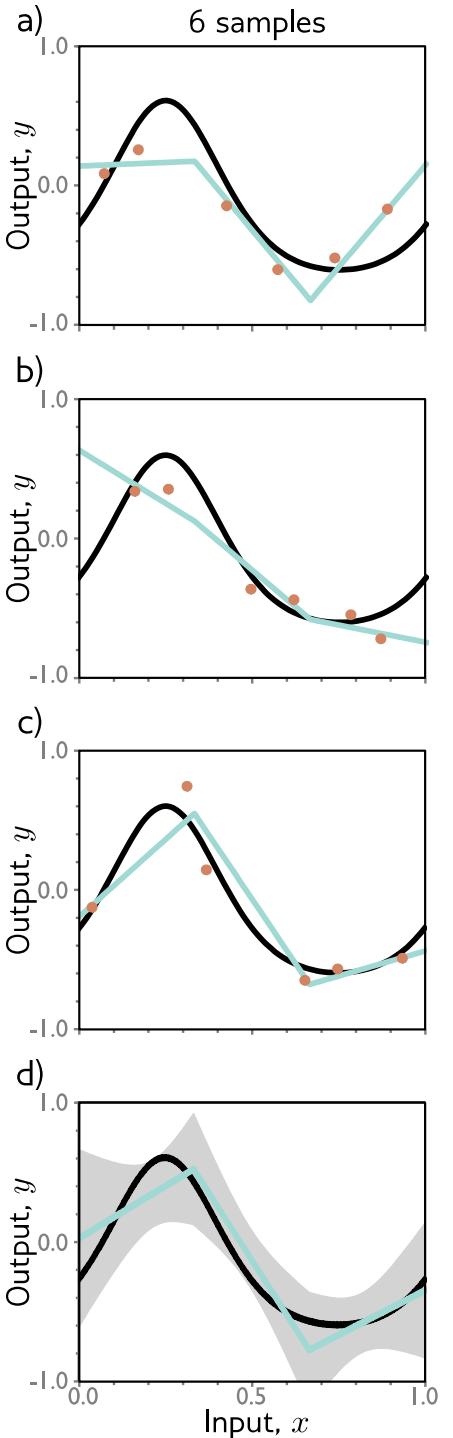
More complex interactions between noise, bias and variance in more complex models.

Any Questions?

???

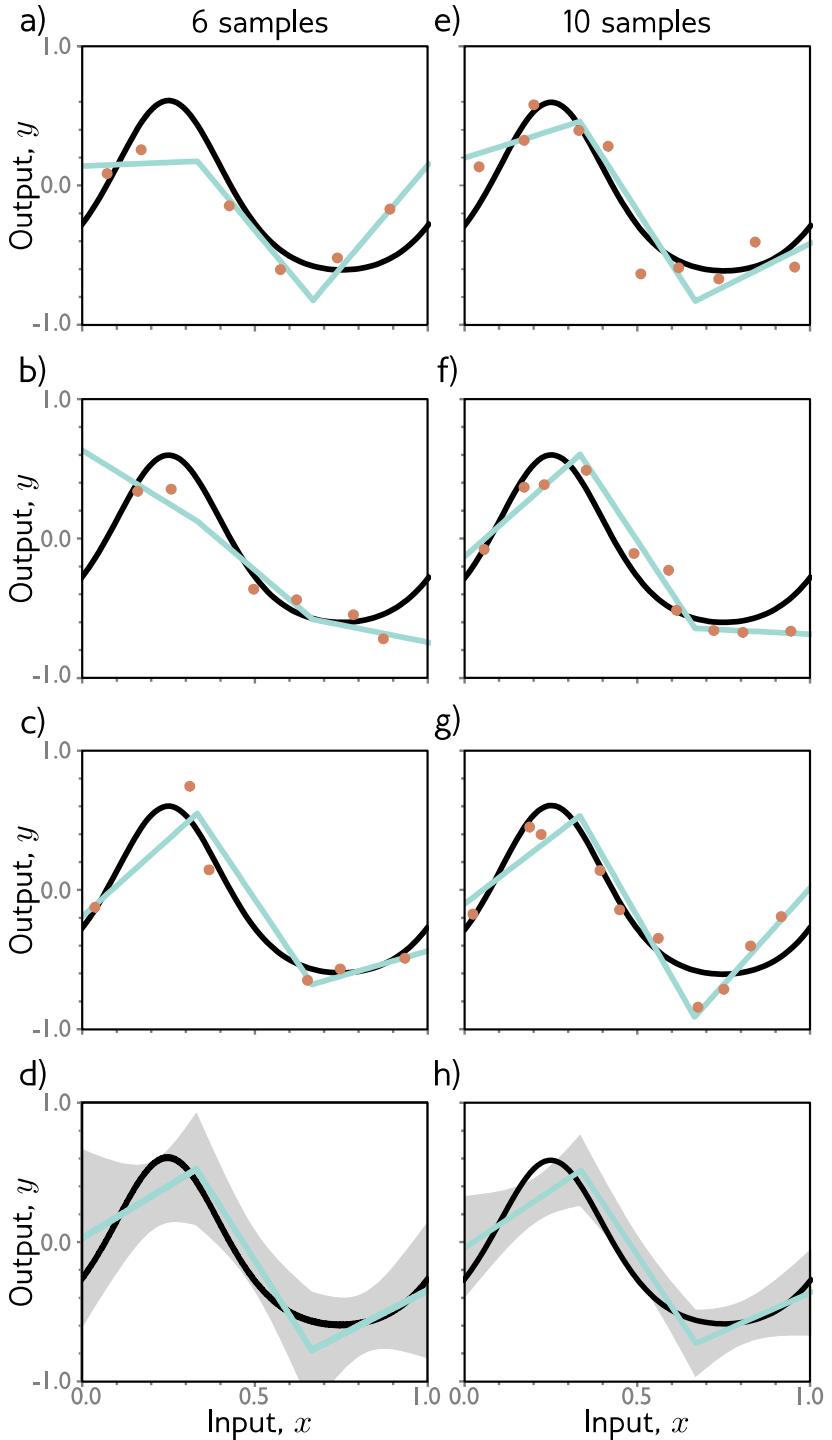
- MNIST1D dataset model and performance
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Variance



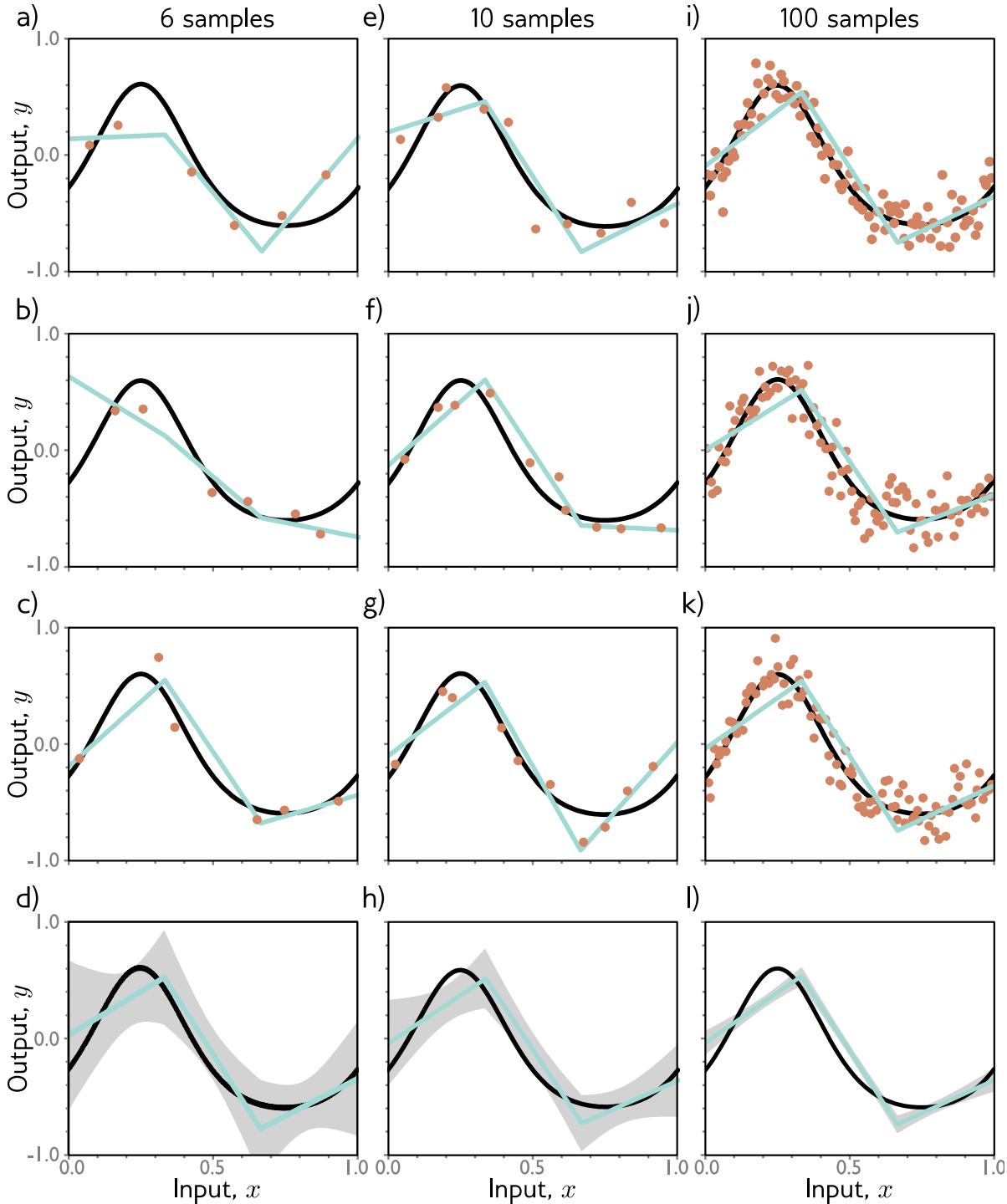
When measuring (capturing) 6 different data samples with a fixed model (e.g. 3 hidden units), we get different optimal fits every time.

Variance



Can reduce variance by adding more samples

Variance



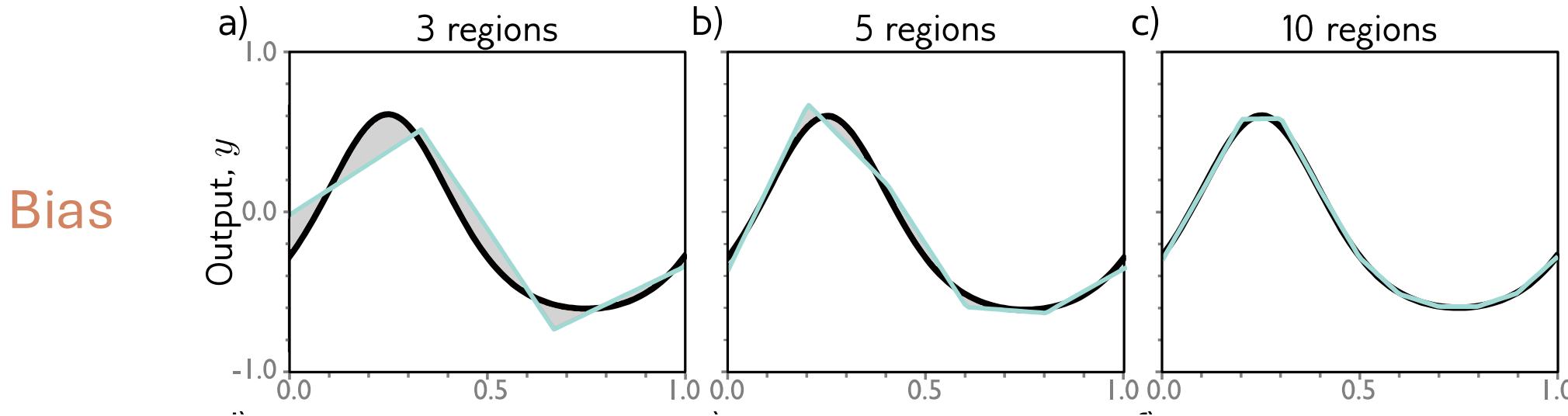
Can reduce variance by adding more samples

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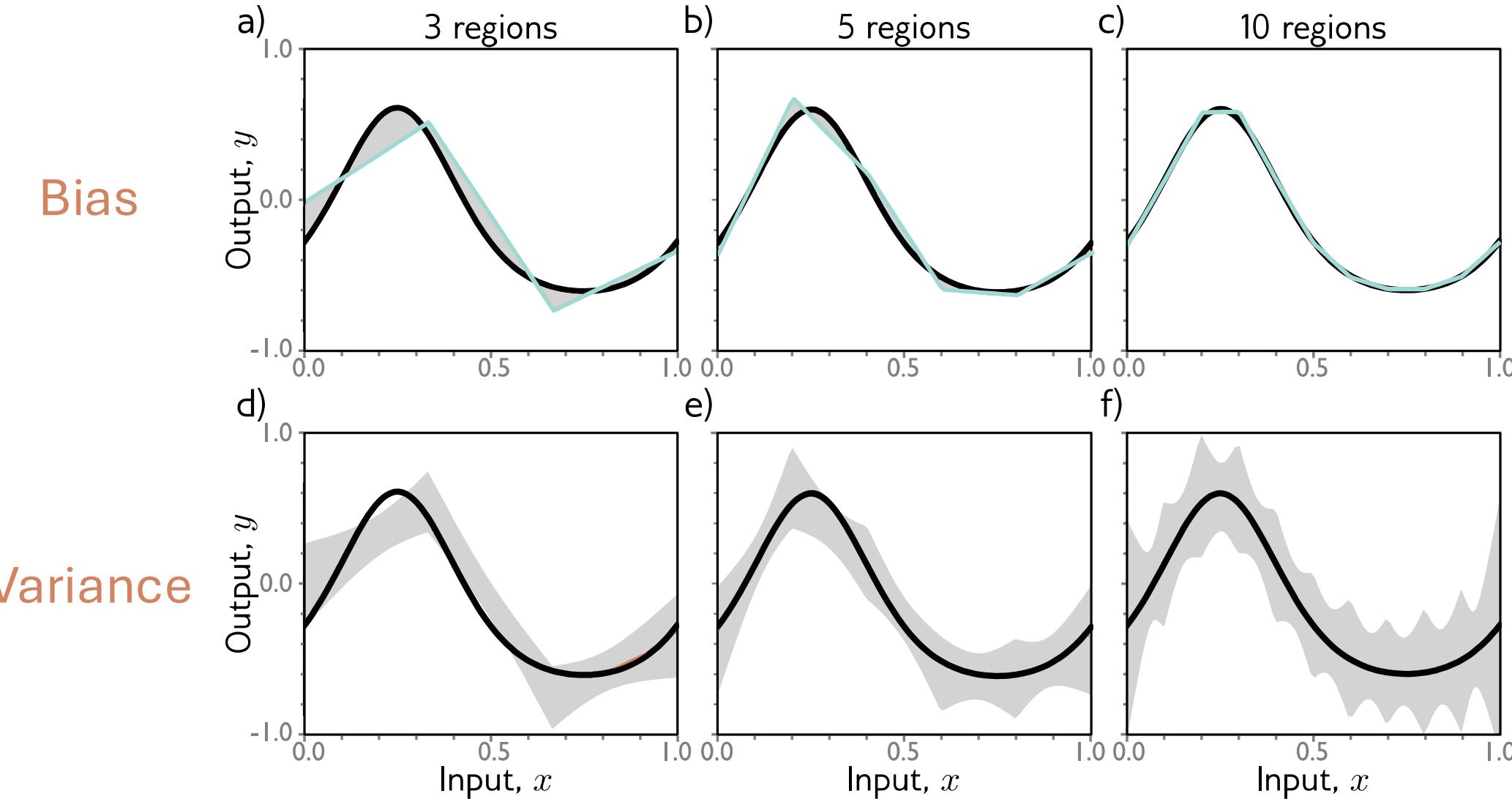
Reducing bias (example with the true function)



We can reduce bias by adding more model capacity.

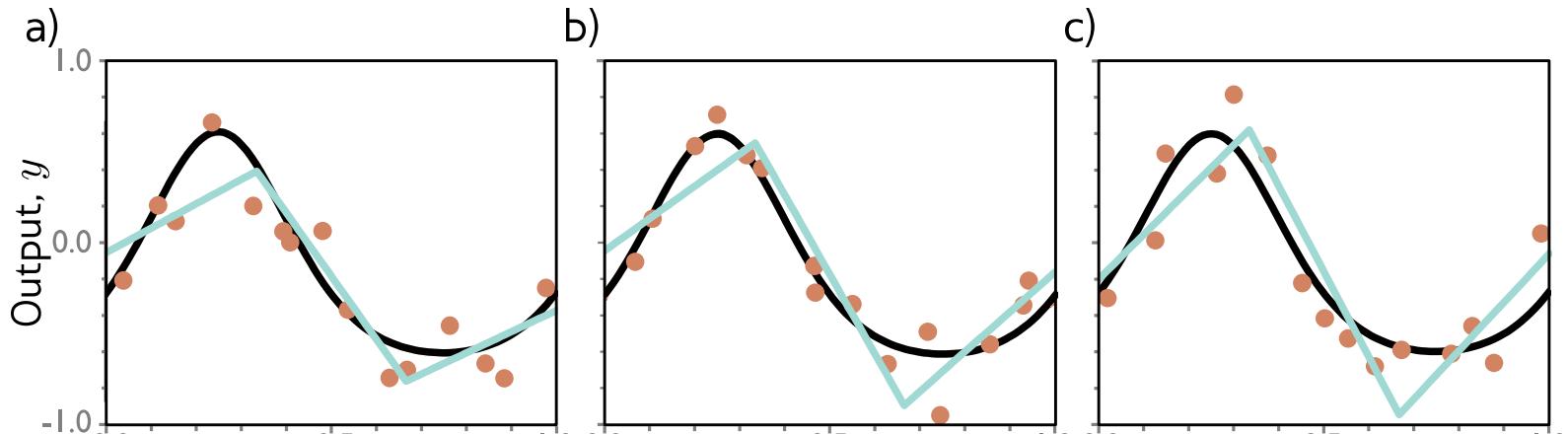
In this case, adding more hidden units.

Reducing bias \rightarrow Increases variance!!

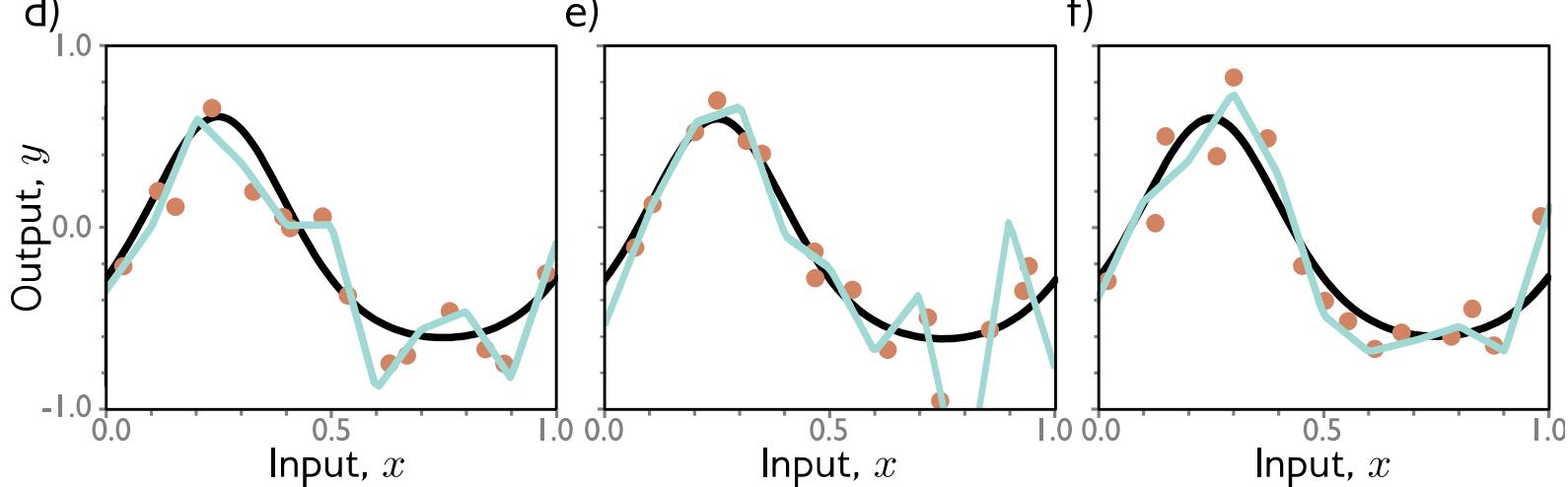


Why does variance increase? Overfitting

3 Regions

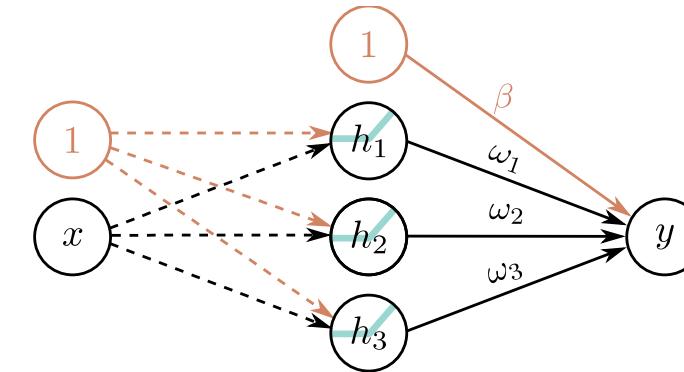
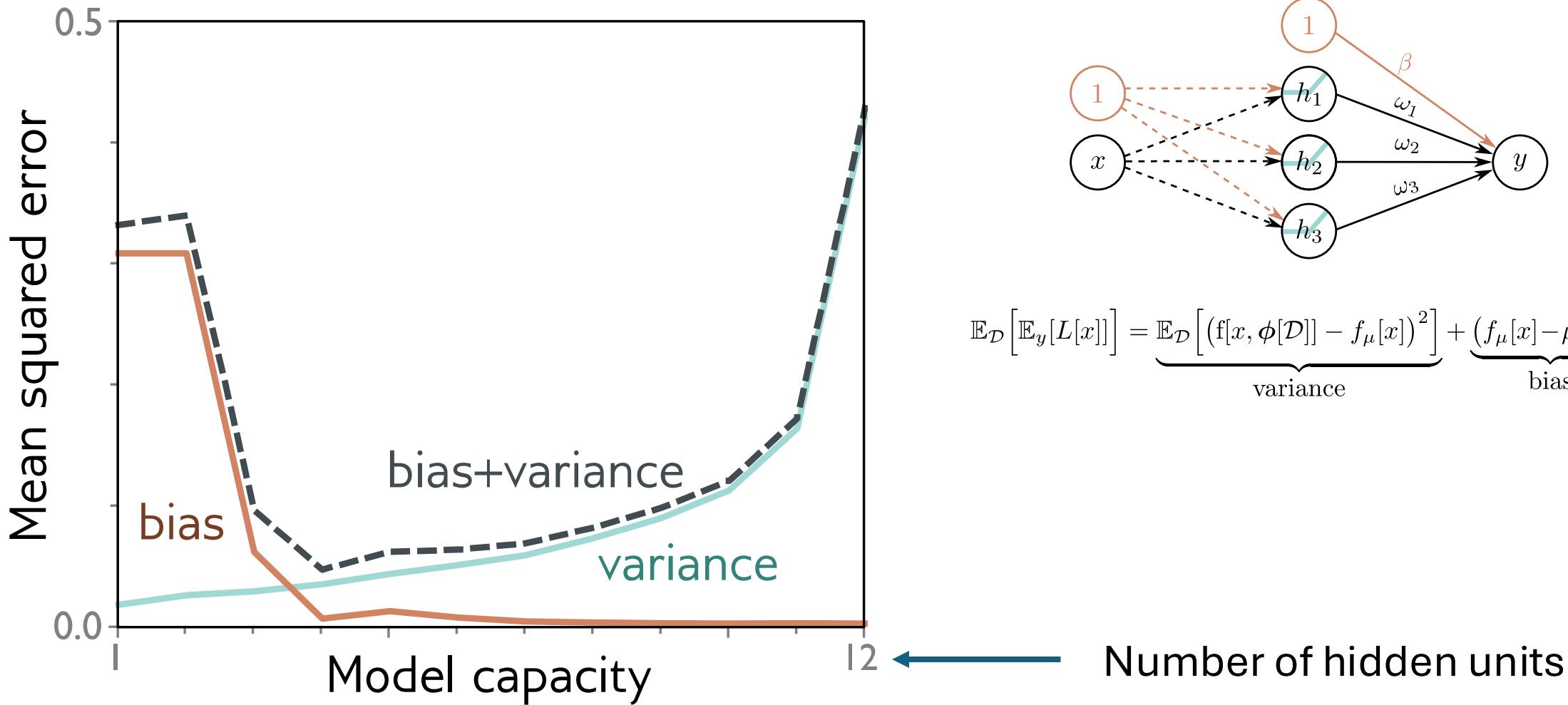


10 Regions



Describes the training data better, but not the true underlying function (black curve)
Many ways to fit a sample of 15 data points

Bias and variance trade-off for the simple linear model



$$\mathbb{E}_{\mathcal{D}} [\mathbb{E}_y [L[x]]] = \underbrace{\mathbb{E}_{\mathcal{D}} [(f[x, \phi[\mathcal{D}]] - f_\mu[x])^2]}_{\text{variance}} + \underbrace{(f_\mu[x] - \mu[x])^2}_{\text{bias}} + \underbrace{\sigma^2}_{\text{noise}}$$

But does picking model capacity to minimize bias & variance hold for more complex data and models?

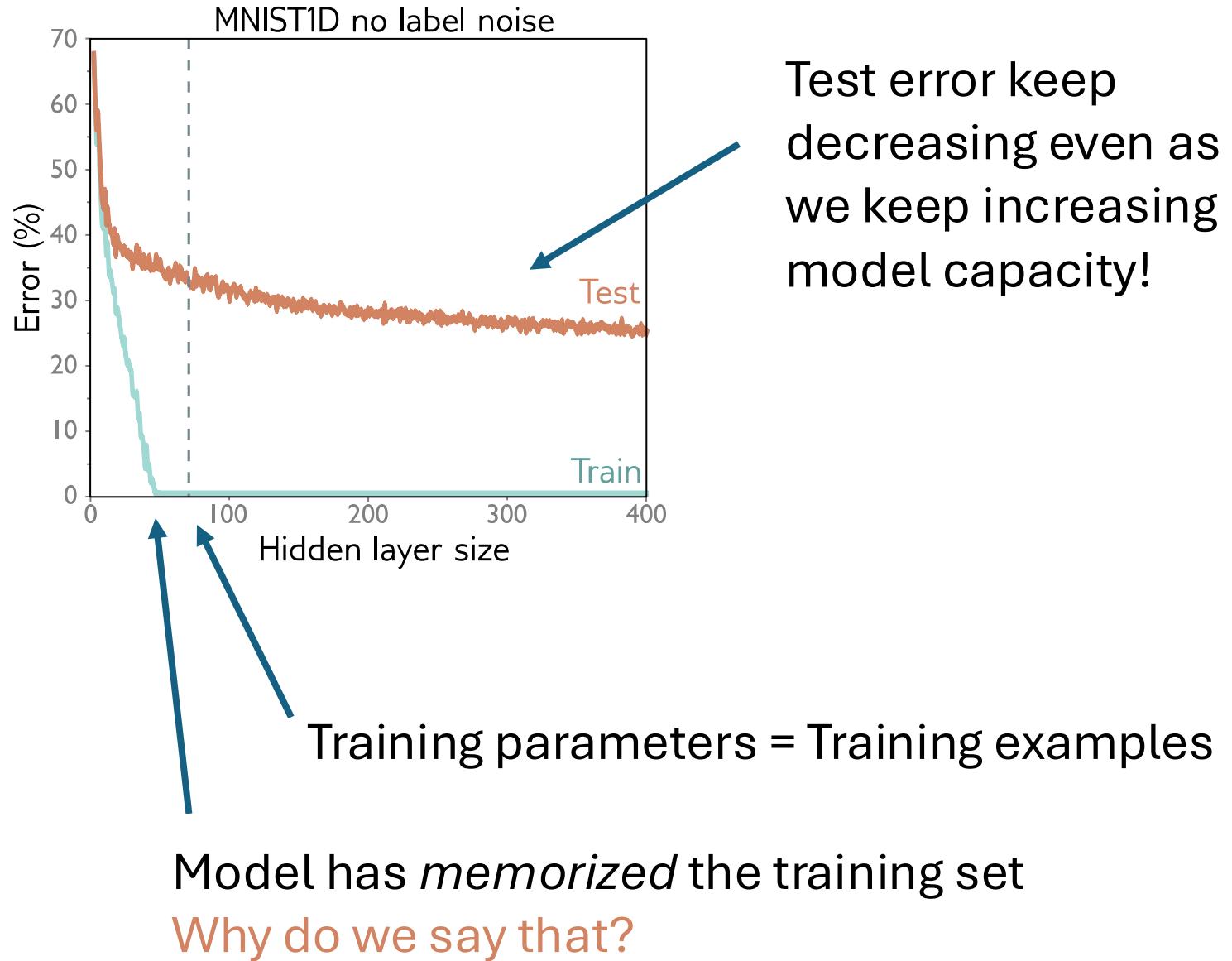
Any Questions?

???

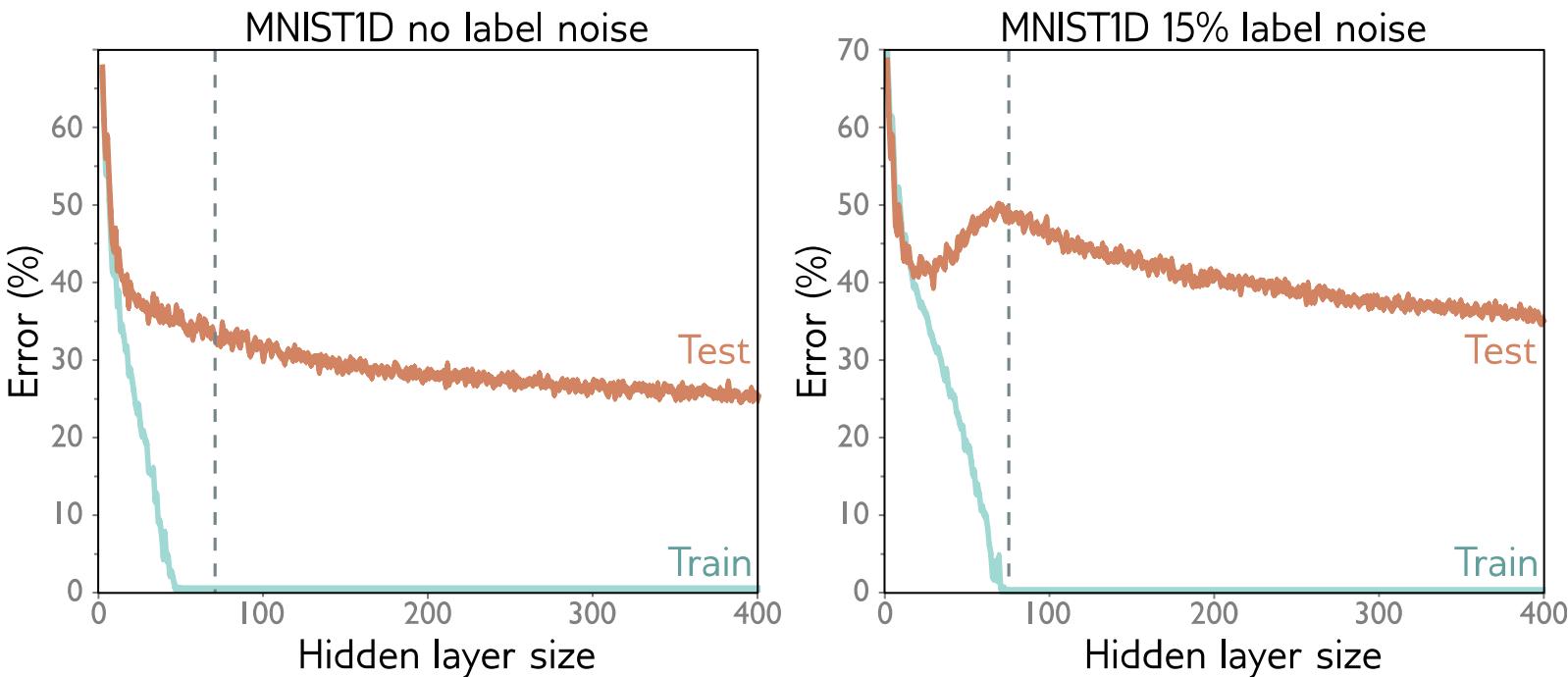
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Train and Test Error versus # of Hidden Layers

- 10,000 training examples
- 5,000 test examples
- Two hidden layers
- Adam optimizer
- Step size of 0.005
- Full batch
- 4000 training steps



Now randomize
15% of the
training labels

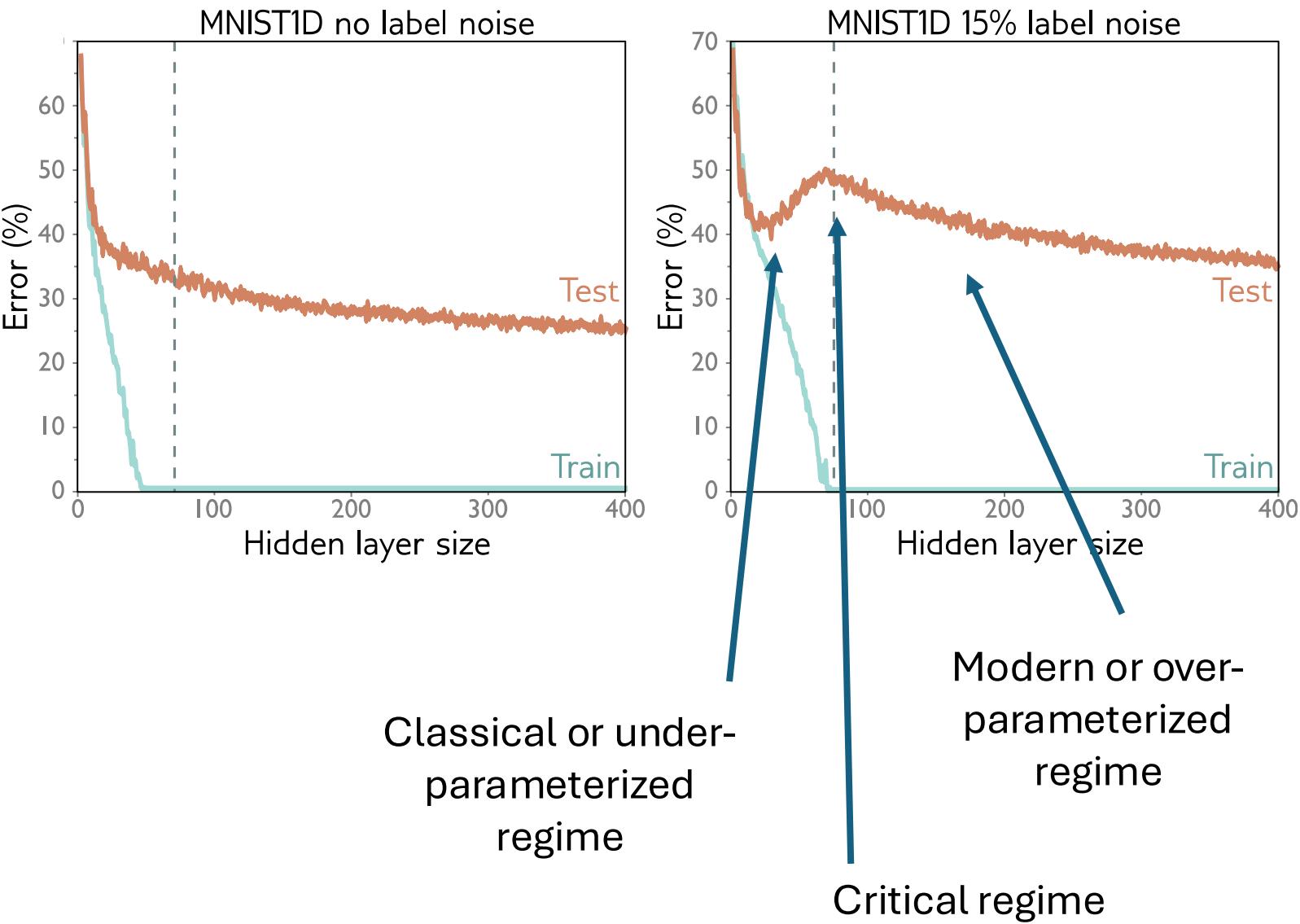


Now we see what looks like bias-variance trade-off as we increase capacity to the point where the model fits training data.

Reminder: vertical dashed line is where:
training parameters = # training samples

But then???

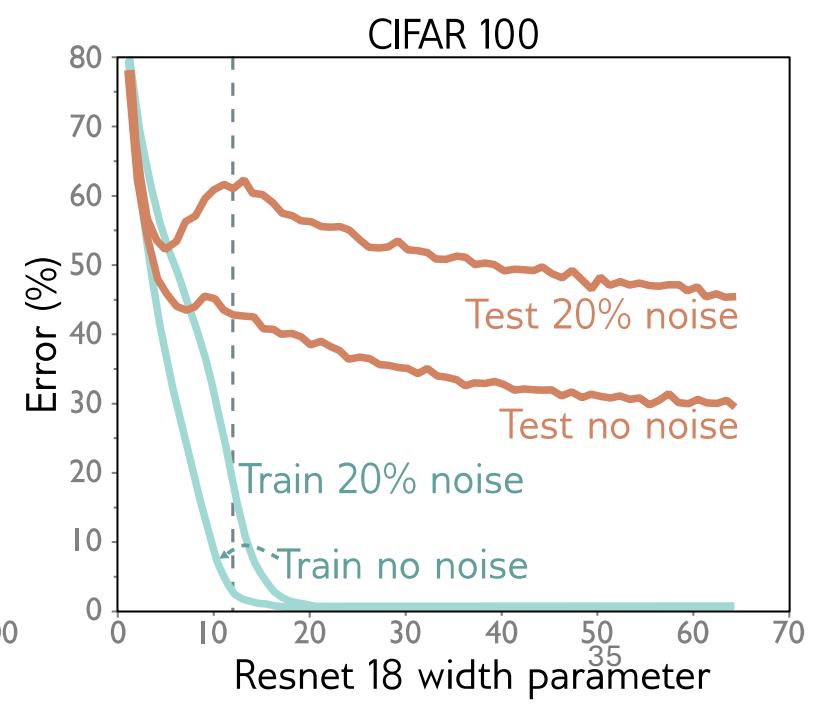
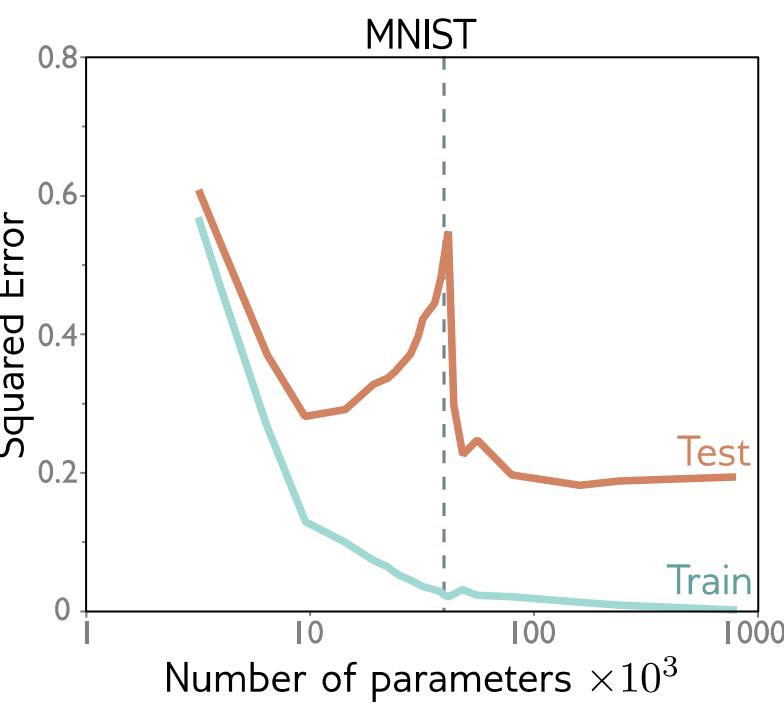
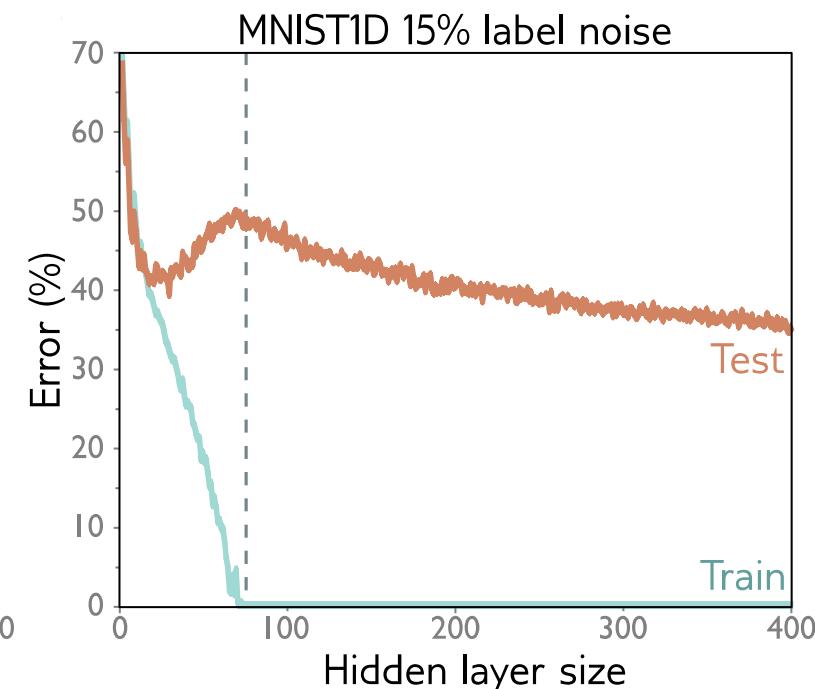
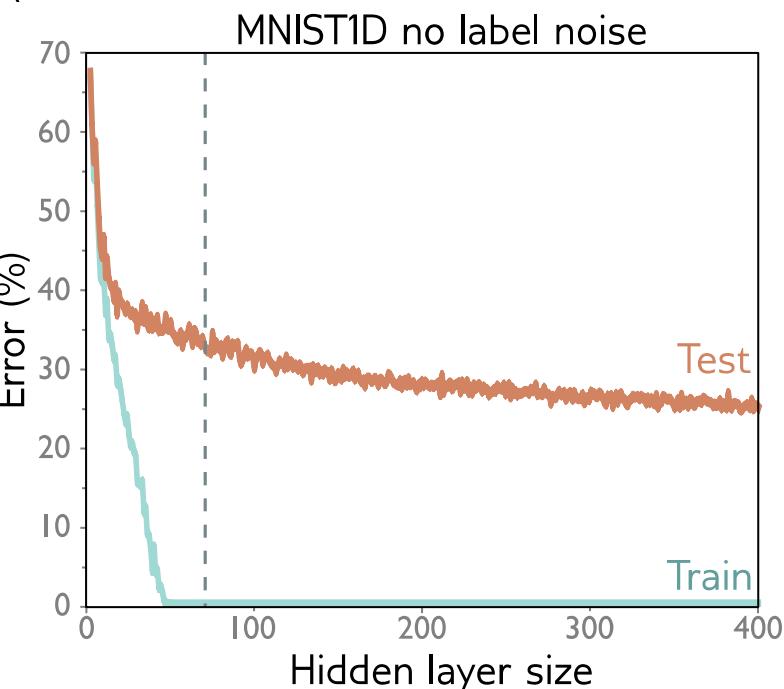
Double Descent



Reminder: vertical dashed line is where:
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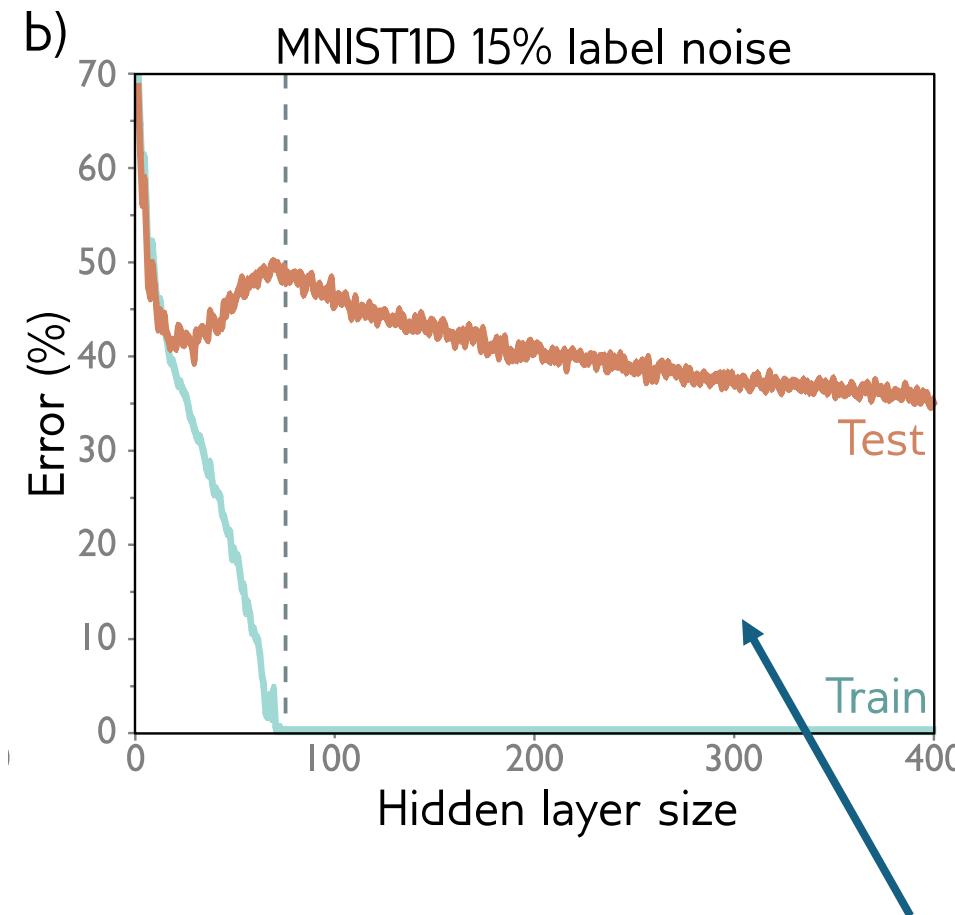
Same phenomenon shows up on MNIST and CIFAR100

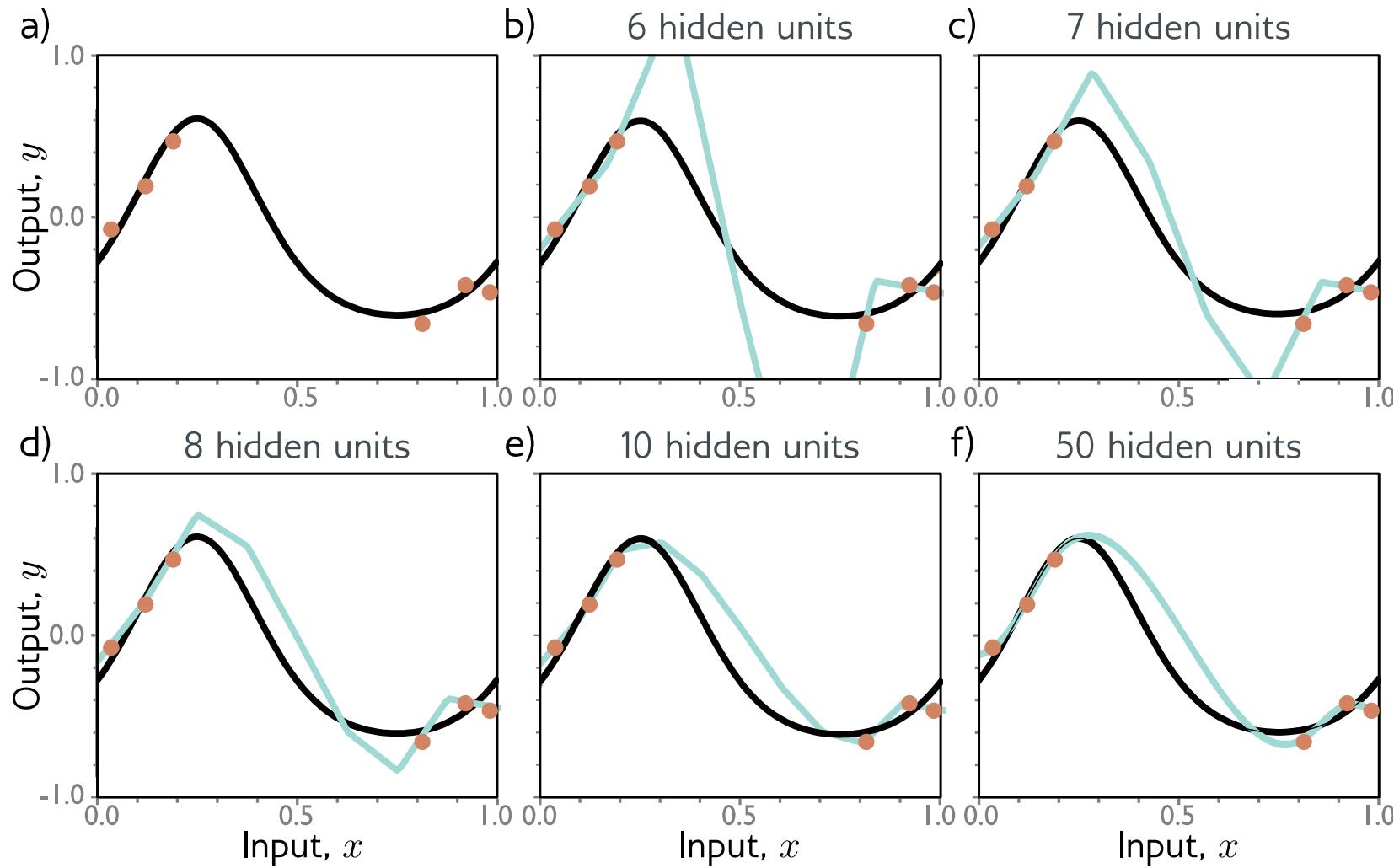
Reminder: vertical dashed line is where:
training parameters = # training samples



Double Descent

- Note that training loss is very close to zero.
- Whatever is happening isn't happening at training data points
- Model never sees test set during training
- Must be happening between the data points??



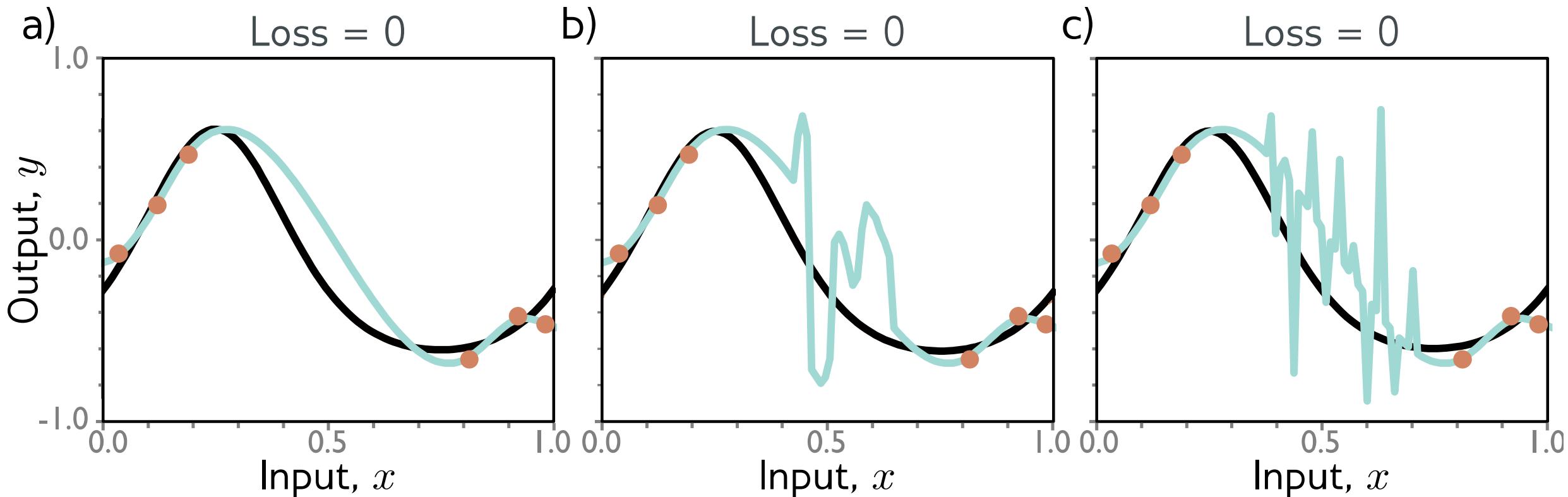


Potential explanation:

- can make smoother functions with more hidden units
- being smooth between the datapoints is a reasonable thing to do

But why?

Next Week: How to bias for smoothness?



- All of these solutions are equivalent in terms of loss.
- Why should the model choose the smooth solution?
- Tendency of model to choose one solution over another is **inductive bias**

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???

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Choosing hyperparameters

- Don't know bias or variance
- Don't know how much capacity to add
- How do we choose capacity in practice?
 - Or model structure
 - Or training algorithm
 - Or learning rate
- Third data set – validation set
 - Train models with different hyperparameters on training set
 - Choose best hyperparameters with validation set
 - Test once with test set

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???

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