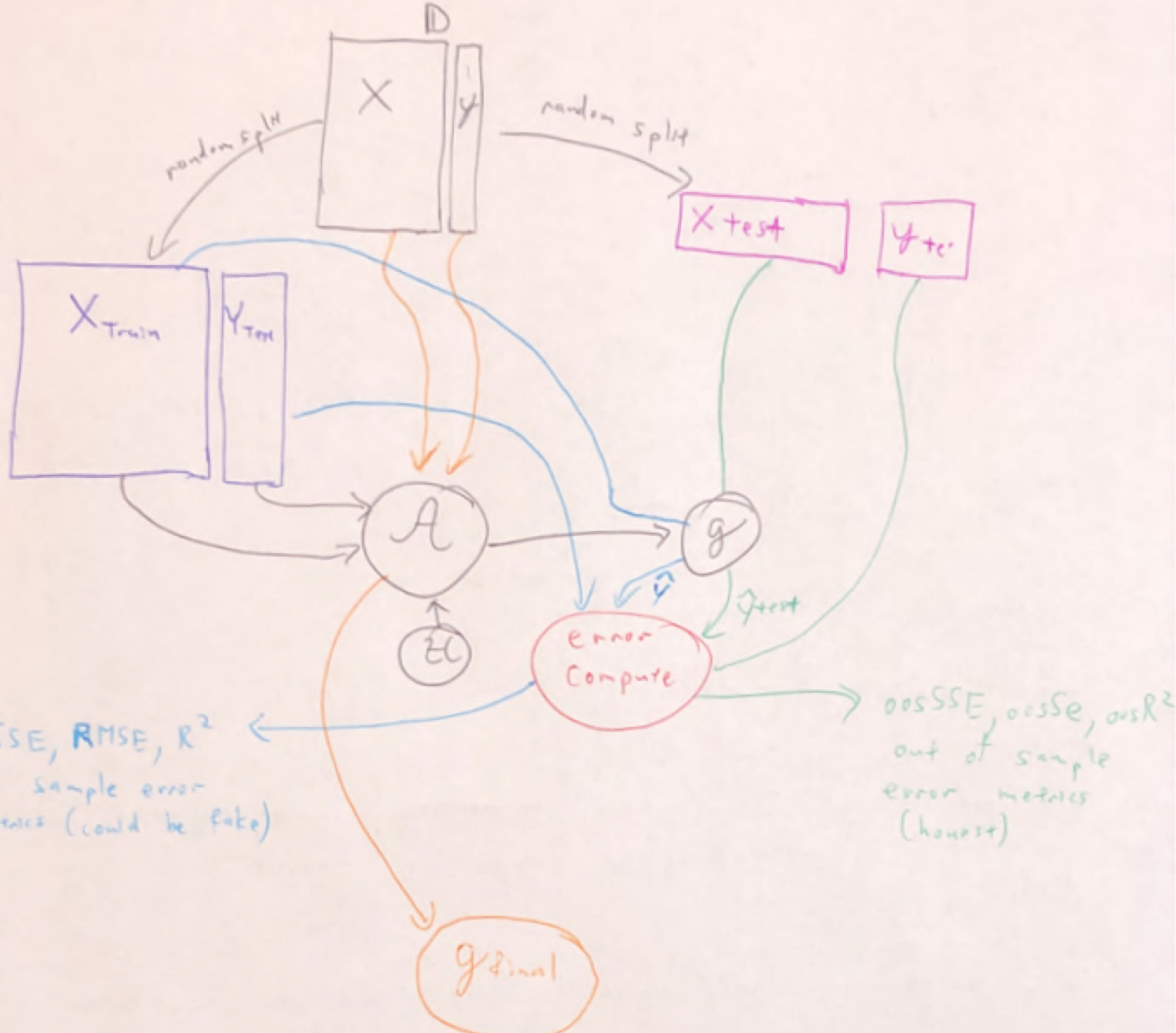
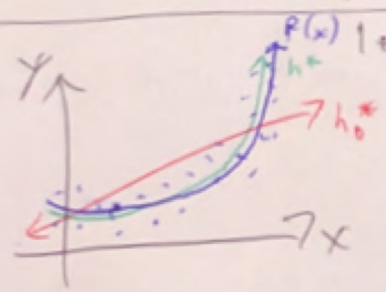
Lecture 13 3/15/21

$K = 10 \Rightarrow$ test set is 10% n.



The g_{final} is the function used for future prediction. Its performance is at least as good as the oos metrics since you're running the same model fitting procedure but now n is slightly higher.



let $p = 1$ feature, $y = g(x) + \underbrace{h^*(x) - g(x)}_{\text{high if } n \text{ not much} > p} + \underbrace{f(x) - h^*(x)}_{\text{misspecification error}} + \underbrace{t(\vec{z}) - f(x)}_{\delta}$

$\mathcal{H}_0 = \{ w_0 + w_1 x : w_0, w_1 \in \mathbb{R} \}$

$\mathcal{H} = \{ w_0 + w_1 x + w_2 x^2 : w_0, w_1, w_2 \in \mathbb{R} \}$

$f(x)$ is not linear and therefore even the best possible linear model (h_0^*) will perform poorly. So why not allow for a more expressive candidate set? We can do that by expanding the basis/complexity in $\mathcal{H}$. For example, we now allow for a quadratic term so we can fit parabolic-shaped curves. This allows us to get closer to the real f (which may be very complex and nonlinear), reducing misspecification error. We now have $p=2$ which is greater than $p_{raw}=1$. We call this a "derived feature" in contrast to a "raw feature" (original). E.g. $x_2 = g(x_1) = x_1^2$. It's a transformation of a raw feature.

You're at liberty to use any transformed features you want. If they're useless, they appear as random noise and you overfit.

Using squares and cubes is a well-known modeling procedure called "polynomial regression".

Is polynomial regression "linear"? Yes and no. "Yes" in the sense that you create a design matrix and use OLS and thus linear in the transformed features but "no" because the g model is not linear in the raw features.

Advanced math note: polynomial regression is a principled approach because of the Weierstrauss Approximation Thm (1885) which says that any continuous function f whose domain is x in $[a,b]$ can be approximated by a polynomial function p_d with arbitrary precision by picking d, its degree:

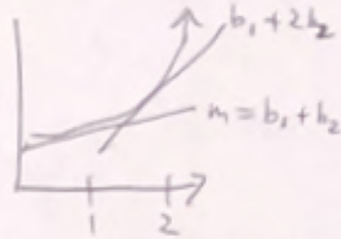
$$\forall \varepsilon > 0 \ \ \forall x \in [a,b] \ \exists d \ \left| f(x) - p_d(x) \right| < \varepsilon.$$

The Stone-Weierstrauss Thm (1937) generalizes the above. One implication of this thm is that a multivariate polynomial function can approximate any continuous function $f(x_1, \ldots, x_p)$. Now do we do a polynomial regression of degree d. E.g. $d=2$.

$$X_{raw} = \begin{array}{c} \begin{array}{cc} & \vec{x}_{\cdot 1} \end{array} \\ \begin{bmatrix} 1 & x_{11} \\ 1 & x_{12} \\ \vdots & \vdots \\ 1 & x_{1n} \end{bmatrix} \\ p_{raw} = 1 \end{array} \xrightarrow{\text{transform}} X = \begin{array}{c} \begin{array}{ccc} & \vec{x}_{\cdot 1} & \vec{x}_{\cdot 2} \end{array} \\ \begin{bmatrix} 1 & x_{11} & x_{11}^2 \\ 1 & x_{12} & x_{12}^2 \\ \vdots & \vdots & \vdots \\ 1 & x_{1n} & x_{1n}^2 \end{bmatrix} \\ p = 2 \end{array}$$

The transformed matrix X is still full rank since a polynomial function cannot be expressed with finite linear terms.

$$\vec{b} = (X^T X)^{-1} X^T \vec{y} = \begin{bmatrix} b_0 \\ b_1 \\ b_2 \end{bmatrix}$$



$$g(x) = \hat{y} = b_0 + b_1 x + b_2 x^2 = b_0 + (b_1 + b_2 x)x$$

Can you make a polynomial regression of degree $d=3$? Yes. Same way! Just make a new feature and cube x_1. How far can you go in OLS? $p = n-1$ i.e $d = n-1$. That would yield a perfect fit. Any higher d, and you can't invert $X^T X$. E.g. $n=5$.

$$X = \begin{bmatrix} 1 & x_{11}^1 & x_{11}^2 & x_{11}^3 & x_{11}^4 \\ 1 & x_{12}^1 & \vdots & \vdots & \vdots \\ 1 & x_{13}^1 & \vdots & \vdots & \vdots \\ 1 & x_{14}^1 & \vdots & \vdots & \vdots \\ 1 & x_{15}^1 & \vdots & \vdots & \vdots \end{bmatrix} \quad \left(1 = x_{11}^0\right)$$

Is this full rank? This is a special matrix called a Vandermonde Matrix and it's proven to be full rank if:

$$\det[X] = \prod_{i=1}^{n} \prod_{j=1}^{n} x_j - x_i \neq 0$$

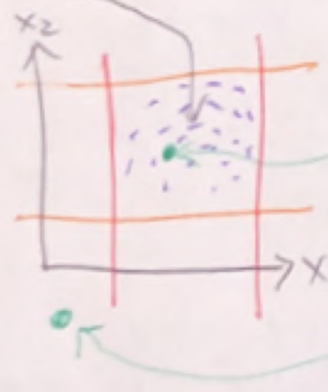
Consider p raw features given by the columns of X.

Define:

$$\text{Range}[X] = [x_{\cdot 1, min}, x_{\cdot 1, max}] \times [x_{\cdot 2, min}, x_{\cdot 2, max}] \times \ldots \times [x_{\cdot p, min}, x_{\cdot p, max}]$$

This is a hyperrectangle representing the space of x-vectors (observations) you've seen in your n examples.

e.g.



"Interpolation" is when you predict for x-vectors inside the Range $[X]$.

"Extrapolation" is when you predict for x-vectors outside the Range $[X]$.

We build models to interpolate. Bad things happen when you extrapolate. Different model fitting procedures ($\mathcal{A}$) extrapolate differently ... beware!

We expanded the complexity of our candidate set $\mathcal{H}$ using polynomials. But we found that high degree polynomials had unintended consequences (Runge's phenomenon). Is there another transformation of raw features that we can employ to expand $\mathcal{H}$? Of course... there are tons of functions! Exponentials, logs, sines etc. Let's examine logs because they are very popular and very useful:

$$\ln(x+1) \approx x - \frac{x^2}{2} + \frac{x^3}{3} - \dots \approx x \text{ if } x \approx 0$$

$$\Rightarrow \ln(x) = \ln((x+1)-1) \approx x-1 \quad \text{e.g. } \ln(1.02) = .019 \approx 1.02-1$$

consider the following linear model:

$$y = b_0 + b_1 \ln(x)$$

$$\Delta x = x_f - x_0 \overset{\text{e.g.}}{=} 1.07 - 1.00$$

$$\Delta y = (\cancel{b_0} + b_1 \ln(x_f)) - (\cancel{b_0} + b_1 \ln(x_0)) = b_1 \ln\left(\frac{x_f}{x_0}\right) \approx b_1 \left(\overbrace{\frac{x_f}{x_0} - 1}^{\%\text{ change in } x}\right)$$

This simple log model can be approx. interpreted as proportional change in x yields a change in y (in y's units) i.e. if x increases by 100%, y goes up by b_1.

Likewise you can do $\ln(y) = b_0 + b_1 x$ and this is approx interpreted as unit change in x yields b_1 proportion change in y and $\ln(y) = b_0 + b_1 \ln(x)$ is approx interpreted as proportional change in x yields b_1 proportion change in y.