CSE 446

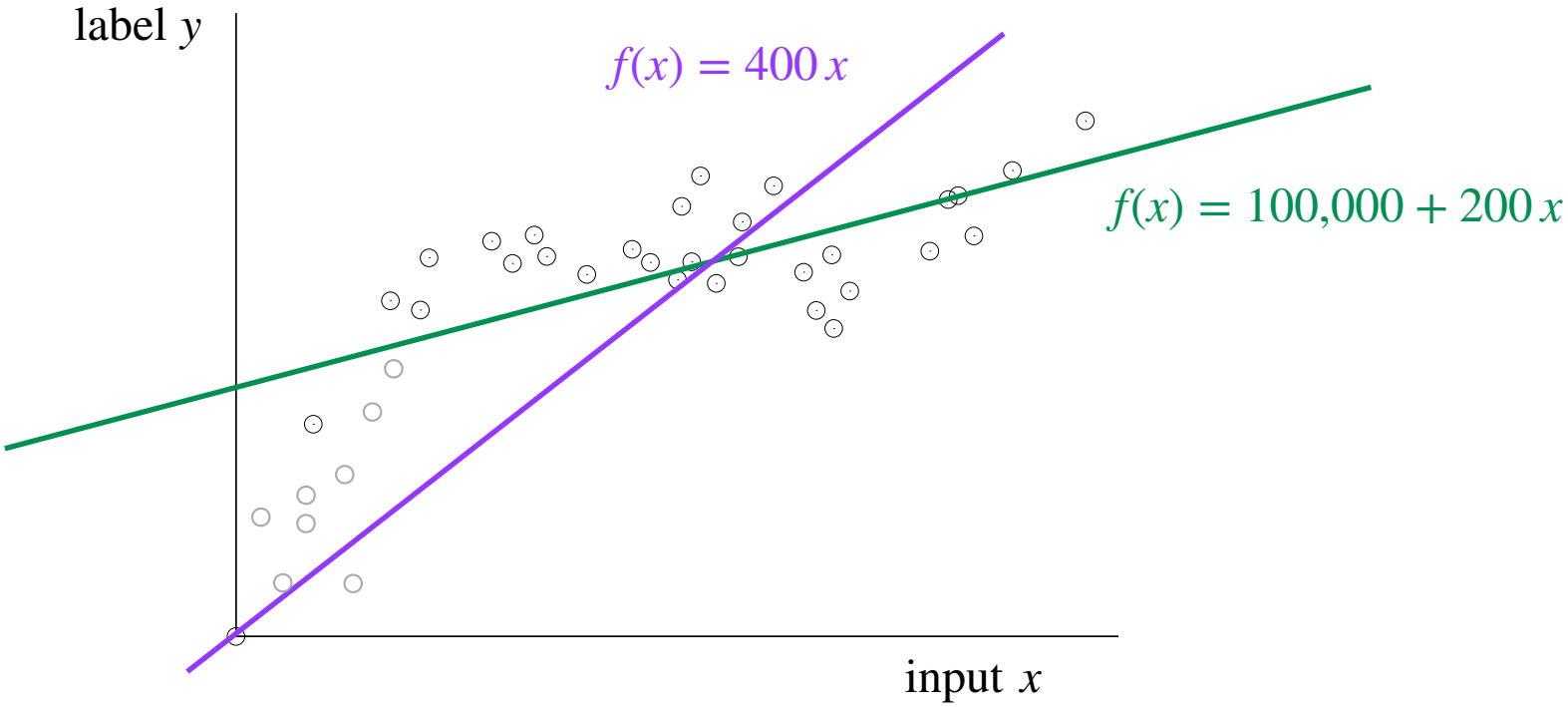
- Linear Regression w/ Basis Functions
- Model Evaluation

Natasha Jaques

UNIVERSITY of WASHINGTON

Polynomial Features

Recap: Linear Regression



- In general high-dimensions, we fit a linear model with intercept

$$y_i \simeq w^T x_i + b\,, \quad \text{or equivalently} \quad y_i = w^T x_i + b + \epsilon_i$$

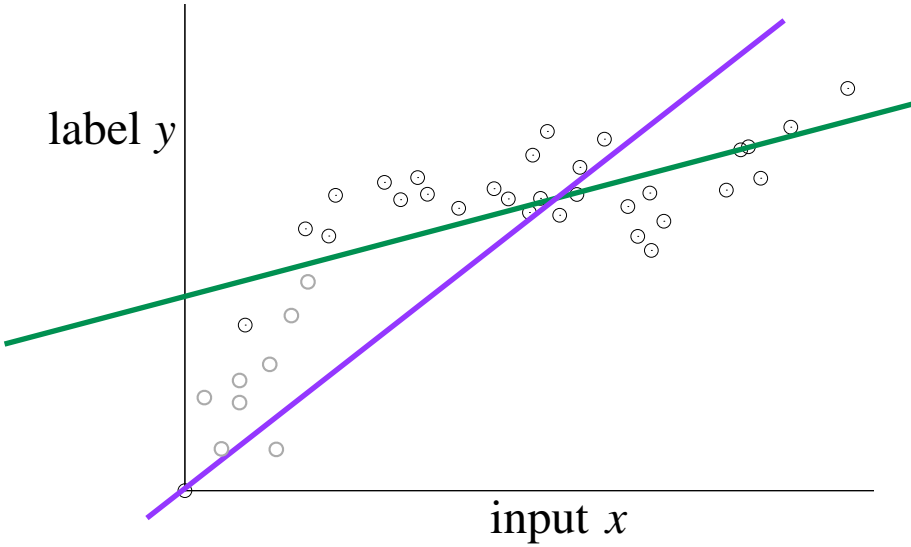
with model parameters $(w \in \mathbb{R}^d, b \in \mathbb{R})$ that minimizes ℓ_2-loss

$$\mathscr{L}(w,b) \;=\; \sum_{i=1}^{n} \underbrace{(y_i - (w^T x_i + b))^2}_{\text{error } \epsilon_i} \qquad \text{\# MSE}$$

Quadratic regression in 1-dimension

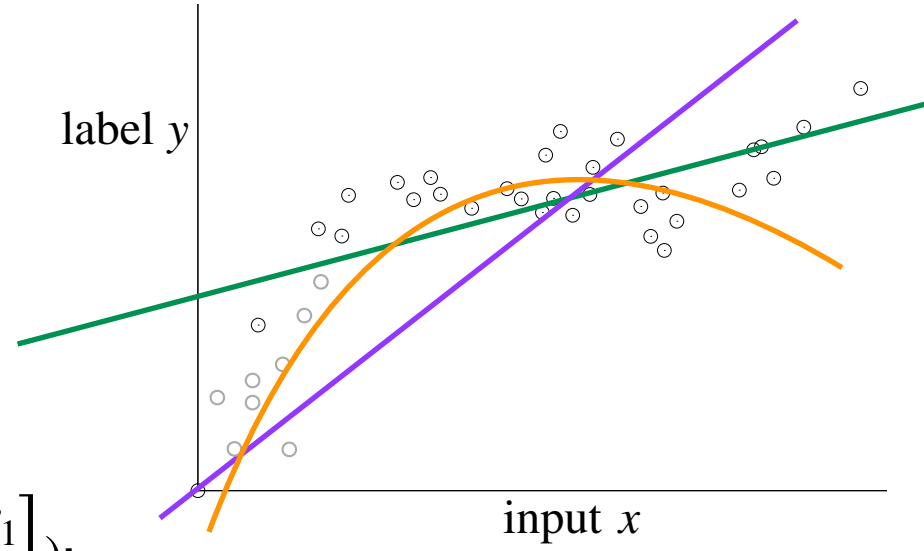
- **Data:** $\mathbf{X} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$, $\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$

- **Linear model with parameter** (b, w_1)**:**
  - $\hat{y}_i = b + w_1 x_i$



Quadratic regression in 1-dimension

- **Data:** $\mathbf{X} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$, $\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$



- **Linear model with parameter** (b, w_1)**:**
  - $\hat{y}_i = b + w_1 x_i$
- **Quadratic model with parameter** $(b, w = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix})$**:**
  - $\hat{y}_i = b + w_1 x_i + w_2 x_i^2$

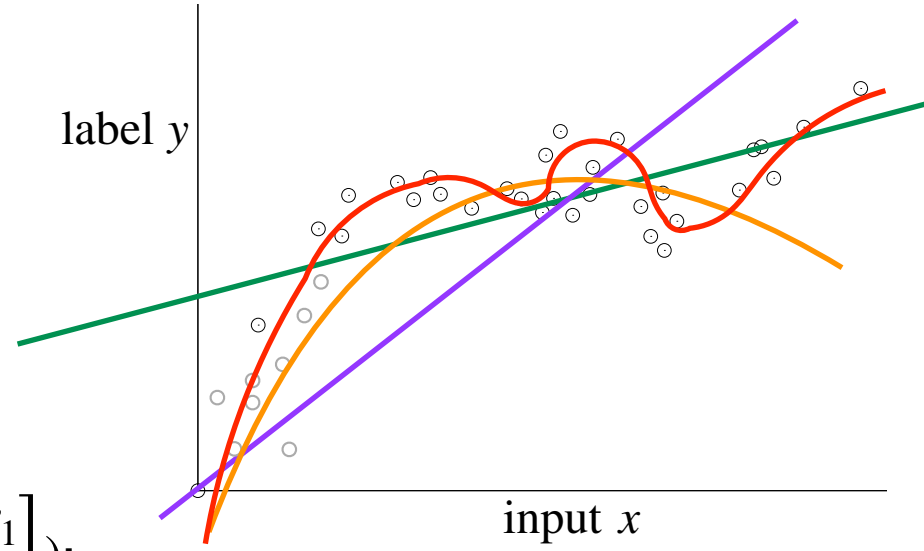
$$h(x_i) = \begin{bmatrix} 1 \\ x_i \\ x_i^2 \end{bmatrix} \quad \hat{y} = h(x_i)^T \begin{bmatrix} b \\ w_1 \\ w_2 \\ \vdots \end{bmatrix}$$

Still linear regression, but on quadratic features

Linear layer fit to non-linear features

Quadratic regression in 1-dimension

- **Data:** $\mathbf{X} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$, $\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$



- **Linear model with parameter** (b, w_1)**:**
  - $\hat{y}_i = b + w_1 x_i$
- **Quadratic model with parameter** $(b, w = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix})$**:**
  - $\hat{y}_i = b + w_1 x_i + w_2 x_i^2$
- **Degree-p polynomial model with *p* parameters**
  - $\hat{y}_i = b + w_1 x_i + w_2 x_i^2 + \ldots + w_p x_i^p$

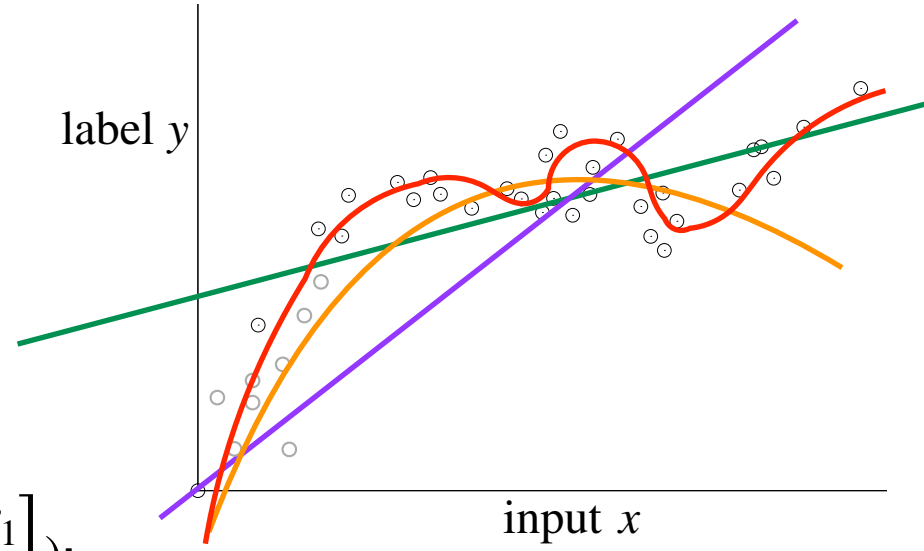
$$h(x_i) = \begin{bmatrix} 1 \\ x_i \\ x_i^2 \end{bmatrix} \quad \hat{y} = h(x_i)^T \begin{bmatrix} b \\ w_1 \\ w_2 \\ \vdots \\ w_p \end{bmatrix}$$

Still linear regression, but on quadratic features

Linear layer fit to non-linear features

Quadratic regression in 1-dimension

- **Data:** $\mathbf{X} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$, $\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$



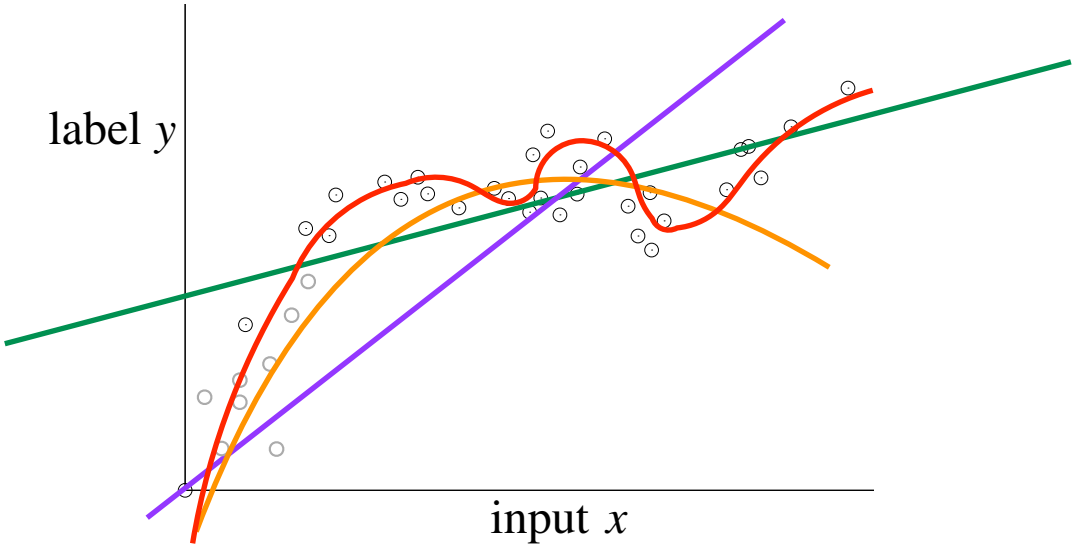
- **Linear model with parameter** (b, w_1)**:**
  - $\hat{y}_i = b + w_1 x_i$
- **Quadratic model with parameter** $(b, w = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix})$**:**
  - $\hat{y}_i = b + w_1 x_i + w_2 x_i^2$
- **Degree-p polynomial model with *p* parameters**
  - $\hat{y}_i = b + w_1 x_i + w_2 x_i^2 + \ldots + w_p x_i^p$
- **General p-features with parameter** $w = \begin{bmatrix} w_1 \\ \vdots \\ w_p \end{bmatrix}$**:**
  - $\hat{y}_i = \langle w, h(x_i) \rangle$ where $h : \mathbb{R} \to \mathbb{R}^p$

$$h(x_i) = \begin{bmatrix} 1 \\ x_i \\ x_i^2 \end{bmatrix} \quad \hat{y} = h(x_i)^T \begin{bmatrix} b \\ w_1 \\ w_2 \\ \vdots \\ w_p \end{bmatrix}$$

Still linear regression, but on quadratic features

Linear layer fit to non-linear features

Quadratic regression in 1-dimension

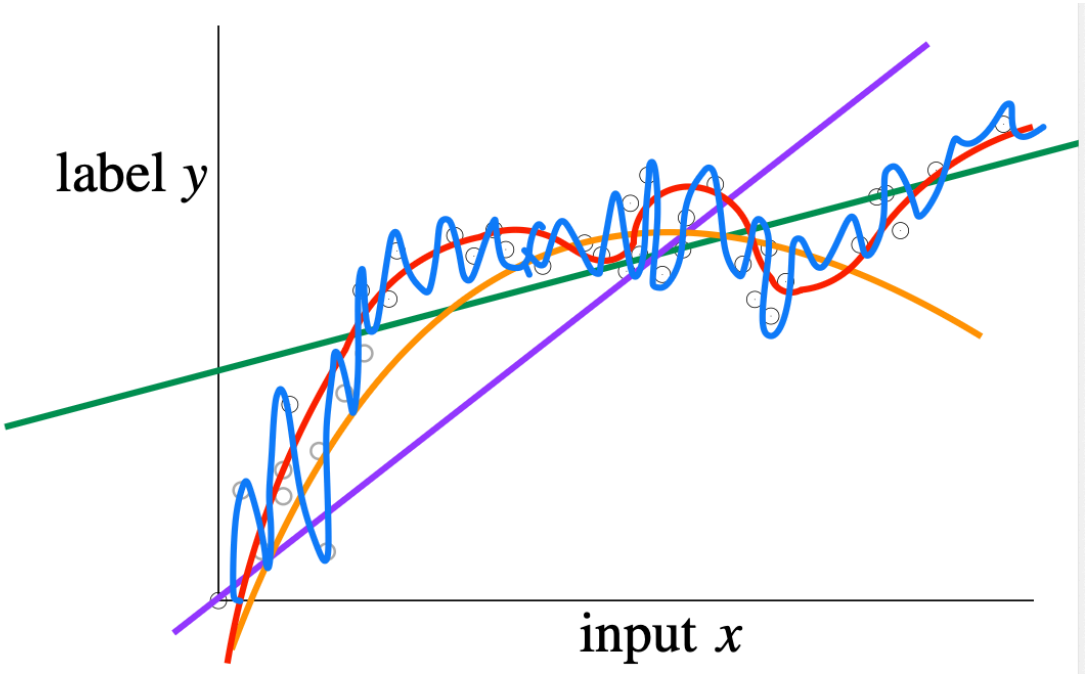


Which line gives us the best fit?

- **Green** & **purple**? Can't capture variance. **Underfitting**
- **Orange**? Can't capture variance. **Underfitting**
- **Red**? Just right?

  Could we take it too far?

Quadratic regression in 1-dimension

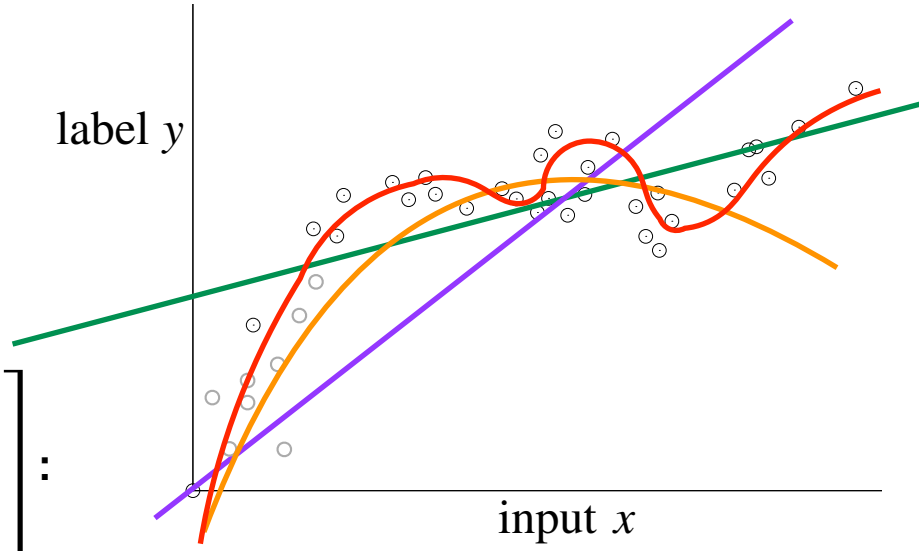


Which line gives us the best fit?

- **Green** & **purple**? Can't capture variance. **Underfitting**
- **Orange**? Can't capture variance. **Underfitting**
- **Red**? Just right?
- **Blue**? Fits random fluctuations / measurement errors in training dataset. **Overfitting.**

Quadratic regression in 1-dimension

- **Data:** $\mathbf{X} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$, $\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$



- **General p-features with parameter** $w = \begin{bmatrix} w_1 \\ \vdots \\ w_p \end{bmatrix}$:
  - $\hat{y}_i = \langle w, h(x_i) \rangle$ where $h : \mathbb{R} \to \mathbb{R}^p$

Note: h can be arbitrary non-linear functions!

$$h(x) = \left[\log(x), x^2, \sin(x), \sqrt{x}\right]^\top$$

Transform features however

How will I know if I have good features?

PLOT PLOT PLOT PLOT PLOT

Breakout discussion:

- When would you use sin(x)?

  # Cyclic data e.g. weather

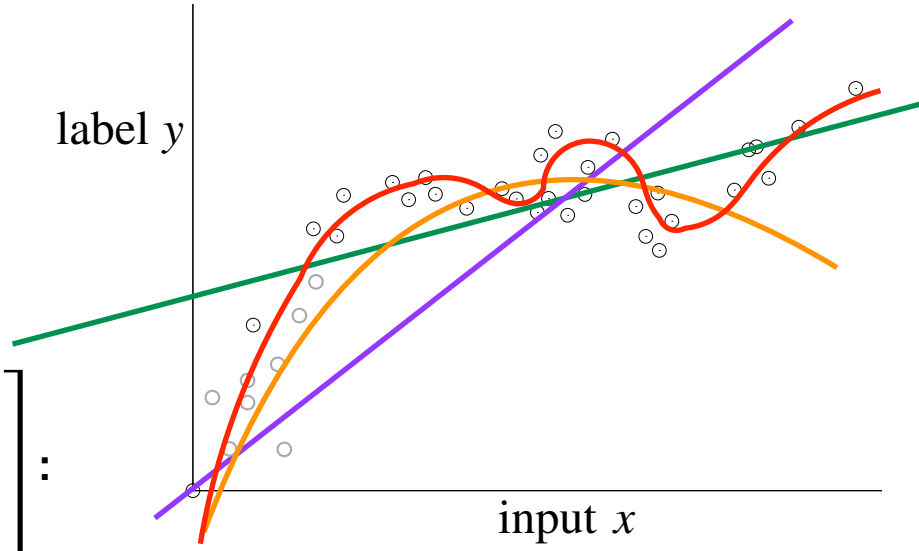
- How should I transform the house feature: zip code?

  # Lat / long

This is the art of feature engineering

Quadratic regression in 1-dimension

- **Data:** $\mathbf{X} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$, $\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$

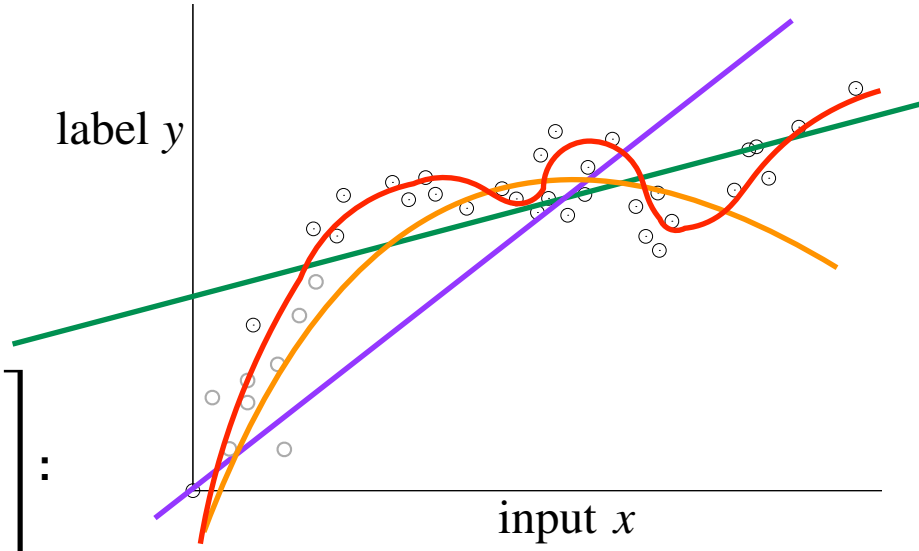


- **General p-features with parameter** $w = \begin{bmatrix} w_1 \\ \vdots \\ w_p \end{bmatrix}$:
  - $\hat{y}_i = \langle w, h(x_i) \rangle$ where $h : \mathbb{R} \to \mathbb{R}^p$

How do we learn w?

Quadratic regression in 1-dimension

- **Data:** $\mathbf{X} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$, $\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$



- **General p-features with parameter** $w = \begin{bmatrix} w_1 \\ \vdots \\ w_p \end{bmatrix}$:
  - $\hat{y}_i = \langle w, h(x_i) \rangle$ where $h : \mathbb{R} \to \mathbb{R}^p$

How do we learn w?

$$\mathbf{H} = \begin{bmatrix} - - h(x_1)^\top - - \\ \vdots \\ - - h(x_n)^\top - - \end{bmatrix} \in \mathbb{R}^{n \times p}$$

$$\widehat{w} = \arg\min_w \|\mathbf{H}w - \mathbf{y}\|_2^2$$

For a new test point x, predict

$\hat{y} = \langle \widehat{w}, h(x) \rangle$

$\hat{w}_{\text{MLE}} = (H^T H)^{-1} H^T y$