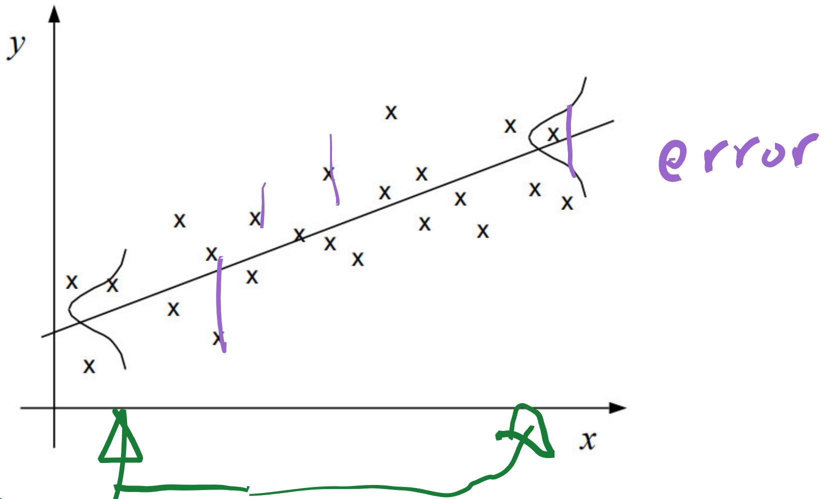
CS 189/289

Today's lecture:

Linear regression (MLE + conditional Gaussians)

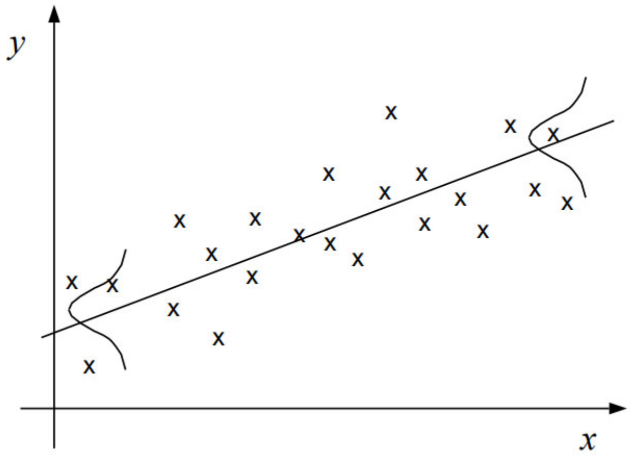
Regression

- *Supervised learning*: data pairs $D = \{(x_i, y_i)\}$, where, x_i may be discrete and/or continuous.
- *Regression:* label, y_i, is a real-valued, e.g., $y_i \in \mathbb{R}$.
- Formally, want $p(y|x)$, the conditional pdf.
- "Point" prediction is then $\hat{y} = E_Y[p(Y|X = x)]$.

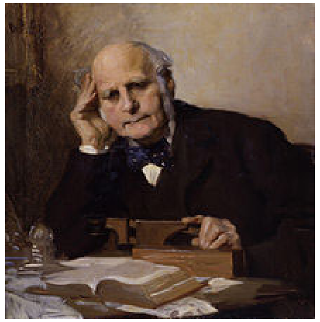


Regression examples

- Covid infection rates from zip code and vaccination rate, etc.
- How much a particular protein will bind to a drug target.
- A person's blood pressure from their genetics.
- Tracking - object location in video at the next time-step.
- Housing prices, crime rates, stock prices, *etc*.
- Earliest regression: Legendre in 1805, and Gauss in 1809, both estimating orbits of bodies about the sun.

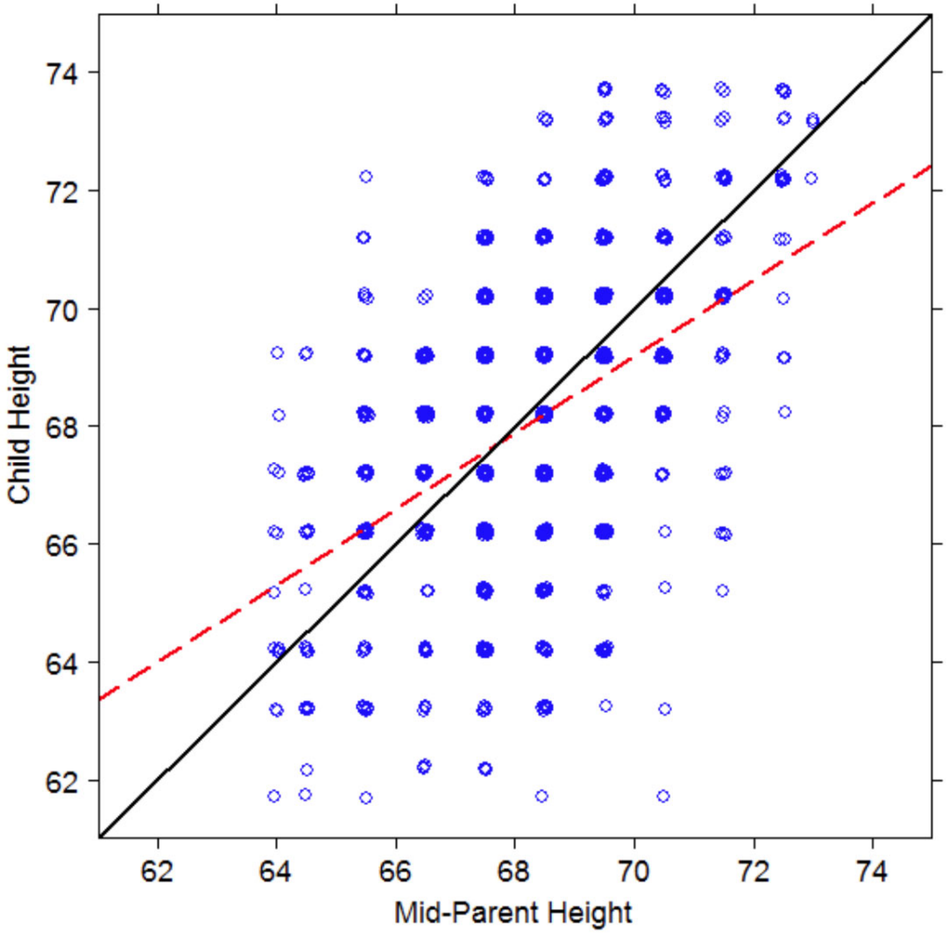


History of the term "Regression"



- Sir Francis Galton (1822-1911) "regression to the mean".

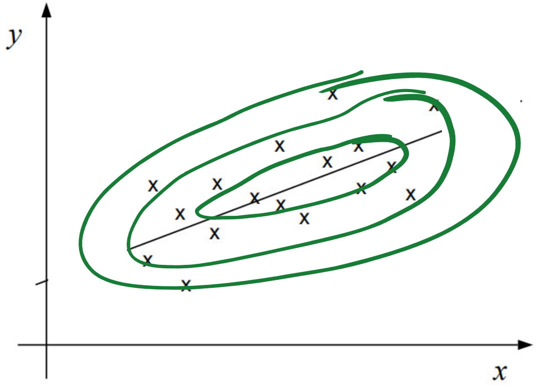
"It appeared from these experiments that the offspring did not tend to resemble their parents in size, but always to be more mediocre than they – to be smaller than the parents, if the parents were large; to be larger than the parents, if the parents were small."



Possible Regression Tactics (to estimate $p(y|x)$)

- Our data are drawn from some distribution, $(X, Y) \sim p(x, y)$.
- What are possible strategies to estimate $p(y|x)$?

1. Estimate $p(x, y|\theta)$ (e.g. MVG for RVs X, Y), and then use fitted model to compute $p(y|x, \hat{\theta}) = \frac{p(y,x|\hat{\theta})}{p(x|\hat{\theta})} = \frac{p(y,x|\hat{\theta})}{\int_y p(y, x|\hat{\theta})dy}$.



Possible Regression Tactics (to estimate $p(y|x)$)

- Our data are drawn from some distribution, $(X_i, Y_i) \sim p(x, y)$.
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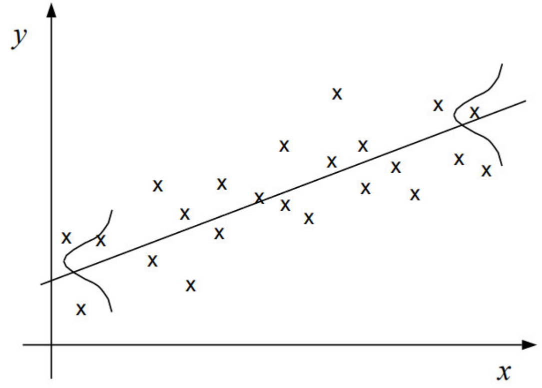
1. Estimate $p(x, y|\theta)$ (e.g. MVG for RVs X, Y), and then use fitted model to compute $p\left(y\middle|x, \hat{\theta}\right) = \frac{p(y,x|\hat{\theta})}{p(x|\hat{\theta})} = \frac{p(y,x|\hat{\theta})}{\int_y p\left(y, x\middle|\hat{\theta}\right)dy}$.
2. Consider the inputs to be fixed, and model only the output as a RV. That is, directly model the conditional $p\left(y\middle|x, \hat{\theta}\right)$.

"*generative*", vs. "*discriminative*"



Linear Regression

- Takes the discriminative approach.
- Predictions are a linear function of the parameters:

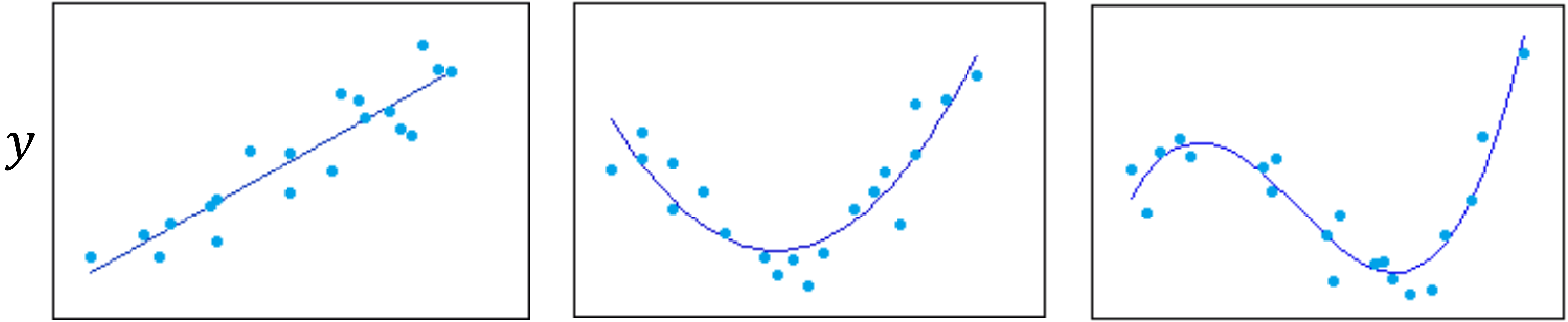
$$\hat{y} = E_Y[p(y|x)] = w^T x + w_0, \text{ for } \boldsymbol{w}, \boldsymbol{x} \in \mathbb{R}^d.$$

- $\boldsymbol{w_0}$ is called the "offset"/"bias"/"intercept".
- Instead of a bias, we can make an extra feature that is always $\mathbf{1}$.
- Now use $\boldsymbol{x'} = [x, 1]$ and $\hat{\boldsymbol{y}} = w^T \boldsymbol{x'}$.

How useful can a linear model be?!

Which of these curves can be modelled by linear regression?

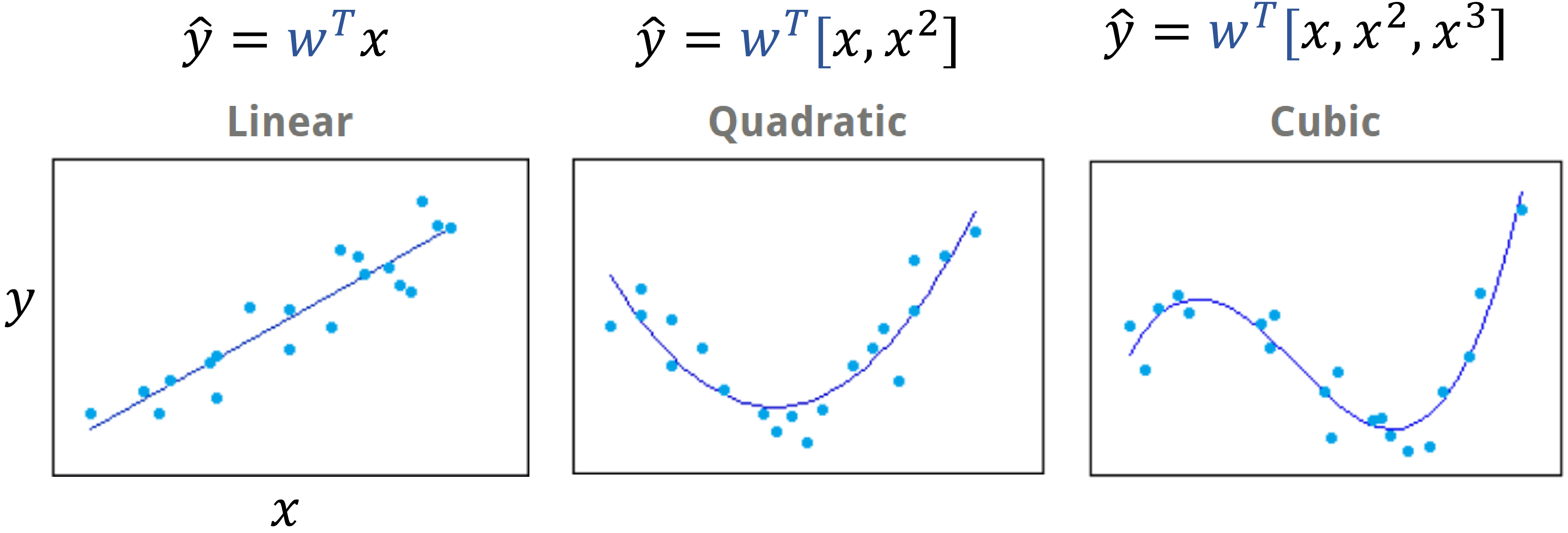
$$\hat{y} = E_Y[p(y|x)] = w^T x + w_0, \text{ for } w, x \in \mathbb{R}^d$$



https://statisticsbyjim.com/regression/curve-fitting-linear-nonlinear-regression/

How useful can a linear model be?!

$w, x \in \mathbb{R}^1$



For full generality, $x \in \mathbb{R}^D$ need the cross-terms and bias terms, e.g., quadratic $[1, x_1, x_2, x_1^2, x_2^2, x_1 x_2]$.

https://statisticsbyjim.com/regression/curve-fitting-linear-nonlinear-regression/

Basis expansion of raw input space

$$x \in \mathbb{R}^{d=2} = [x_1, x_2] \rightarrow [1, x_1, x_2, x_1 x_2, x_1^2, x_2^2] \in \mathbb{R}^{k=6}$$

Polynomial expansion of order 2 (i.e. quadratic)

- Denote *basis expansion* of the (raw) input features: $\Phi(x): \mathbb{R}^d \rightarrow \mathbb{R}^k$.

For $d = 1$, polynomial expansions of order $k = 2, 3$:

- For a quadratic expansion, $\Phi(x) = [1, x, x^2]$, and $k = 2$.
- For a cubic expansion, $\Phi(x) = [1, x, x^2, x^3]$, and $k = 3$.

- For a linear/identity basis expansion, $\Phi(x) = x$, and $k = d$.

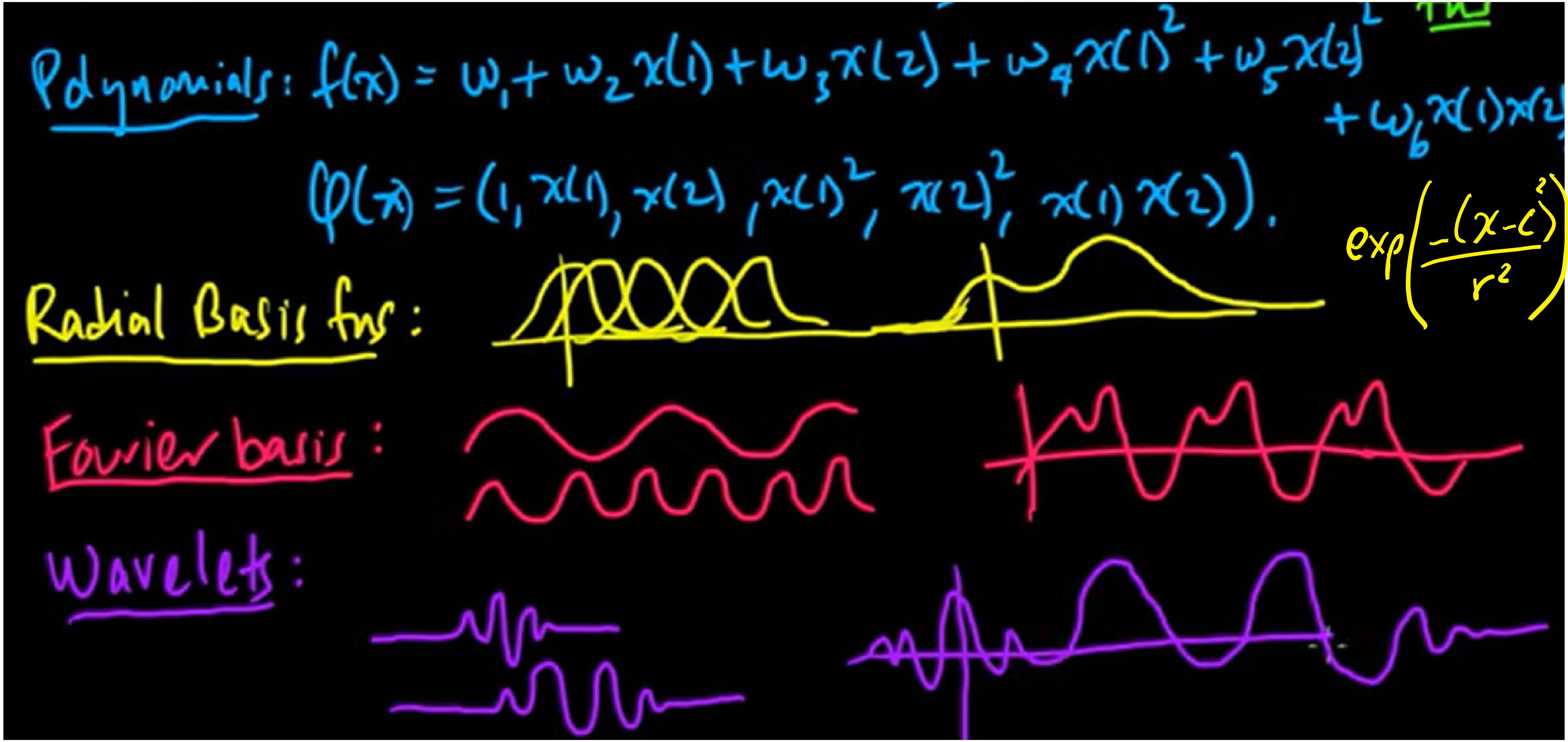
Basis expansion of raw input space

Basis functions are pre-determined, so just a notational change:

$$\hat{y} = E_Y[p(y|x)] = w^T \Phi(x), \text{ for } w \in \mathbb{R}^k, x \in \mathbb{R}^d$$

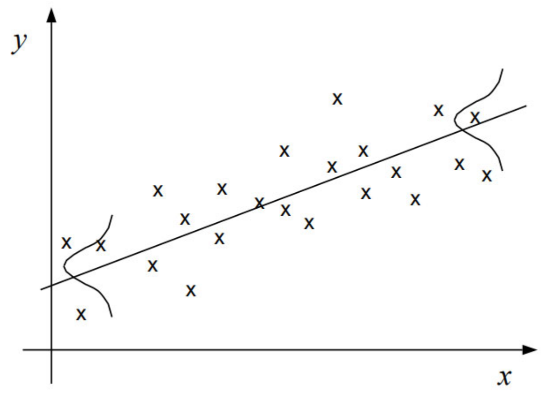
In this lecture, for simplicity of notation, we will assume that this expansion has already been done, and just write $\hat{y} = w^T x$.

Many basis possible functions!



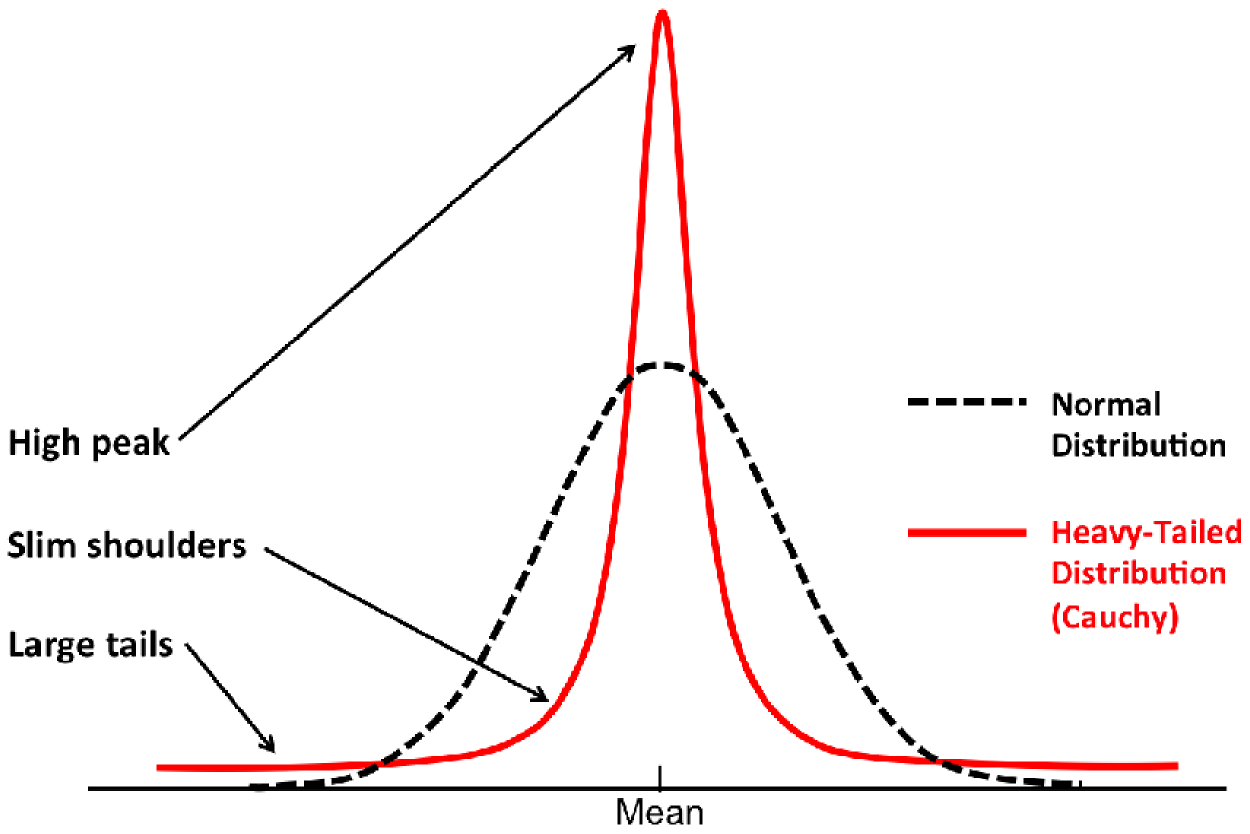
Specific form of linear regression

- So far we said linear regression is $\hat{y} = E_Y[p(y|x)] = E[p(y|x)] = w^T x$.
- But what do we use for $p(y|x)$?
- Standard linear regression uses a Gaussian $p(y|x) = N(y|w^T x, \sigma^2)$.
- Equivalent to $Y = w^T x + \epsilon$, with $\epsilon \sim N(0, \sigma^2)$.
- Which is equivalent to $Y - w^T x = \epsilon \sim N(0, \sigma^2)$.
- Alternate forms give "heavier tails" to the distribution of the "residual".



Aside: heavy-tailed distribution

- More of the mass lies further from the center of mass.
- Heavy-tailed noise models outliers better than a Gaussian.



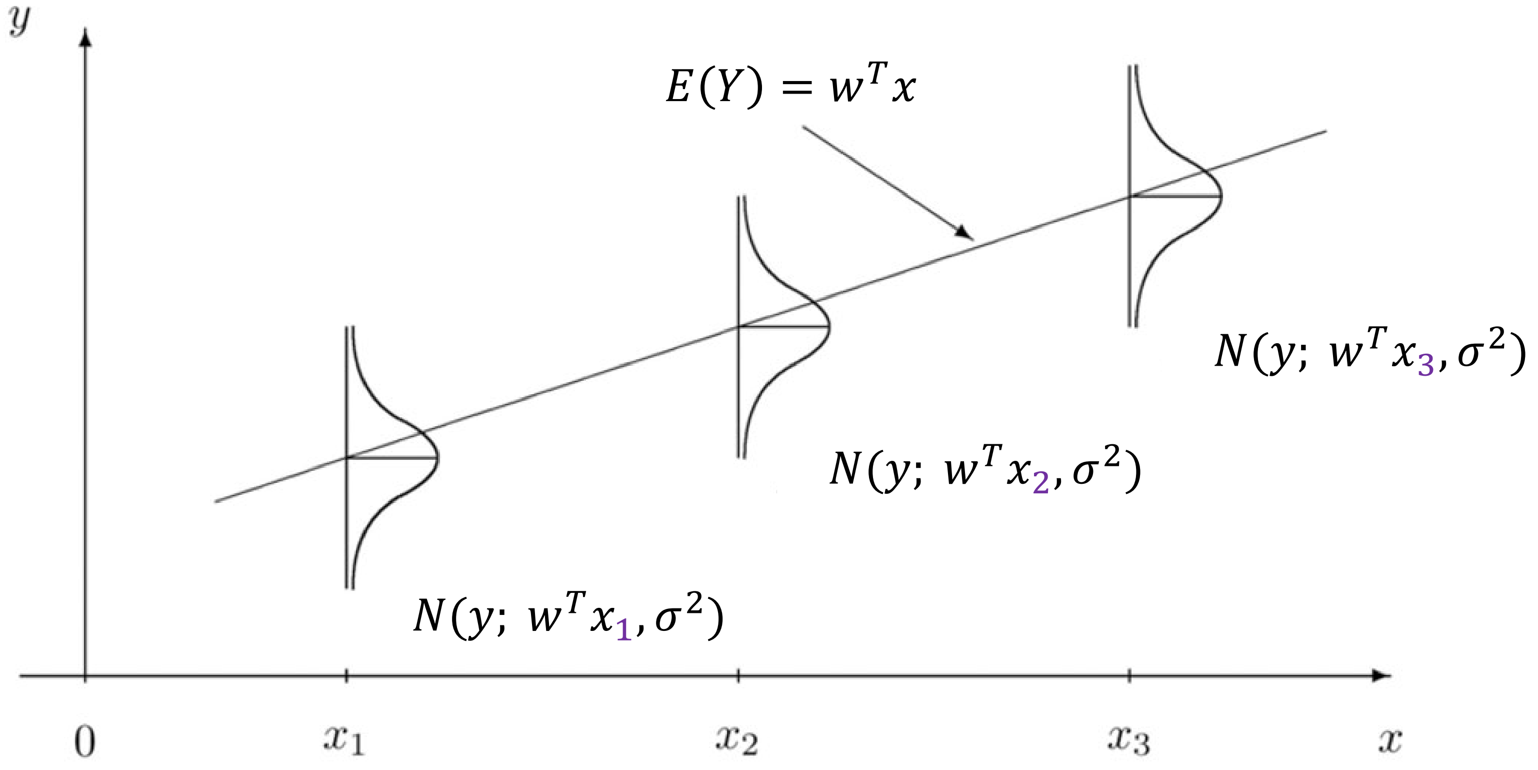
$$Y - w^T x = \epsilon \sim N(0, \sigma^2)$$

$$Y - w^T x = \epsilon \sim Cauchy(0, \sigma^2)$$

https://www.semanticscholar.org/paper/The-Normal-Distribution-.-.-.-or-Another-Brandenburger-Weston/b0a227e36d655c0dceaeb774225e0b4fb6cda8ed/figure/2

Gaussian linear regression, $p(y|x) = N(y|w^T x, \sigma^2)$

For every value $X = x$, the target variable, Y, takes on a Gaussian distribution with the same variance, σ^2:



https://sdcastillo.github.io/PA-R-Study-Manual/introduction-to-modeling.html

"Training" a Gaussian linear regression model

How will we fit the regression model, $p(y|x) = N(y|w^T x, \sigma^2)$?

MLE: $\theta_{MLE} = (w_{MLE}, \sigma^2_{MLE}) = \underset{(w,\sigma^2)}{\arg\max} \log p(D = \{(x_i, y_i)_{i=1}^n\}|\theta)$

$$= \underset{(w,\sigma^2)}{\arg\max} \sum_{i=1}^n log\, p(y_i|x_i, \theta)$$

$$= \underset{(w,\sigma^2)}{\arg\max} \sum_{i=1}^n log\, N(y_i|w^T x_i, \sigma^2)$$

$$= \underset{(w,\sigma^2)}{\arg\max} \sum_{i=1}^n log\left(\frac{1}{\sqrt{2\pi\sigma^2}}\right) - \frac{1}{2\sigma^2}\sum_{i=1}^n (y_i - w^T x_i)^2$$

$$= \underset{(w,\sigma^2)}{\arg\max}\, n\, log\left(\frac{1}{\sqrt{2\pi\sigma^2}}\right) \qquad - \frac{1}{2\sigma^2}\sum_{i=1}^n (y_i - w^T x_i)^2$$

If we assume σ^2 is known…

"Training" a Gaussian linear regression model

If we assume $\boldsymbol{\sigma^2}$ is known…

$$(w_{MLE}, \sigma^2_{MLE}) = \arg\max_{(w,\sigma^2)} n \log\left(\frac{1}{\sqrt{2\pi\sigma^2}}\right) - \frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i - w^T x_i)^2$$

… then estimating $\boldsymbol{w}$ above is the same as

$$= \arg\min_{w} \sum_{i=1}^{n}(y_i - w^T x_i)^2$$

$$= \arg\min_{w} \sum_{i=1}^{n}(y_i - \widehat{y_i})^2$$

"least squares" loss function!

$$p(y|x) = N(y|w^T x, \sigma^2)$$

"Training" a Gaussian linear regression model

$$w_{\text{MLE}} = \arg\min_w \sum_{i=1}^{n} (y_i - w^T x_i)^2$$

Lets re-write this loss in "vectorized" form:

First, define:

$$\begin{pmatrix} y_1 - w^T x_1 \\ \vdots \\ y_n - w^T x_n \end{pmatrix} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix} - \begin{pmatrix} x_1^T w \\ \vdots \\ x_n^T w \end{pmatrix} = y - \begin{pmatrix} x_1^T \\ \vdots \\ x_n^T \end{pmatrix} w = y - Aw$$

$$\underbrace{w^T x_i}_{\text{Scalar}} = \underbrace{x_i^T w}_{}$$

"Training" a Gaussian linear regression model

$$\mathrm{w}_{\mathrm{MLE}} = \arg\min_{w} \sum_{i=1}^{n} (y_i - w^T x_i)^2$$

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$$\underbrace{w^T x_i}_{\text{scalar}} = \underbrace{x_i^T w}_{\text{scalar}}$$

A is called the "design matrix"

"Training" a Gaussian linear regression model

$$\arg\min_{w} \sum_{i=1}^{n} (y_i - w^T x_i)^2$$

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$$w^T x_1 = x_1^T w$$

Scalar

A is called the "design matrix"

Then, we can re-write the loss as

$$\arg\min_{w} (y - Aw)^T (y - Aw)$$

$$= \arg\min_{w} \|y - Aw\|_2{}^2$$

"Training" a Gaussian linear regression model

So want to minimize

$$\mathcal{L} = (y - Aw)^T(y - Aw) \qquad (y \in \mathbb{R}^n, A \in \mathbb{R}^{n\times d}, w \in \mathbb{R}^{d\times 1})$$

$$= (y^T - (Aw)^T)(y - Aw)$$

$$= y^T y - w^T A^T y - y^T Aw + w^T A^T Aw$$

$$= y^T y - 2w^T A^T y + w^T A^T Aw$$

$$\begin{pmatrix} x_1^T \\ \vdots \\ x_n^T \end{pmatrix}$$

A

To minimize, we want to set $\frac{\partial \mathcal{L}}{\partial w} = \mathbf{0}$.

This is most easily achieved by using the rules of vector calculus, so lets do a quick refresher.

$$p(y|x) = N(y|w^T x, \sigma^2)$$

Refresher on vector calculus

Some "rules" for taking gradients with respect to vectors.

- e.g., for vectors $\boldsymbol{a}, \boldsymbol{b} \in \mathbb{R}^{d\times 1}$, so that $\boldsymbol{a}^T\boldsymbol{b} \in \mathbb{R}$,

$$\frac{\partial(a^T b)}{\partial a_j} = \frac{\partial(a_1 b_1 + a_2 b_2 + \cdots a_d b_d)}{\partial a_j} = b_j$$

Thus,

$$\frac{\partial(a^T b)}{\partial a} = \frac{\partial(a_1 b_1 + a_2 b_2 + \cdots a_d b_d)}{\partial a} = b \in \mathbb{R}^{d\times 1}$$

(not true for $\boldsymbol{a}\boldsymbol{b}^T$ which is a matrix, be careful!)

$$= \frac{\partial(b^T a)}{\partial a}$$

Useful cheat sheet: https://cs.nyu.edu/~roweis/notes/matrixid.pdf

Refresher on vector calculus

For vector $x \in \mathbb{R}^{d\times 1}$, and matrix $\Sigma \in \mathbb{R}^{d\times d}$

$$\frac{\partial x^T \Sigma x}{\partial x} = (\Sigma + \Sigma^T)x$$

Thus, if Σ is symmetric such that $\Sigma = \Sigma^T$ then

$$\frac{\partial x^T \Sigma x}{\partial x} = 2\Sigma x$$

(similar to the scalar version: $\frac{\partial(ax^2)}{\partial x} = 2ax$)

"Training" a Gaussian linear regression model

So want to minimize

$(y \in \mathbb{R}^n, A \in \mathbb{R}^{n \times d}, w \in \mathbb{R}^{d \times 1})$

$$\begin{pmatrix} x_1^T \\ \vdots \\ x_n^T \end{pmatrix} = A$$

$$\begin{aligned}
\mathcal{L} = \ & (y - Aw)^T (y - Aw) \\
&= (y^T - (Aw)^T)(y - Aw) \\
&= y^T y - w^T A^T y - y^T A w + w^T A^T A w \\
&= y^T y - 2 w^T A^T y + w^T A^T A w
\end{aligned}$$

To minimize, we want to set $\frac{\partial \mathcal{L}}{\partial w} = \mathbf{0}$.

"Training" a Gaussian linear regression model

So want to minimize

$(y \in \mathbb{R}^n, A \in \mathbb{R}^{n \times d}, w \in \mathbb{R}^{d \times 1})$

$$\begin{pmatrix} x_1^T \\ \vdots \\ x_n^T \end{pmatrix} = A$$

$$\mathcal{L} = (y - Aw)^T (y - Aw)$$
$$= (y^T - (Aw)^T)(y - Aw)$$
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$$= y^T y - 2 w^T A^T y + w^T A^T A w$$

To minimize, we want to set $\frac{\partial \mathcal{L}}{\partial w} = \mathbf{0}$.

$$\nabla_w \mathcal{L} = \begin{bmatrix} \partial \mathcal{L} / \partial w_1 \\ \partial \mathcal{L} / w_2 \\ \vdots \\ \partial \mathcal{L} / w_d \end{bmatrix} = \left[-2A^T y + 2A^T A w \right]$$

$$= \underbrace{-A^T y + A^T A w}_{d \times 1}$$

"Training" a Gaussian linear regression model

So want to minimize

$$\mathcal{L} = (y - Aw)^T(y - Aw)$$
$$= (y^T - (Aw)^T)(y - Aw)$$
$$= y^T y - w^T A^T y - y^T A w + w^T A^T A w$$
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To minimize, we want to set $\frac{\partial \mathcal{L}}{\partial w} = 0$.

$$\nabla_w \mathcal{L} = \begin{bmatrix} \partial\mathcal{L}/\partial w_1 \\ \partial\mathcal{L}/\omega_2 \\ \vdots \\ \partial\mathcal{L}/\omega_d \end{bmatrix} = \left[-2A^T y + 2A^T A w\right]$$

$$= \underbrace{-A^T y + A^T A w}_{d \times 1}$$

set to 0

$$-A^T y + A^T A w = 0$$
$$A^T A w = A^T y$$
$$\boxed{w = (A^T A)^{-1} A^T y}$$

"left pseudo-inverse" of A

$$(A^T A)^{-1} A^T * A = I$$

$$A^{+} A = I$$

$$\begin{pmatrix} x_1^T \\ \vdots \\ x_n^T \end{pmatrix} = A$$

rectangular

so no A^{-1}!

"Training" a Gaussian linear regression model

$$\begin{pmatrix} x_1^T \\ \vdots \\ x_n^T \end{pmatrix} = A$$

- We still need to check if the critical point, $w = (A^T A)^{-1} A^T y$ is minimum of the squared error loss.
- Recall $\nabla_w \mathcal{L} = -2A^T y + 2A^T A w$
- So Hessian matrix ($\nabla_w^2 \mathcal{L}$) is $2A^T A$. When is $A^T A$ PD?
- When the features are independent (when it has full rank).
- σ^2 from MLE as well is just the mean squared residual, $\sigma^2 = \frac{1}{N} \sum_i (y_i - w^T x)^2$.

$$\nabla_w \mathcal{L} = \begin{bmatrix} \partial \mathcal{L}/\partial w_1 \\ \partial \mathcal{L}/w_2 \\ \vdots \\ \partial \mathcal{L}/w_d \end{bmatrix} = \begin{bmatrix} -2A^T y + 2A^T A w \end{bmatrix} = \underbrace{-A^T y + A^T A w}_{d \times 1}$$

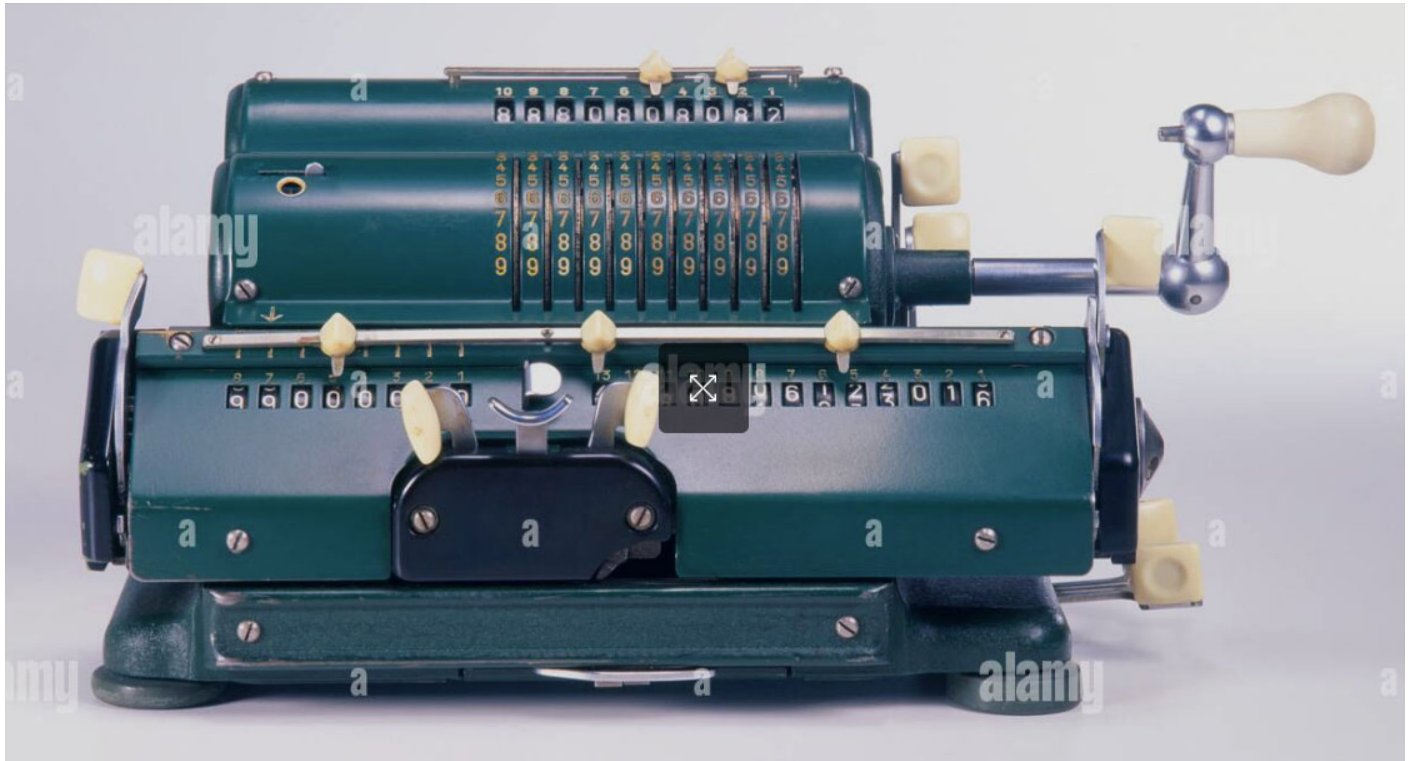
$$-A^T y + A^T A w = 0$$

$$A^T A w = A^T y$$

$$\boxed{w = (A^T A)^{-1} A^T y}$$

Regression in 1950s

Electromechanical desk "calculators" were used, and it could take up to 24 hours to receive the result from one regression.



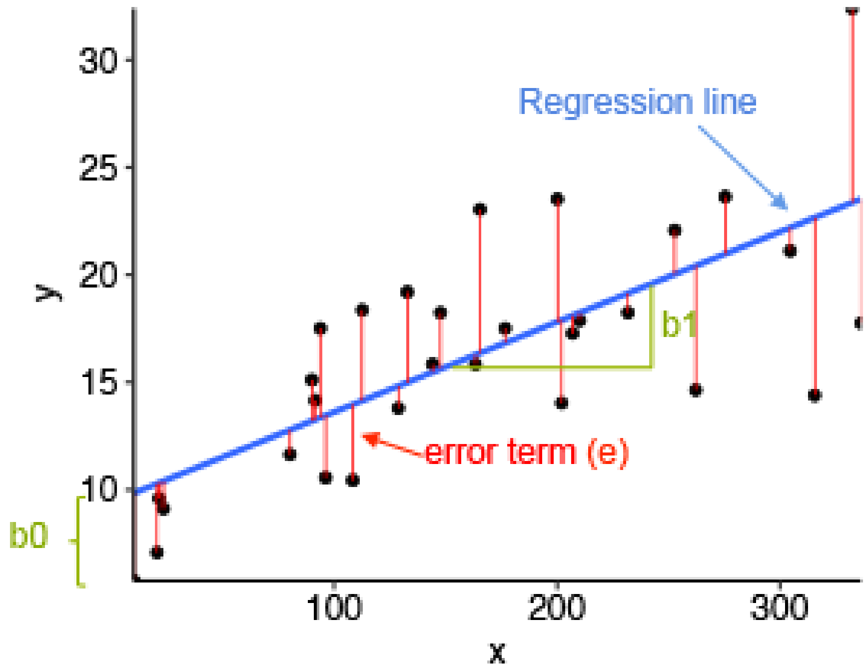
Geometric view of linear regression

- We're trying to predict all our training data labels correctly, such that $y_i = w^T x_i$ for all $i \in [1 \dots n]$.
- In vector form, this means we're looking for

$$\begin{pmatrix} x_1^T \\ \vdots \\ x_n^T \end{pmatrix} = A$$

$$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix} = Aw = \begin{bmatrix} x_1^T \\ x_2^T \\ \vdots \\ x_N^T \end{bmatrix} w$$

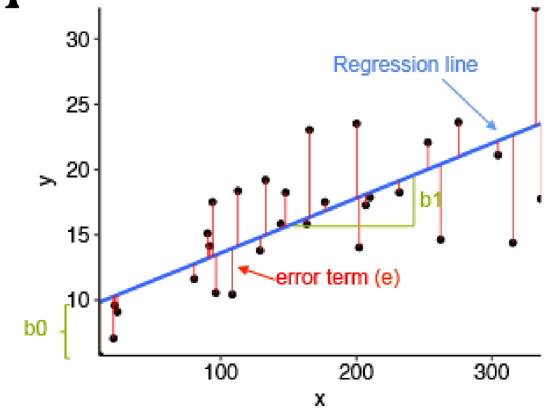
Generally not possible because of noise; or incorrect model (e.g. all features).



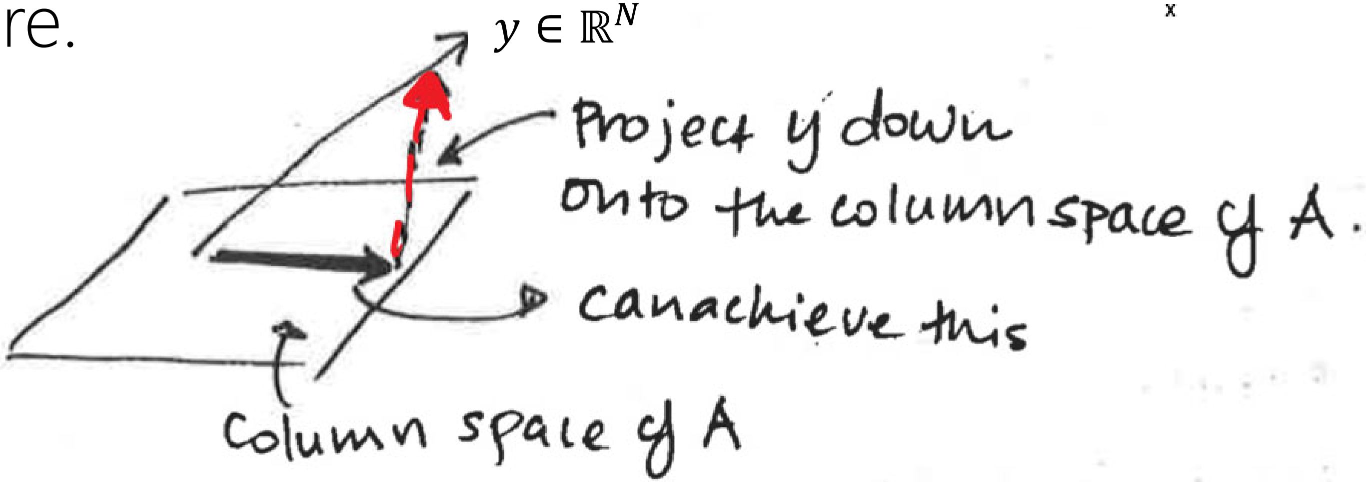
https://www.analyticsvidhya.com/blog/2021/06/25-questions-to-test-your-skills-on-linear-regression-algorithm/

Geometric view of linear regression, $y = Aw$

- So lets think about the error vector ($\mathbf{e} \equiv y - \hat{y} = y - Aw, \in \mathbb{R}^{n \times 1}$).
- A "good" setting of w minimizes the length of $\mathbf{e}$.
- The length is minimized when e lies $\perp$ to column space of A
- Thus we seek w such that $A^T e = 0 = A^T(y - Aw)$.
- Thus $A^T y - A^T A w = 0$.
- Thus $A^T y = A^T A w$ (same as from MLE/least squares)!
- Thus $w = (A^T A)^{-1} A^T y$, as before.



$$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix} = Aw = \begin{bmatrix} x_1^T \\ x_2^T \\ \vdots \\ x_N^T \end{bmatrix} w$$



Using basis expansions instead of x_i

$$\begin{pmatrix} x_1^T \\ \vdots \\ x_n^T \end{pmatrix} = A$$

- $\{\mathrm{x_j}\} \to \{\Phi(x_j)\}$?
- Just define $\mathbf{A}$ with $\Phi^{\mathrm{T}}(\mathrm{x_j})$ instead of x_j because $\Phi(x)$ is fixed ahead of time, so its like someone just gave us different raw inputs x.

$$x = \Phi[x_1, x_2] = [1, x_1, x_2, x_1 x_2, x_1^2, x_2^2] \in \mathbb{R}$$

Polynomial expansion of order 2 (i.e. quadratic)

What can go wrong in linear regression

$$\begin{pmatrix} x_1^T \\ \vdots \\ x_n^T \end{pmatrix} = A$$

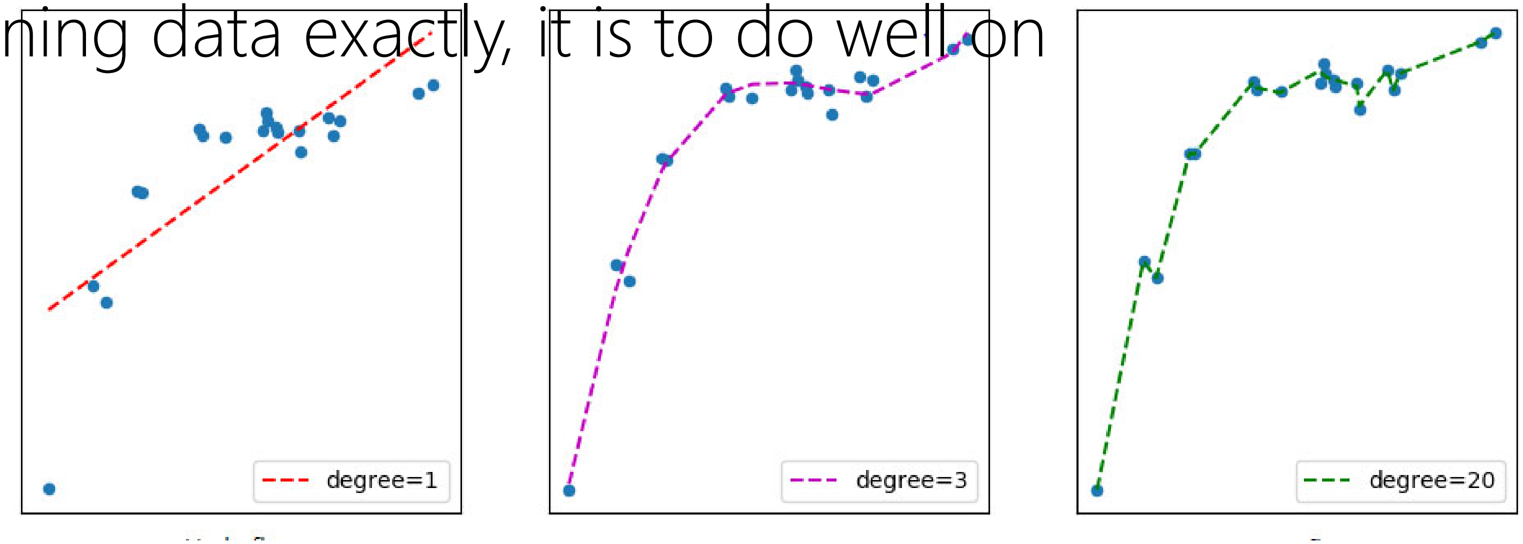
When can we invert $A^T A \in \mathbb{R}^{d \times d}$ (for d features)? $(A \in \mathbb{R}^{N \times d})$

- Consider the decomposition we learned last class:
- $A^T A = \Sigma = QDQ^T$ for diagonal D containing eigenvalues, and orthonormal Q.
- Then we had that $(A^T A)^{-1} = QD^{-1}Q^T$. So if $A^T A$ has any zero eigenvalues we cannot invert it (there are ∞ equally good solutions w then).
- (Could use Moore-Penrose pseudo inverse.)
- This degeneracy occurs when the features in A, for the given data $\{x_j\}$ are linearly dependent.
- e.g., when $d > n$ (then $rank(A^T A) < n$, but needs to be D, i.e. “full rank” to avoid zero eigenvalues).
- What about when $d = n$?

What can go wrong in linear regression

As we add higher and higher order polynomials, a few things happen:

1. # features, $\boldsymbol{d}$ gets bigger and bigger.
2. For $\boldsymbol{d} \geq \boldsymbol{n}$ can perfectly fit any data (*i.e.*, polynomials are a complete basis).
3. Even when we don't perfectly fit the training data, we are still in danger of overfitting (worse prediction on test set). Our goal is not to fit a line through the training data exactly, it is to do well on unseen test cases!



https://towardsdatascience.com/polynomial-regression-bbe8b9d97491

What can go wrong in linear regression

Two main categories of fixes:

1. Remove features until the problem is well behaved.
2. Leave the features as they are, but add constraints to the system to “tighten it up” (aka “regularization”).

1) Is called “feature selection”, e.g. “forward selection”, “backward selection”, etc.

(Moore-Penrose inverse is not a general fix for ML models, only works for linear regression.)

A thought experiment

Consider:

- Use MLE on data, $D = \{x_i, y_i\}$ to get $\hat{y}_i = p_\theta(y|\Phi(x))$ using linear regression.
- Assume an abundance of data (millions of data points), and only 100 parameters.
- Suppose get accuracy $\mp$\$1000 of sale price when applying to held out part of our data.
- Can we assume this model will get $\mp$\$1000 on any test set that may come in the future?

Actual *vs.* predicted sale price of house

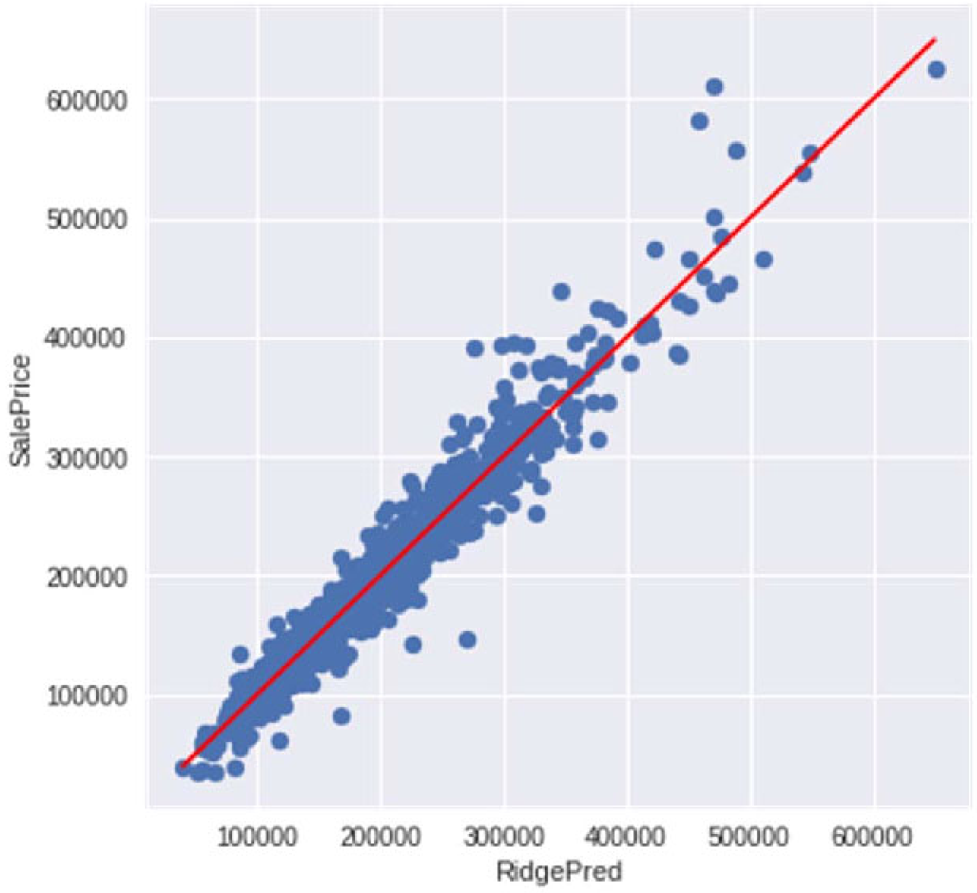


Fig. 4 Ridge Prediction for Training Data.

Causation vs correlation

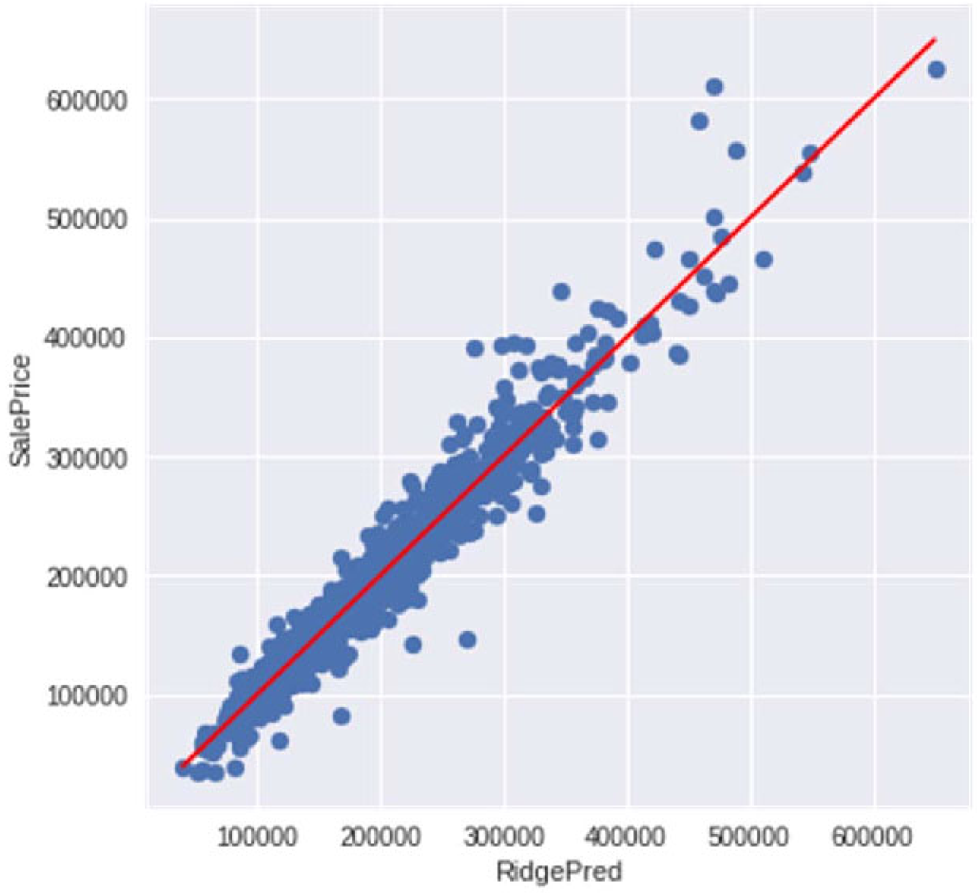
Breakingviews

Zillow’s failed house flipping

Reuters

WSJ NOV. 2021 : *“The company expects to record losses of more than $500 million from home-flipping by the end of this year and is laying off a quarter of its staff.”*

Actual *vs.* predicted sale price of house



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