LECTURE 15

# Bias and Variance

Exploring the different sources of error in the predictions that our models make.

# What is a random variable?

A random variable is a **numerical function of a random sample.**

Another name for a numerical function of a sample is a "statistic."

We typically denote random variables with uppercase letters late in the alphabet (e.g. $X$, $Y$).

Why **random**? Because the sample on which it is a function was drawn at random.

Why **variable**? Because its value depends on how the sample came out.

# Definition of expectation

The **expectation** of a random variable X is the weighted average of the values of X, where the weights are the probabilities of the values.

The most common formulation applies the weights one possible value at a time:

$$\mathbb{E}(X) = \sum_{\substack{\text{all possible} \\ x}} x\mathbb{P}(X = x)$$

However, an equivalent formulation applies the weights one sample at a time:

$$\mathbb{E}(X) = \sum_{\substack{\text{all samples} \\ s}} X(s)\mathbb{P}(s)$$

# Linearity

Two of the properties we just established were

- Linear transformations apply to expectations.
- Expectation is additive.

Combining these gives us a single property, which is sometimes referred to as the **linearity of expectation**. For any random variables X, Y and constants a, b:

$$E(aX + bY) = aE(X) + bE(Y)$$

This more general form won't appear often in this class, but it is good to be aware of.

# Definition of variance

- Variance is the **expected squared deviation from the expectation** of X.
- It is defined as follows:

$$\mathbb{V}ar(X) = \mathbb{E}((X - \mathbb{E}(X))^2)$$

- The units of the variance are the square of the units of X.
- To get back to the right scale, we look at the **standard deviation** of X:

$$\mathbb{SD}(X) = \sqrt{\mathbb{V}ar(X)} = \sqrt{\mathbb{E}((X - \mathbb{E}(X))^2)}$$

- Both standard deviation and variance must be non-negative.

# Interpretation of variance

- The main use of variance is to **quantify chance error**.
  - How far away from the expectation can X be, just by chance?

- By Chebyshev's inequality:
  - No matter what the shape of the distribution of X is,
  - The vast majority of the probability lies in the interval "expectation plus or minus a few SDs".
  - Specifically, if $\mu$ = E[X] and $\sigma$ = SD[X], then $P(|X - \mu| \geq k\sigma) \leq \frac{1}{k^2}$ .

# An alternative calculation

There's a more convenient form of variance for use in calculations.

$$\mathbb{V}ar(X) = \mathbb{E}(X^2) - (\mathbb{E}(X))^2$$

To derive this, we make repeated use of the linearity of expectation. (A more detailed walkthrough is in the lecture video.)

$$\begin{aligned} Var(X) &= E((X - E(X))^2) \\ &= E\big(X^2 - 2XE(X) + (E(X)^2)\big) \\ &= E(X^2) - 2E(X)E(X) + (E(X))^2 \\ &= E(X^2) - (E(X))^2 \end{aligned}$$

# An alternative calculation

$$\mathbb{V}ar(X) = \mathbb{E}(X^2) - (\mathbb{E}(X))^2$$

For example, to compute the variance of one roll of a die, we can find

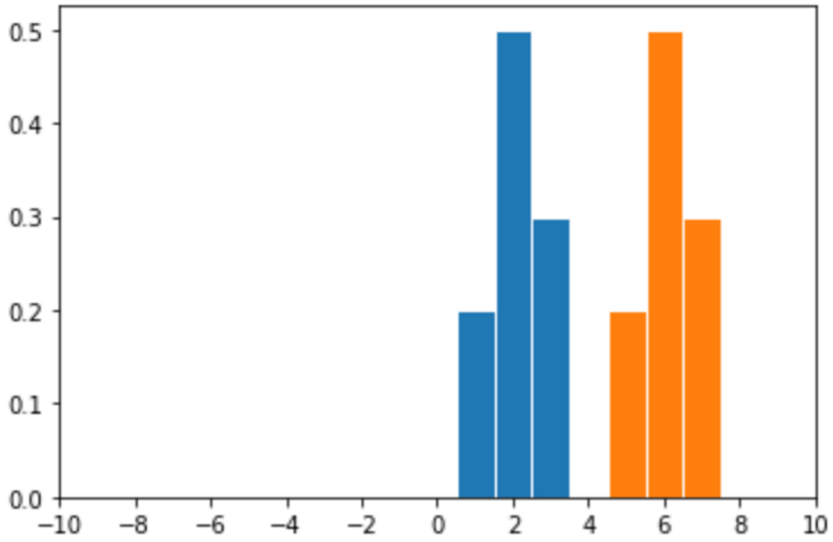
$$Var(X) = (1^2 + 2^2 + 3^2 + 4^2 + 5^2 + 6^2) \cdot \frac{1}{6} - (3.5)^2 = 2.92$$

- This formulation also makes clear that if X is **centered**, i.e. E(X) = 0, then Var(X) = E(X²).
- Since Var(X) is non-negative, this property also shows us that $E(X^2) \geq (E(X))^2$ . Equality is if and only if X is a constant.
- If you know the expectation and variance of a random variable, you can easily determine the expectation of its square: $\mathbb{E}(X^2) = \mathbb{V}ar(X) + (\mathbb{E}(X))^2$ .

# Linear transformations

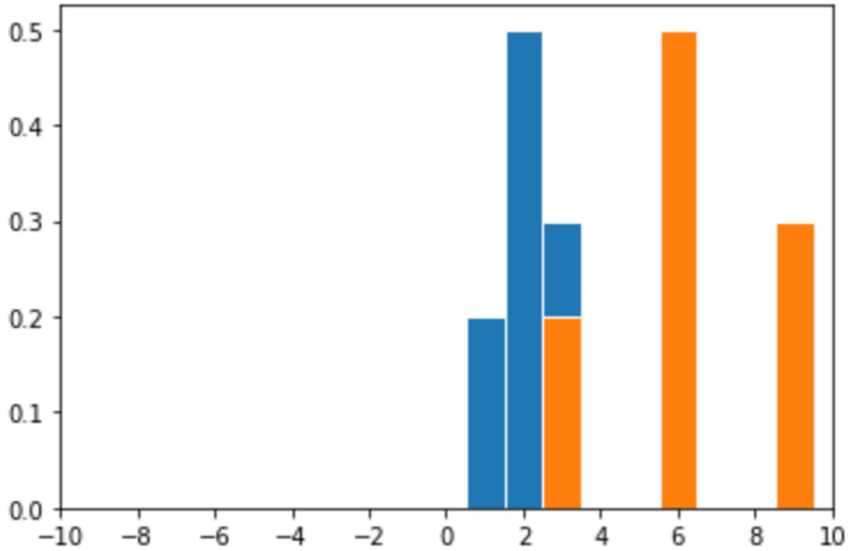
We know that $\mathbb{E}(aX + b) = a\mathbb{E}(X) + b$ . In order to compute Var(aX + b), consider:

A shift by **b** units **does not** affect spread:




Here, the distribution of X is in blue, and the distribution of X+4 is in orange.

But scaling by **a** units **does** affect spread:




The distribution of X is in blue, and the distribution of 3X is in orange.

# Linear transformations

We know that $\mathbb{E}(aX + b) = a\mathbb{E}(X) + b$ .

In order to compute Var(aX + b), consider:

- A shift by **b** units **does not** affect spread. Thus, Var(aX + b) = Var(aX).
- The multiplication by **a does** affect spread!

Then,

$$\begin{aligned} Var(aX + b) = Var(aX) &= E((aX)^2) - (E(aX))^2 \\ &= E(a^2X^2) - (aE(X))^2 \\ &= a^2\left(E(X^2) - (E(X))^2\right) \\ &= a^2 Var(X) \end{aligned}$$

In summary:

$$\mathbb{V}ar(aX + b) = a^2\mathbb{V}ar(X)$$
$$\mathbb{SD}(aX + b) = |a|\mathbb{SD}(X)$$

Don't forget the absolute values and squares!

# Standardization of random variables

X in **standard units** is the random variable $X_{su} = \dfrac{X - \mathbb{E}(X)}{\mathbb{SD}(X)}$ .

- $X_{su}$ measures X on the scale **"number of SDs from expectation**."
- It is a linear transformation of X. By the linear transformation rules for expectation and variance:

$$\mathbb{E}(X_{su}) = 0, \quad \mathbb{SD}(X_{su}) = 1$$

- Since $X_{su}$ is centered (has expectation 0):

$$\mathbb{E}(X_{su}^2) = \mathbb{V}ar(X_{su}) = 1$$

**You should prove these facts yourself.**

# Variance of a sum, Covariance

# Recap

Thus far, we've established the following:

- Linear transformations of random variables apply to their expectation.

$$\mathbb{E}(aX + b) = a\mathbb{E}(X) + b$$

- Expectation is additive.

$$\mathbb{E}(X + Y) = \mathbb{E}(X) + \mathbb{E}(Y)$$

- Linear transformations of random variables transform their variance as follows:

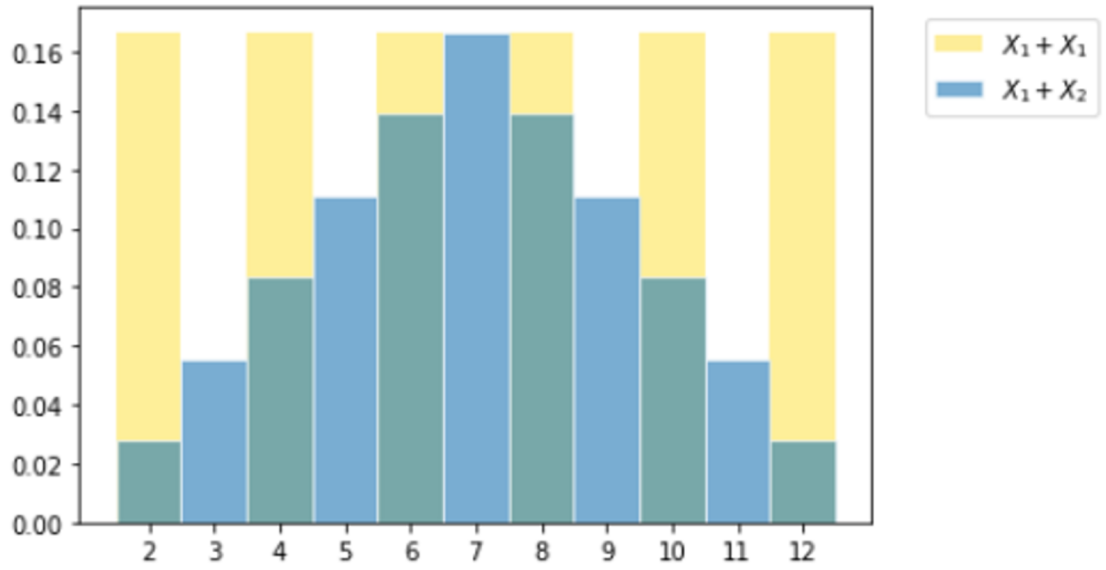
$$\mathbb{V}ar(aX + b) = a^2\mathbb{V}ar(X)$$

**We haven't yet talked about the variance of a sum of random variables.** Let's now do that!

# Distributions of sums

Suppose $X_1$ and $X_2$ are the numbers on two rolls of a die.

- **$X_1$ and $X_2$ have the same distribution** (they are both Uniform in {1, 2, 3, 4, 5, 6}).
- But the **distributions of $X_1 + X_1$ and $X_1 + X_2$ are different**.
- Both $X_1 + X_1$ and $X_1 + X_2$ have the same expectation (7).
- But $X_1 + X_2$ seems to have less spread, indicating that $X_1 + X_1 = 2X_1$ has a larger variance.



# Variance of a sum

The variance of a sum is affected by the dependence between the two random variables that are being added. Let's expand out the definition of Var(X + Y) to see what's going on.

Let $\mu_x = E[X], \mu_y = E[Y]$ .

$$
\begin{aligned}
Var(X+Y) &= E\big[(X+Y-E(X+Y))^2\big] \\
&= E\big[((X-\mu_x)+(Y-\mu_y))^2\big] \\
&= E\big[(X-\mu_x)^2 + 2(X-\mu_x)(Y-\mu_y) + (Y-\mu_y)^2\big] \\
&= E\big[(X-\mu_x)^2\big] + E\big[(Y-\mu_y)^2\big] + 2E\big[(X-\mu_x)(Y-\mu_y)\big] \\
&= Var(X) + Var(Y) + 2E\big[(X-E(X))(Y-E(Y))\big]
\end{aligned}
$$

By the linearity of expectation, and the substitution.

We see that the variance of a sum is equal to the sum of variances, PLUS this weird term...

# Covariance

The covariance of two random variables is their **expected product of deviations**.

$$\mathbb{C}ov(X, Y) = \mathbb{E}((X - \mathbb{E}(X))(Y - \mathbb{E}(Y)))$$

- It is a generalization of variance. Note: $\mathbb{C}ov(X, X) = \mathbb{V}ar(X)$.
- Using the linearity of expectation and some algebra, you can show the following equality, which is a generalization of the alternative calculation for variance:

$$\mathbb{C}ov(X, Y) = \mathbb{E}(XY) - \mathbb{E}(X)\mathbb{E}(Y)$$

- To see whether variance is ever additive, we need to look at covariance differently.

# When is variance additive?

For any two random variables X and Y:

$$\mathbb{V}ar(X+Y) = \mathbb{V}ar(X) + \mathbb{V}ar(Y) + 2\mathbb{C}ov(X,Y)$$

In order for variance to be additive, the covariance between X and Y needs to be 0.

$$\mathbb{V}ar(X+Y) = \mathbb{V}ar(X) + \mathbb{V}ar(Y) \iff \mathbb{C}ov(X,Y) = 0$$

When is the covariance between two random variables 0?

- A sufficient condition is that X and Y are **independent**. If X and Y are independent, knowing the value of X tells you nothing about the value of Y. Independence is a **strong statement**.
- This is not the only case when the covariance is 0, as we will shortly see.

Sometimes called the **addition rule for variance**:

$$\mathbb{V}ar(X+Y) = \mathbb{V}ar(X) + \mathbb{V}ar(Y) \text{ if } X \text{ and } Y \text{ are independent}$$

# Correlation

The units of the covariance are hard to interpret (e.g. “inch pounds”). In order to get rid of the units, we can scale it:

$$\begin{aligned}
\frac{\mathbb{C}ov(X,Y)}{\mathbb{SD}(X)\mathbb{SD}(Y)} &= \frac{\mathbb{E}((X-\mathbb{E}(X))(Y-\mathbb{E}(Y)))}{\mathbb{SD}(X)\mathbb{SD}(Y)} \\
&= \mathbb{E}\left(\frac{X-\mathbb{E}(X)}{\mathbb{SD}(X)} \cdot \frac{Y-\mathbb{E}(Y)}{\mathbb{SD}(Y)}\right) \\
&= \mathbb{E}(X_{su}Y_{su}) \\
&= r(X,Y)
\end{aligned}$$

Recall: correlation is the average product in standard units. This is the random variable equivalent of that!

**Correlation** is covariance scaled by the two SDs.

# Uncorrelated random variables

The correlation between X and Y is

$$r(X,Y) = \frac{\mathbb{C}ov(X,Y)}{\mathbb{SD}(X)\mathbb{SD}(Y)}$$

This means that either both correlation and covariance are 0, or neither are.

$$\mathbb{C}ov(X,Y) = 0 \iff r(X,Y) = 0$$

- “Covariance equal to 0” is the same as “**uncorrelated**”.
- **Independent random variables are uncorrelated**.
- But not all uncorrelated random variables are independent!
  - For instance: Let X be uniform on {-1, 1}. X and $X^2$ are uncorrelated, but dependent.

# More properties of sums

# Addition rule for variance

If X and Y are **uncorrelated** (in particular, if they are **independent**), then

$$\mathbb{V}ar(X+Y) = \mathbb{V}ar(X) + \mathbb{V}ar(Y)$$

Therefore, under the same conditions,

$$\mathbb{SD}(X+Y) = \sqrt{\mathbb{V}ar(X) + \mathbb{V}ar(Y)} = \sqrt{(\mathbb{SD}(X))^2 + (\mathbb{SD}(Y))^2}$$

- Uncorrelated random variables are like orthogonal vectors.

# I.I.D. sample sum

- "i.i.d." is short for "independent and identically distributed".
- Draws at random with replacement from a population are i.i.d.
- Let the sample $X_1, X_2, \ldots, X_n$ be i.i.d. draws from a numerical population that has mean $\mu$ and SD $\sigma$.
- Let the sample sum be $S_n = \sum_{i=1}^{n} X_i$.

Then, $\mathbb{E}(S_n) = n\mu, \quad \mathbb{V}ar(S_n) = n\sigma^2, \quad \mathbb{SD}(S_n) = \sqrt{n}\sigma$

SD is not additive, even when each RV in the sum is independent.

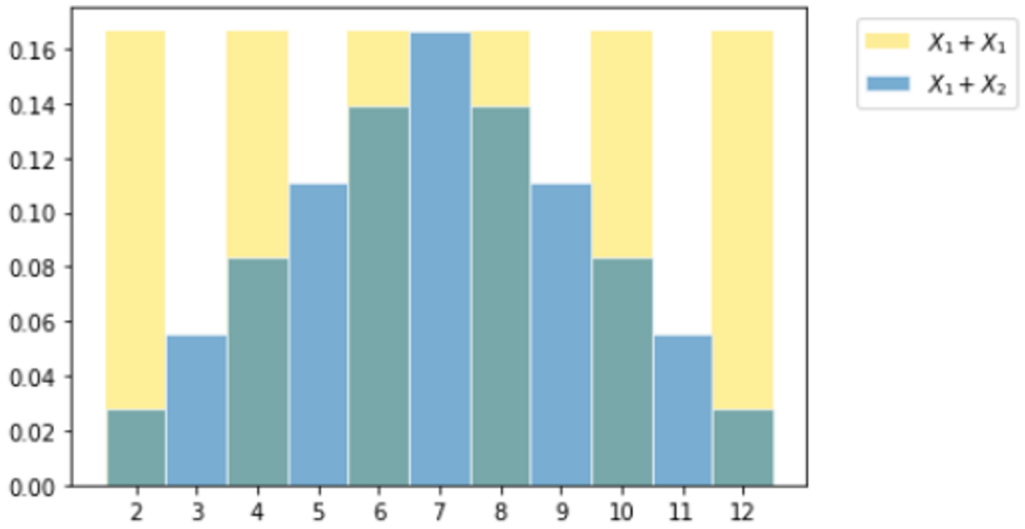
# An example revisited

Suppose $X_1$ and $X_2$ are the numbers on two rolls of a die. $X_1$ and $X_2$ have the same expectation and variance:

$\mathbb{E}(X_1) = 3.5 = \mathbb{E}(X_2) \qquad \mathbb{SD}(X_1) = 1.71 = \mathbb{SD}(X_2)$

$X_1 + X_1$ and $X_1 + X_2$ have the same expectation:

$\mathbb{E}(X_1 + X_1) = 2 \times 3.5 = 7 = \mathbb{E}(X_1 + X_2)$




But their variances (and hence SDs) are different:

$\mathbb{SD}(X_1 + X_1) = \mathbb{SD}(2X_1) = 2 \times 1.71 = 3.42$

$\mathbb{SD}(X_1 + X_2) = \sqrt{2} \times 1.71 = 2.42$

Since $X_1$ and $X_2$ are independent, we can use the result from the previous slide.

As we reasoned about earlier, the spread of $X_1 + X_2$ is less than the spread of $X_1 + X_1$.

# Variance of the Bernoulli distribution

En-route to computing the variance of the binomial distribution, let's first compute the variance of the Bernoulli (p) distribution. We can do this using the alternate calculation for variance.

$$E(X) = p$$

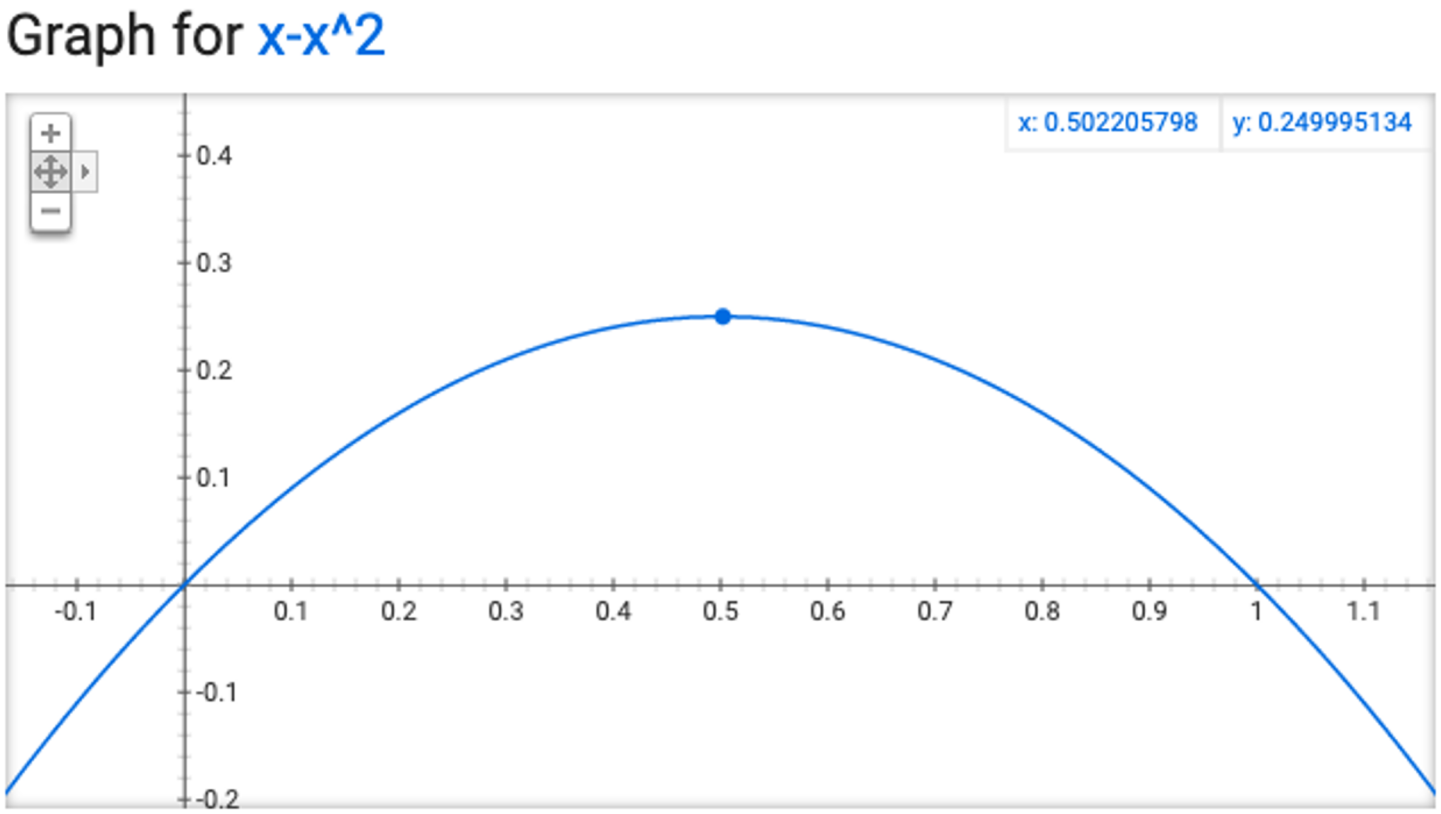
$$E(X^2) = 1^2 \cdot p + 0^2 \cdot (1 - p) = p$$

Putting these together:

$$Var(X) = E(X^2) - (E(X))^2 = p - p^2 = p(1 - p)$$

# A quick bit of intuition - when is Var(Ber(p)) maximal?

$$Var(X) = p - p^2 = p(1-p)$$




ps - tip, plot above: google(plot x - x^2)

# Variance of the binomial distribution

Let X have the **binomial (n, p)** distribution. We know that X is the number of “successes” in n independent trials of some event, each of which occur with probability p.

- Each trial can be thought of as a single Bernoulli (p) trial.
- We can then write:

$$X = I_1 + I_2 + \cdots + I_n$$

where $I_j$ is the **indicator** of success on trial j. $I_j$ = 1 if trial j is a success, and 0 else.

- For each j, $\mathbb{E}(I_j) = p, \quad \mathbb{V}ar(I_j) = p(1-p)$ .
- As established before, $\mathbb{E}(X) = np$ .
- Using the fact that each indicator is independent:

$$\mathbb{V}ar(X) = np(1-p), \quad \mathbb{SD}(X) = \sqrt{np(1-p)}$$

# Distribution of sample means

# Sample mean

Earlier, we looked at the expectation and SD of the sample sum. Let's explore the sample mean.

- Consider an i.i.d. sample $X_1, X_2, \ldots, X_n$.
- For each i, $E(X_i) = \mu, \quad SD(X_i) = \sigma$.
- Define:

$$S_n = \sum_{i=1}^{n} X_i, \quad \bar{X}_n = \frac{1}{n} S_n$$

- The sample mean is a linear transformation of the sample sum (scaled by 1/n).
  - By linear transformation rules:

$$\mathbb{E}(\bar{X}_n) = \mu, \quad \mathbb{SD}(\bar{X}_n) = \frac{\sigma}{\sqrt{n}}$$

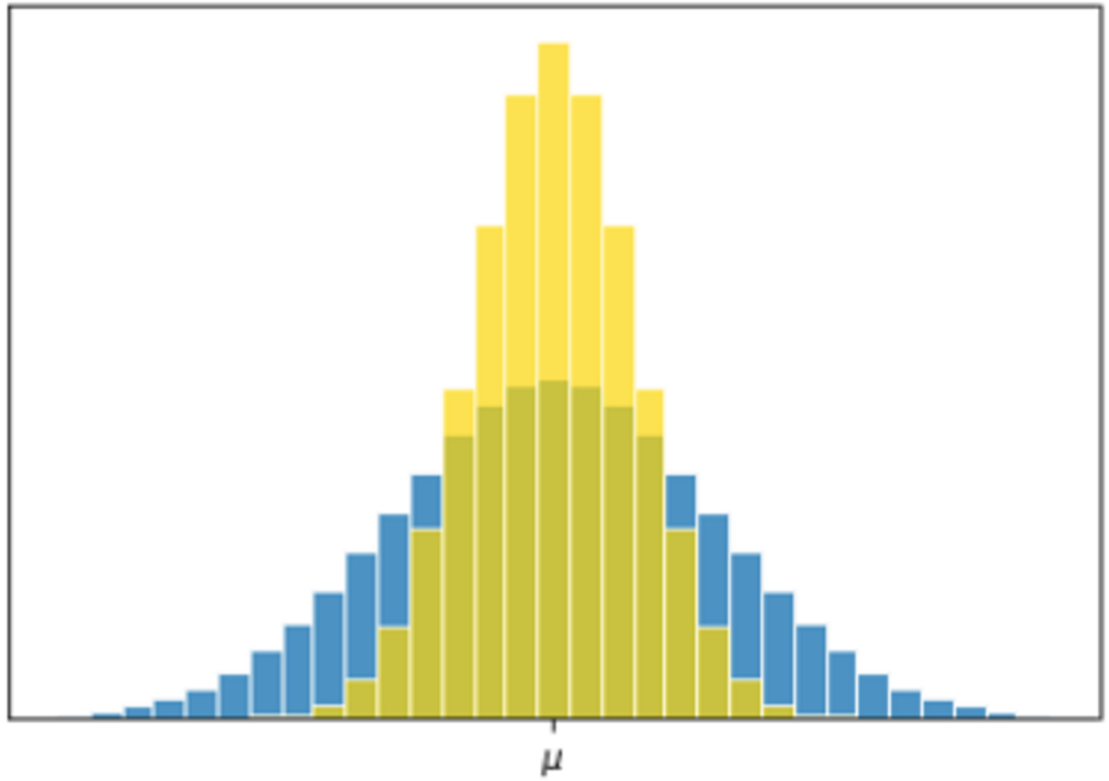
# Accuracy of the sample mean

- Our goal will often be to estimate some characteristic of a population.
  - For instance, the average height of undergrad students.
  - To do this, we typically go out and collect a single sample. It has just one average.
  - Since that sample was random, it *could have* come out differently. As such, we need to look at the distribution of all possible sample means.
- For any sample size, the expected value of the sample mean is the population mean.
  - $\mathbb{E}(\bar{X}_n) = \mu$ .
  - We call the sample mean an unbiased estimator of the population mean.

# Shape of the distribution

- As the sample size increases, the SD of the sample mean decreases.
    - The sample mean is more likely to be close to the population mean if we have a larger sample size.
- **Square root law:** If you increase the sample size by a factor, the SD decreases by the square root of the factor.

$$\mathbb{SD}(\bar{X}_n) = \frac{\sigma}{\sqrt{n}}$$




Here are the distributions of two sample means. Both are drawn from the same population, but with different sample sizes.

# Central limit theorem

The **central limit theorem (CLT)** states that no matter what population you are drawing from, the probability distribution of **the sum of an i.i.d. sample is roughly normal** if the sample size is large.

- Since the sample mean is a linear transformation of the sample sum, the sample mean is also roughly normal (with scaled parameters).

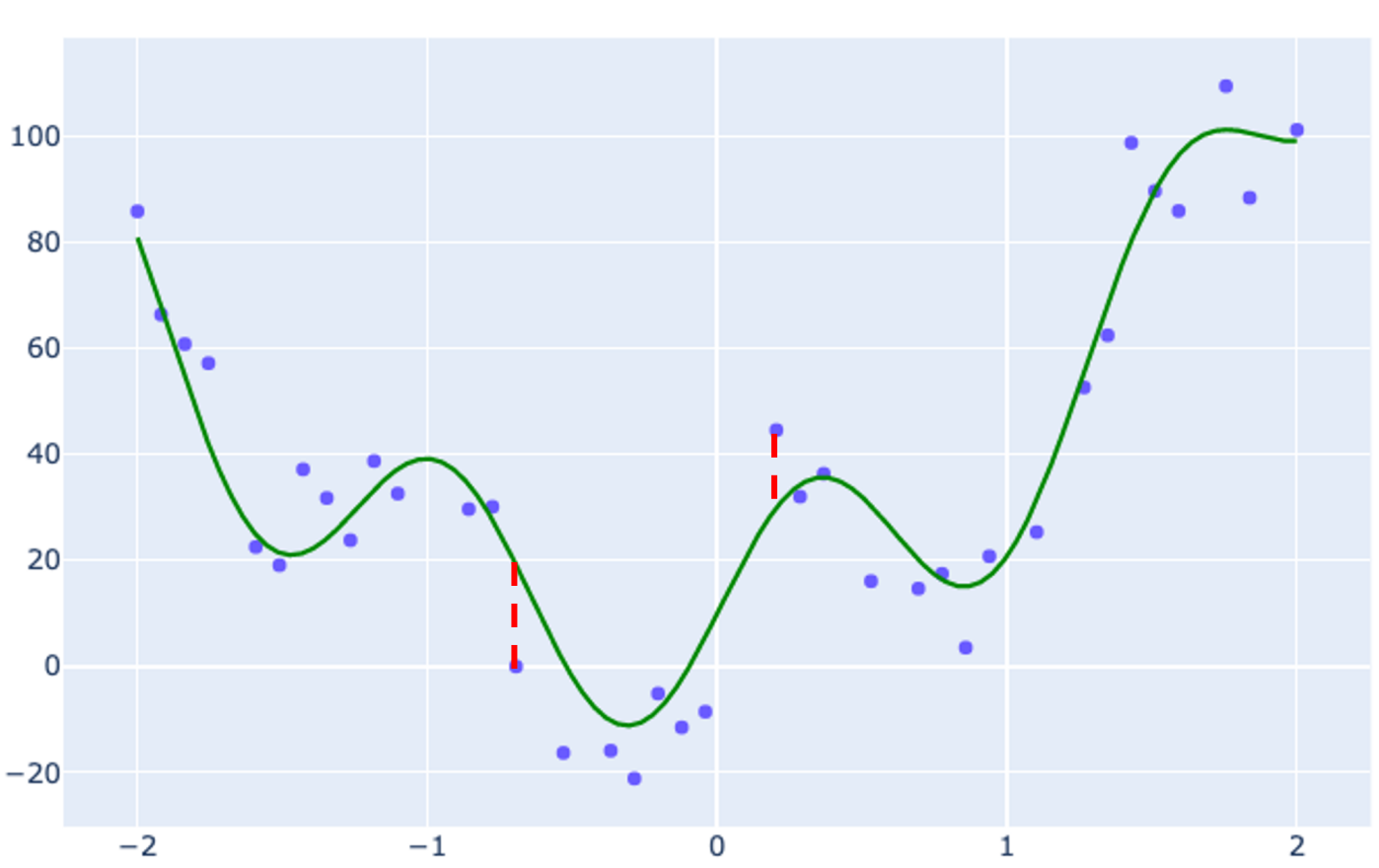
# Bias and Variance in Modeling

# Questions

- **How** can we describe the randomness in our data generation process?
- **What** does it mean for a new individual to be "similar" to those for whom we already have data?
- **What** are the main sources of error in prediction?
- **Why** do these errors occur, and how can we reduce them?
- **How** do all the different errors affect our overall risk?

# Assumptions of Randomness

# Data Generation Process




- True relation $g$
- For each individual,
  - fixed value of $x$ and hence also $g(x)$
  - Random error $\epsilon$
  - Observation is

$$Y = g(x) + \epsilon$$

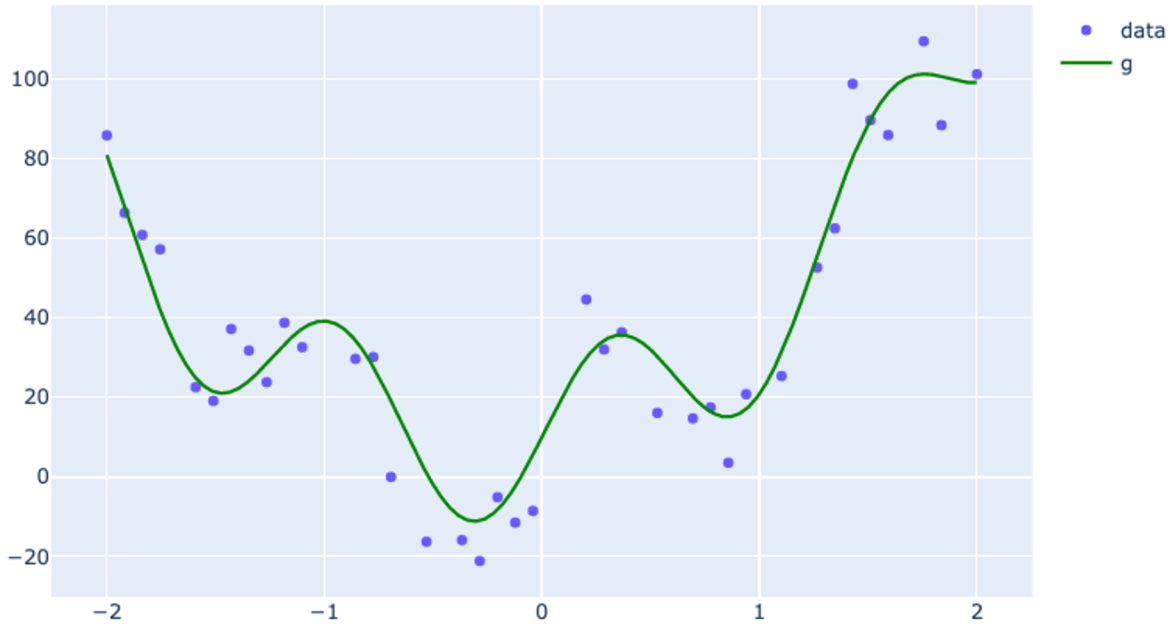
Errors have expectation 0 and are i.i.d. across individuals

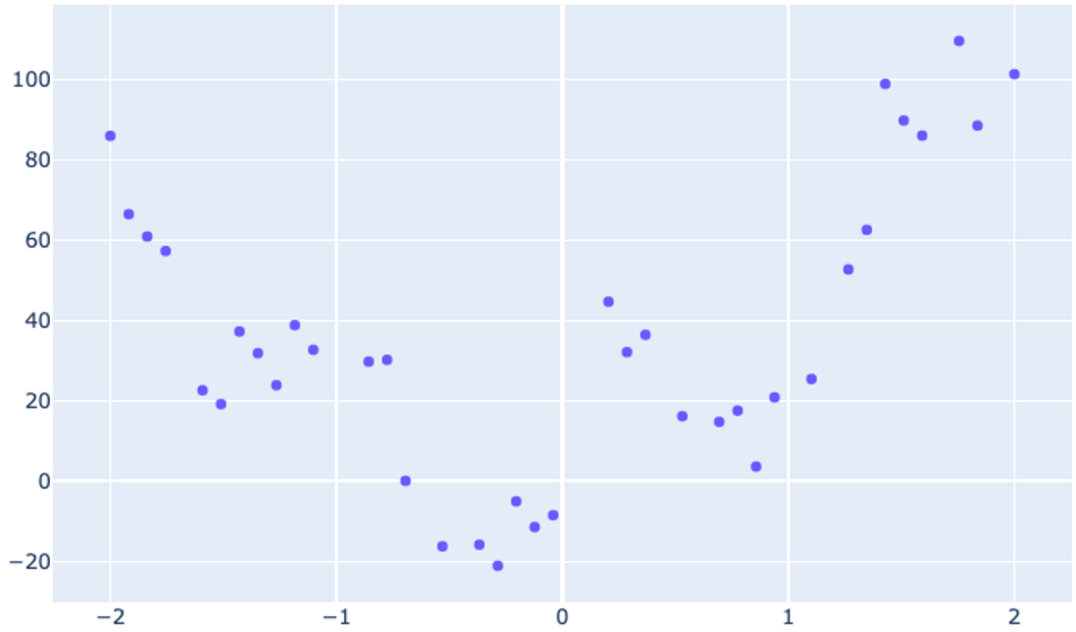
# The Data

At each $x$,

- truth = $g(x)$
- noise = $\epsilon$
- Observation $Y = g(x) + \epsilon$

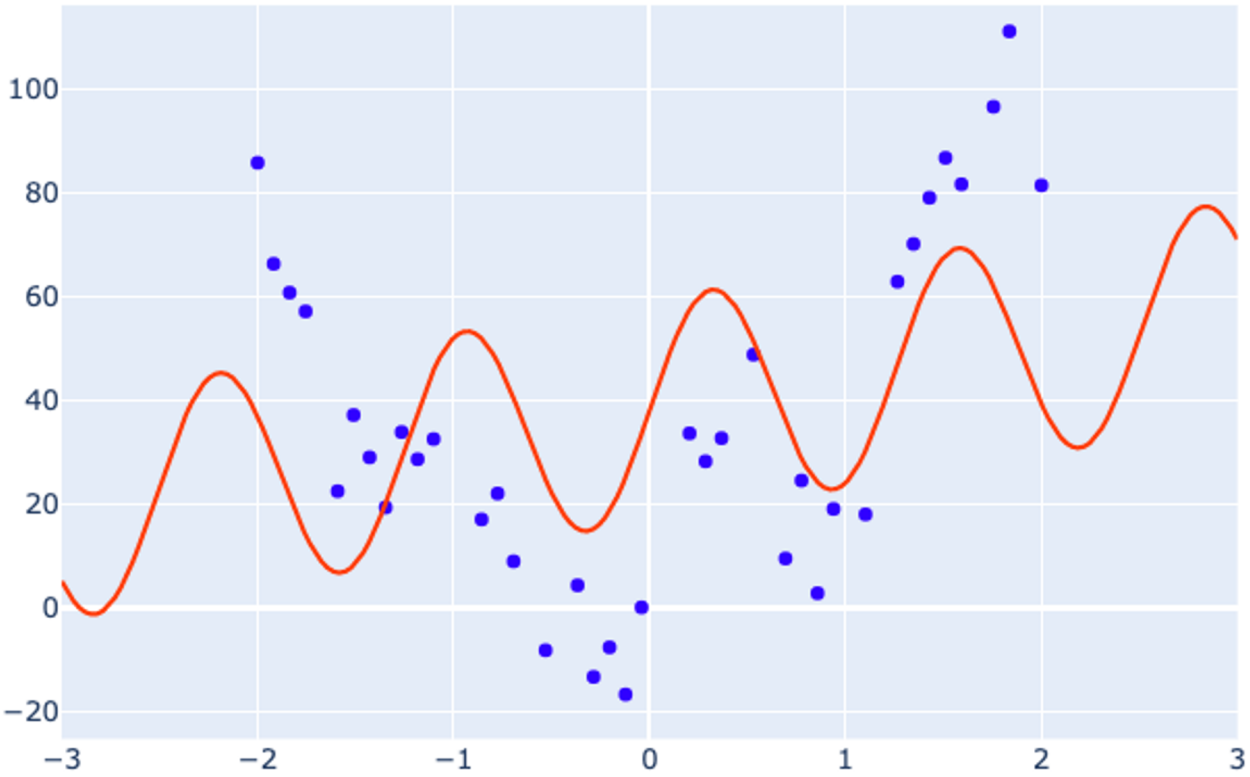
We only see $Y$



# Our Predictions

We choose a model and fit it to our data.
The red line is our fitted function.




At every $x$, our prediction for $Y$ is

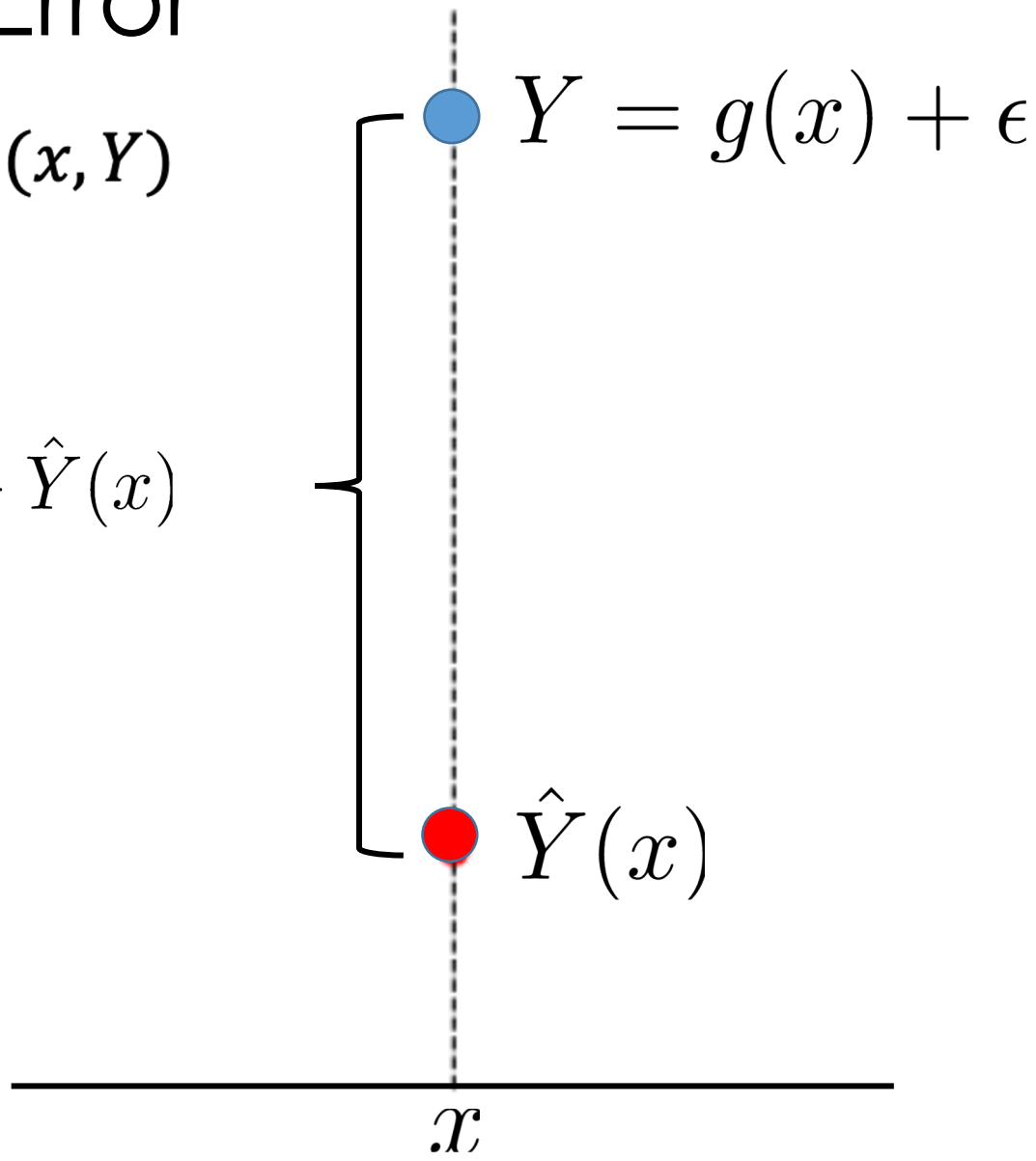
- The height of the red line at $x$
- Denote this $\hat{Y}(x)$

# Measuring Prediction Error

# Prediction Error

New individual: $(x, Y)$

error = $Y - \hat{Y}(x)$



# Model Risk

- For a new individual at $(x, Y)$:
- Mean squared error of prediction

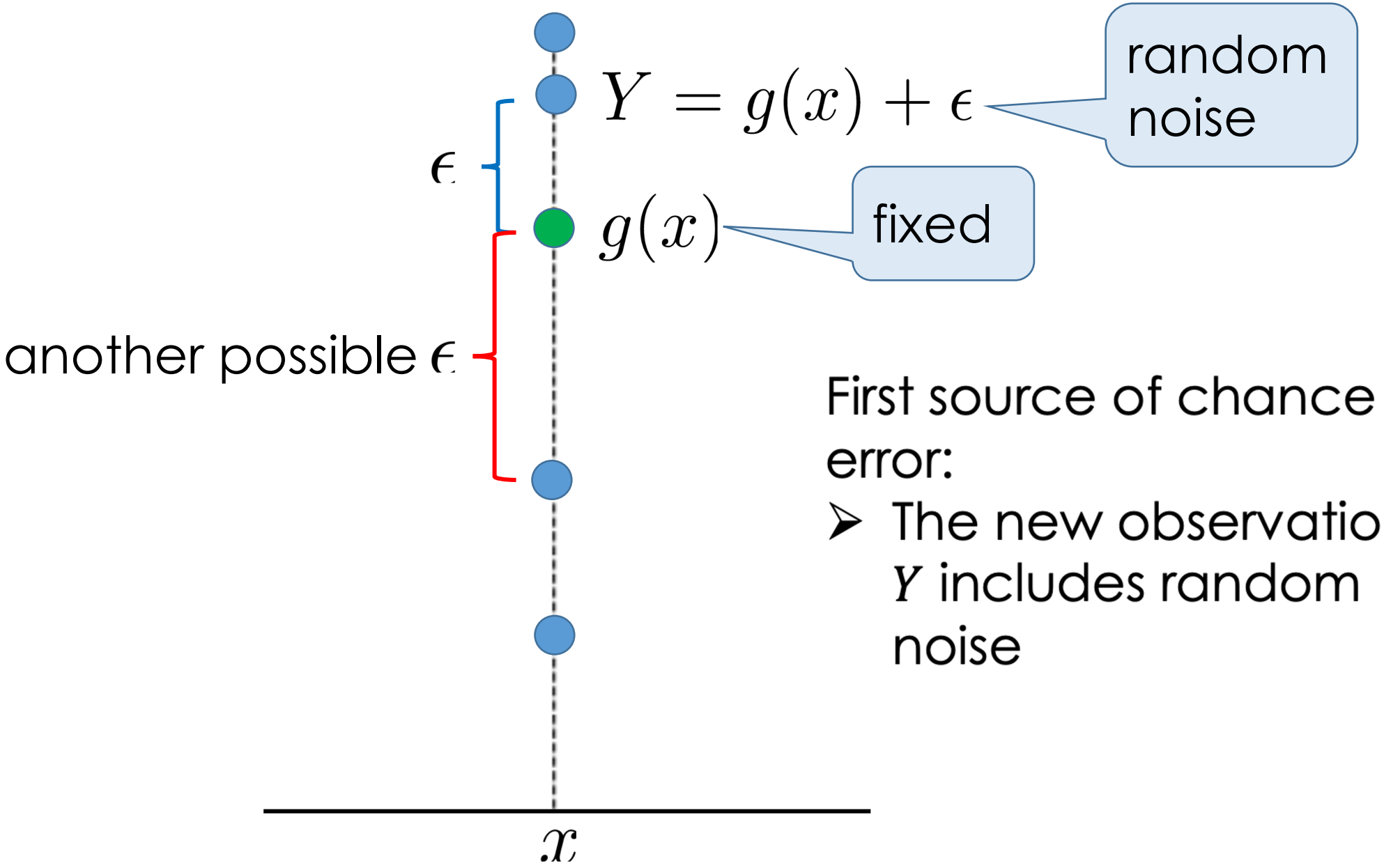
$$\text{model risk} = \mathbb{E}((Y - \hat{Y}(x))^2)$$

- The expectation is an average over all samples:
  - all possible samples we could have got for fitting our model
  - all possible new observations at the fixed $x$

# Two Kinds of Error

- Chance error:
  - Due to randomness alone
  - In the new observations
  - Also in the sample we used for fitting our model
- Bias:
  - Non-random error
  - Due to our model being different from the true underlying function $g$

# Chance Error in the New Observation




First source of chance error:

- The new observation $Y$ includes random noise

# Observation Variance

- The new observation is $Y$
- $Y = g(x) + \epsilon$
- $\epsilon$ is random $\quad \mathbb{E}(\epsilon) = 0 \qquad \mathbb{V}ar(\epsilon) = \sigma^2$

$$\mathbb{V}ar(Y) = \mathbb{V}ar(g(x) + \epsilon) = \mathbb{V}ar(\epsilon) = \sigma^2$$

$$\text{observation variance} = \sigma^2$$

# Reasons and Remedies

Some reasons:

- Measurement error
- Missing information acting like noise

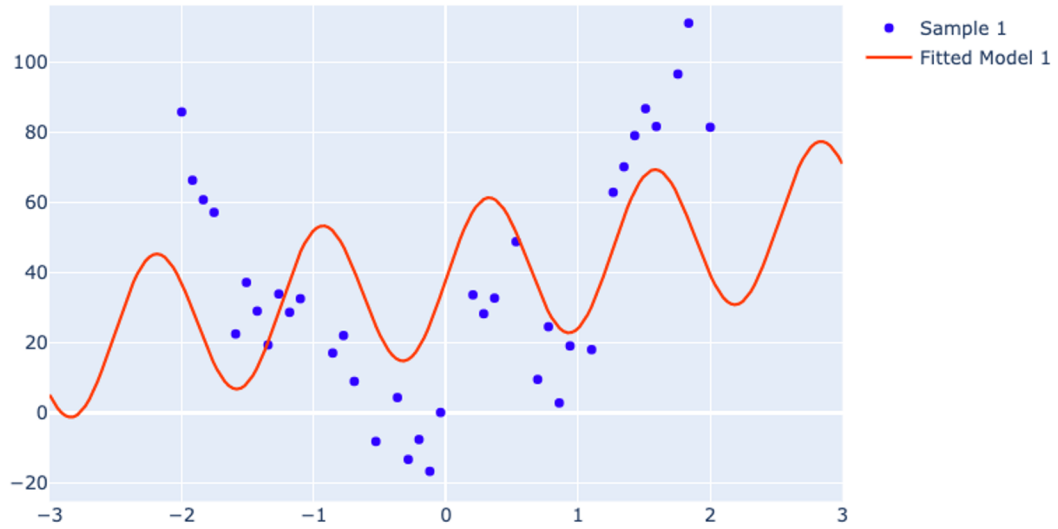
Could try to get more precise measurements

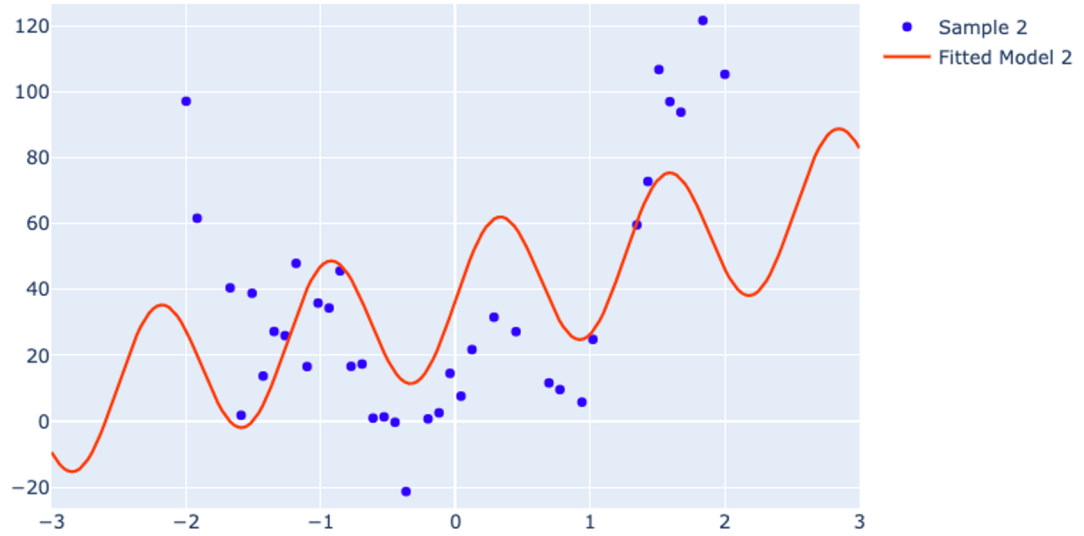
Often this is beyond the control of the data scientist.

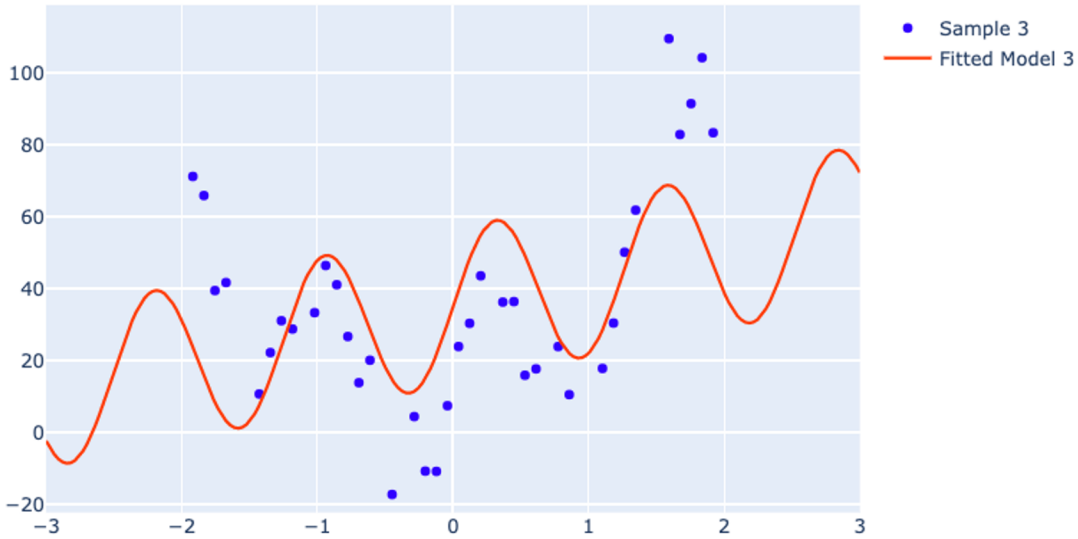
# Chance Error in Our Fitted Model

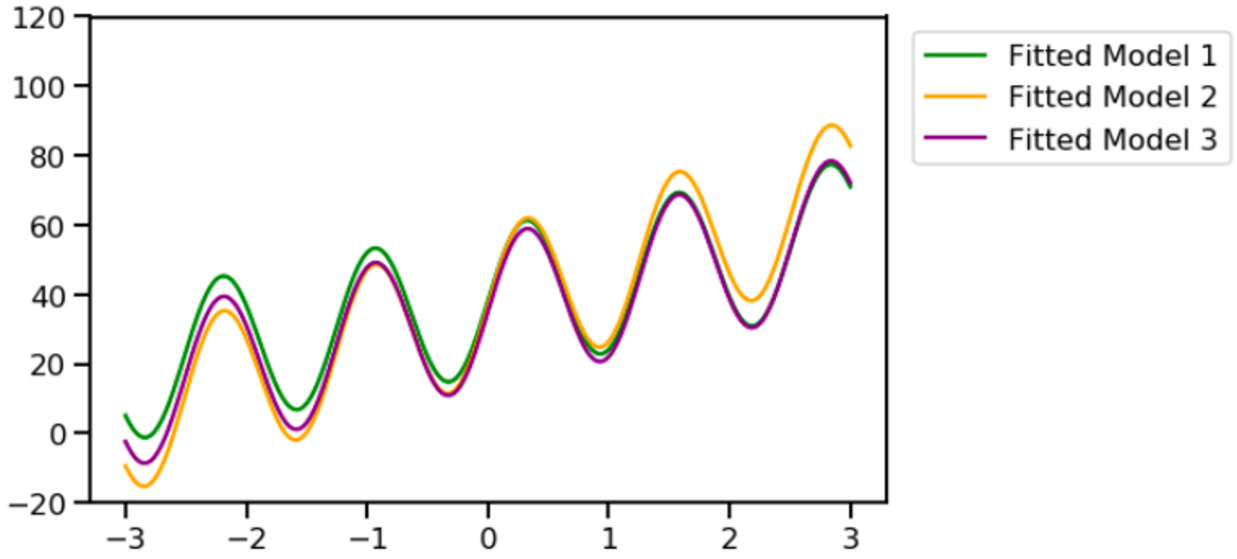
# Model Variability

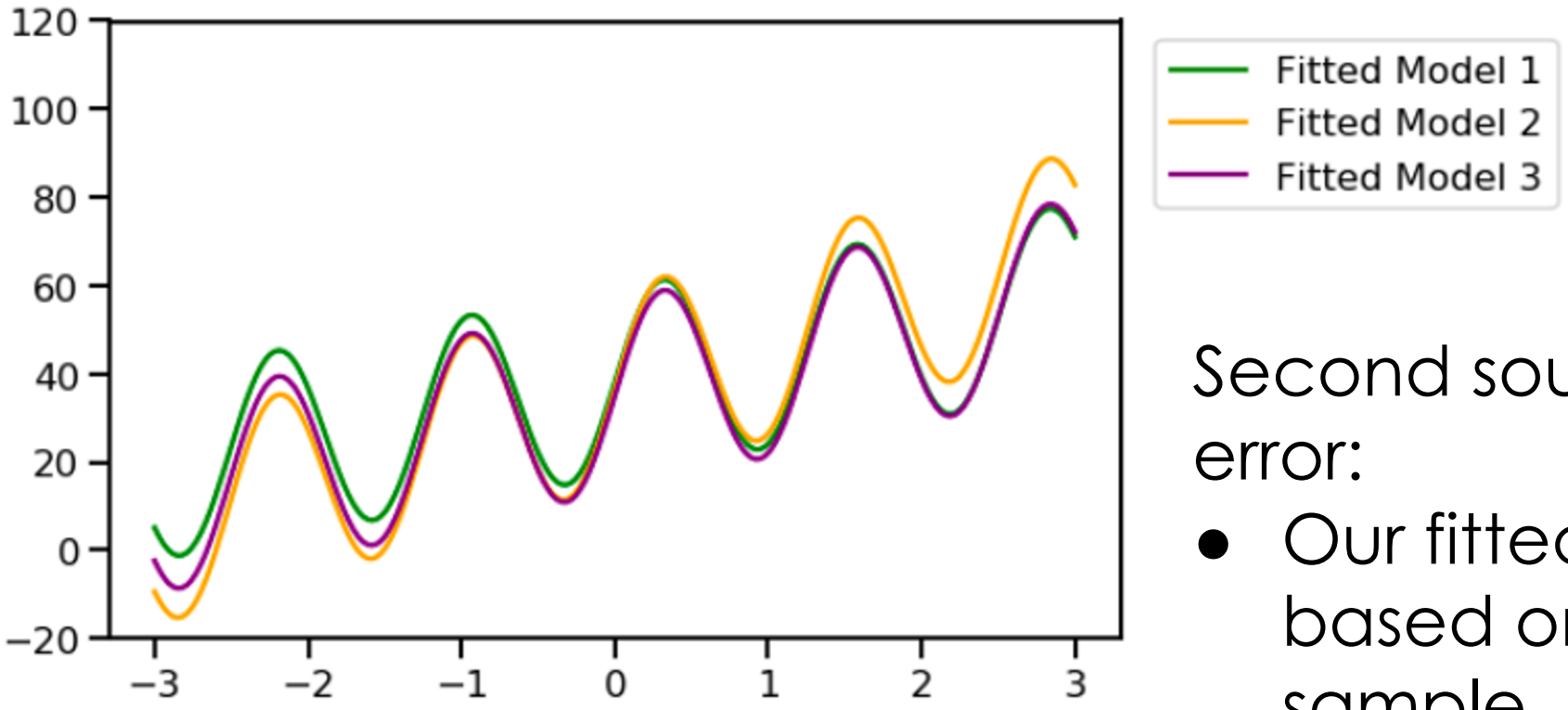
## $\hat{Y}$ depends on the sample






Second source of chance error:

- Our fitted model is based on a random sample
- The sample could have come out differently
- Then the fitted model would have been different

# Model Variance

- Our prediction at $x$ is $\hat{Y}(x)$

- The average of these predictions across all possible samples is $\mathbb{E}(\hat{Y}(x))$

- The variance of our prediction is

$$\text{model variance} = \mathbb{V}ar(\hat{Y}(x)) = \mathbb{E}\big((\hat{Y}(x) - \mathbb{E}(\hat{Y}(x)))^2\big)$$

# Reasons and Remedies

Main reason:

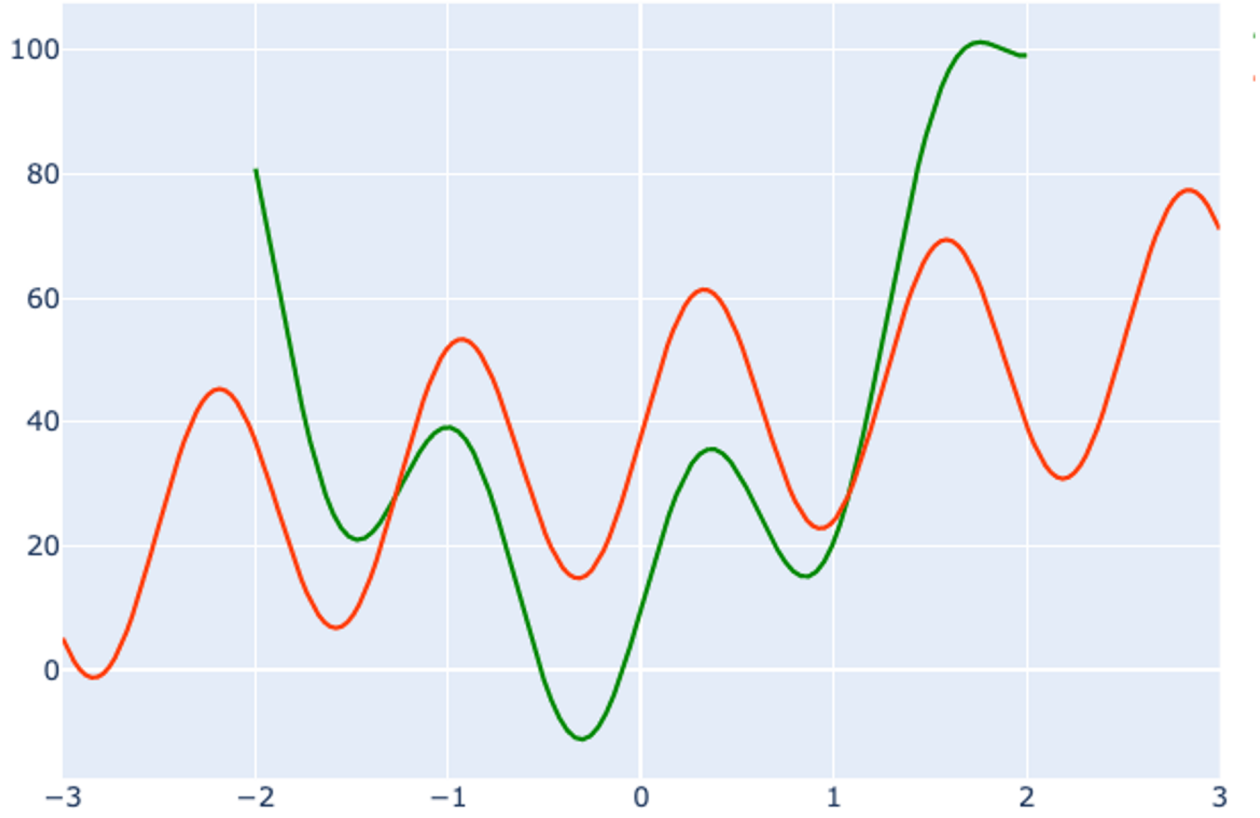
- Overfitting: small differences in random samples lead to large differences in the fitted model

Remedy:

- Reduce model complexity
- Don’t fit the noise

# Bias

# Our Model Versus the Truth




- The green line is the fixed truth $g$
- The red line is our fitted model
- Bias measures how far off these two are, on average over all possible samples

# Model Bias

- The difference between our predicted value and the true $g(x)$
  - averaged over all possible samples

$$\mathbb{E}(\hat{Y}(x) - g(x)) = \mathbb{E}(\hat{Y}(x)) - g(x)$$

$$\text{model bias} = \mathbb{E}(\hat{Y}(x)) - g(x)$$

- Bias depends on $x$ but is **not random**
  - If positive, the model tends to overestimate at $x$
  - If negative, the model tends to underestimate at $x$

# Reasons and Remedies

Some reasons:

- Underfitting
- Lack of domain knowledge

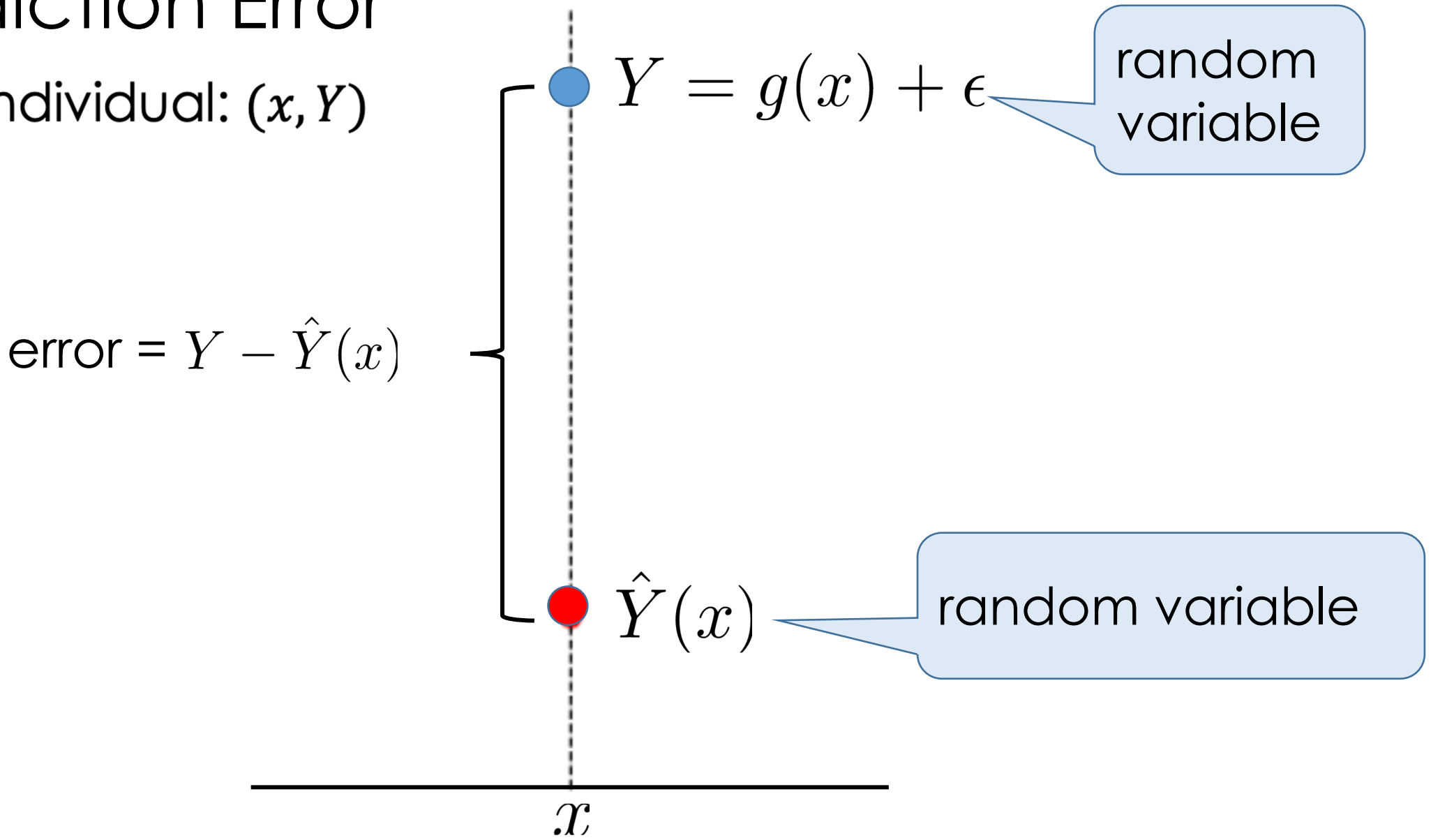
Remedies:

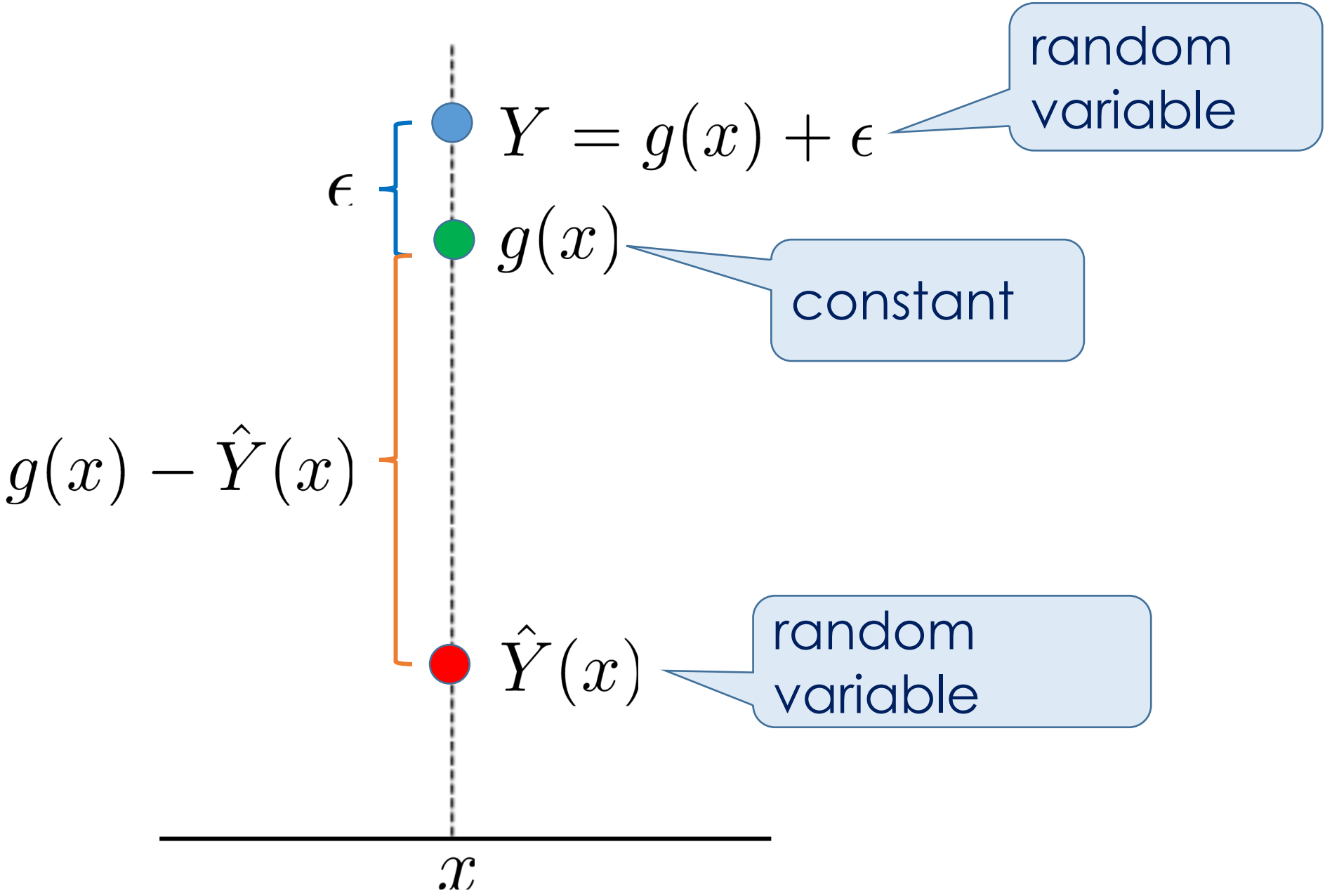
- Increase model complexity (but don't overfit)
- Consult domain experts to see which models make sense

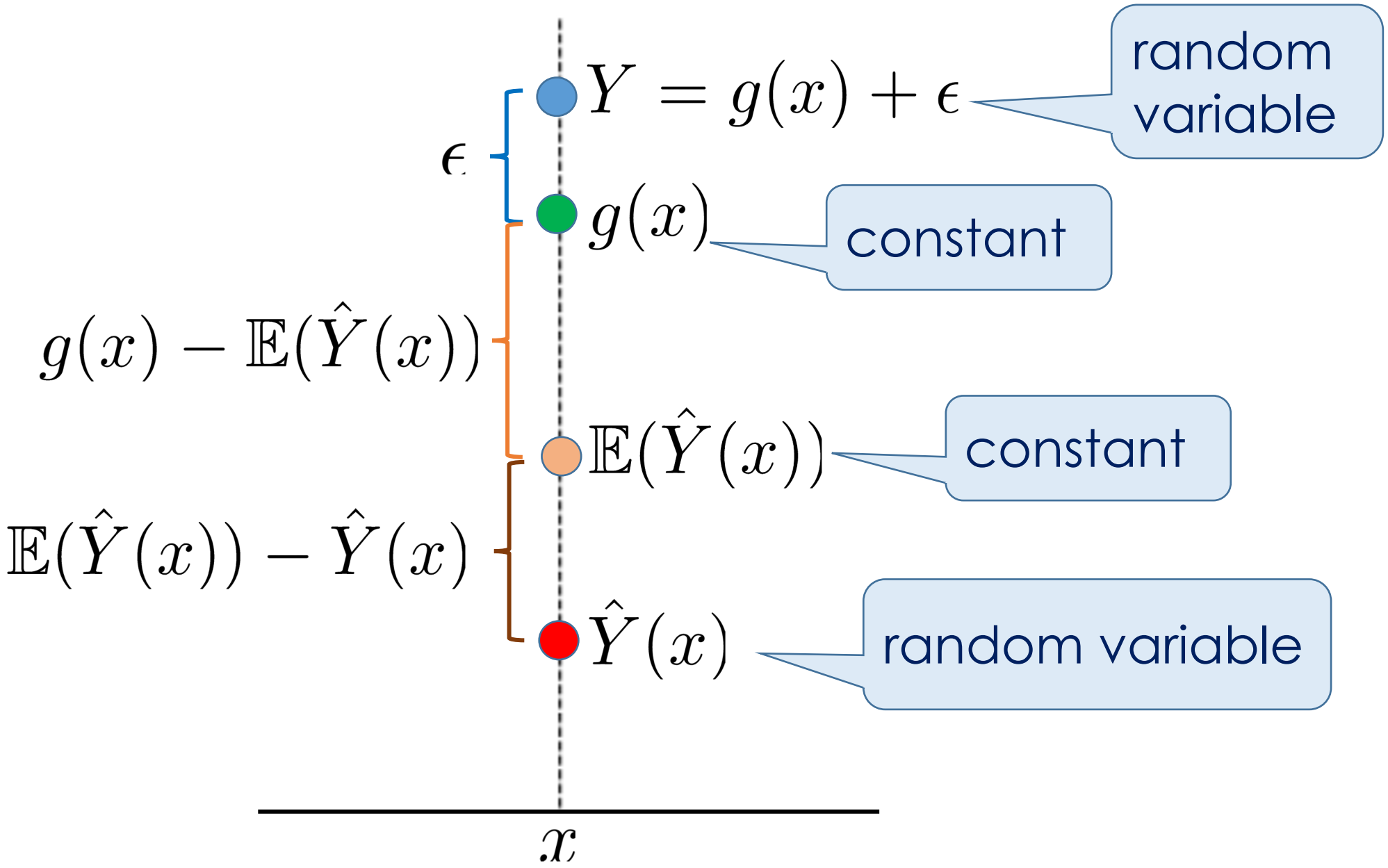
# Components of Prediction Error

# Prediction Error

New individual: $(x, Y)$




$Y = g(x) + \epsilon$
random variable
$\epsilon$
$g(x)$
constant
$g(x) - \hat{Y}(x)$
$\hat{Y}(x)$
random variable
$x$


$Y = g(x) + \epsilon$
random variable
$\epsilon$
$g(x)$
constant
$g(x) - \mathbb{E}(\hat{Y}(x))$
$\mathbb{E}(\hat{Y}(x))$
constant
$\mathbb{E}(\hat{Y}(x)) - \hat{Y}(x)$
$\hat{Y}(x)$
random variable
$x$

# Decomposition of Model Risk

# Decomposition of Error and Risk

Decomposition of the prediction error into three pieces:

$$Y - \hat{Y}(x) \;=\; \epsilon \;+\; (g(x) - \mathbb{E}(\hat{Y}(x))) \;+\; (\mathbb{E}(\hat{Y}(x)) - \hat{Y}(x))$$

Decomposition of the model risk into three pieces:

$$\begin{aligned}\mathbb{E}\big((Y - \hat{Y}(x))^2\big) &= \mathbb{E}(\epsilon^2) \\ &\quad + (g(x) - \mathbb{E}(\hat{Y}(x)))^2 \\ &\quad + \mathbb{E}\big((\mathbb{E}(\hat{Y}(x)) - \hat{Y}(x))^2\big)\end{aligned}$$

The cross-product terms are 0

$$\text{model risk} = \sigma^2 + (\text{model bias})^2 + \text{model variance}$$

# Bias Variance Decomposition

$$\text{model risk} = \text{observation variance} + (\text{model bias})^2 + \text{model variance}$$

$$\mathbb{E}\big((Y - \hat{Y}(x))^2\big) \;=\; \sigma^2 \;+\; (\mathbb{E}(\hat{Y}(x)) - g(x))^2 \;+\; \mathbb{E}\big((\hat{Y}(x) - \mathbb{E}(\hat{Y}(x)))^2\big)$$

Note: these three terms are dimensionally consistent.

# Predicting by a Function with Parameters

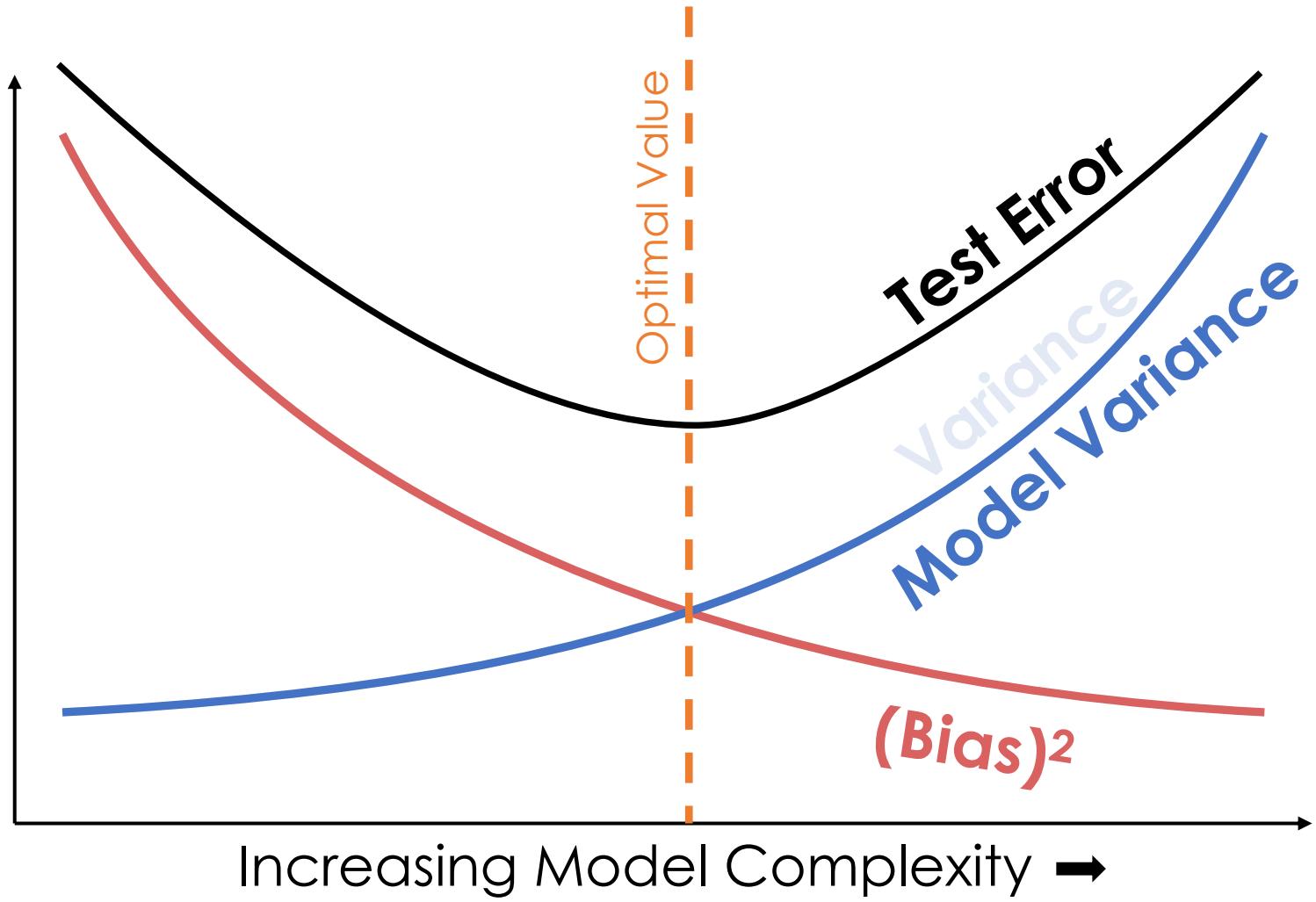
If our model is a non-random function $f$ that has an unknown parameter vector $\theta$

- $\theta$ is not random but has to be estimated from the sample
- The estimate $\hat{\theta}$ is random
- So our fitted function $f_{\hat{\theta}}$ is random and is just another name for $\hat{Y}$

$$\mathbb{E}\big((Y - f_{\hat{\theta}}(x))^2\big) \;=\; \sigma^2 \;+\; (\mathbb{E}(f_{\hat{\theta}}(x)) - g(x))^2 \;+\; \mathbb{E}\big((f_{\hat{\theta}}(x) - \mathbb{E}(f_{\hat{\theta}}(x)))^2\big)$$

# Summary for Modeling

# Bias Variance Plot



# Modeling Goals

- Try to minimize all three of observation variance, model bias, and model variance.

*But*

- Observation variance is often out of our control
- Reducing complexity to reduce model variance can increase bias
- Increasing model complexity to reduce bias can increase model variance
- Domain knowledge matters: the right model structure!