香港科技大學
THE HONG KONG
UNIVERSITY OF SCIENCE
AND TECHNOLOGY

COMP 5212
Machine Learning
Lecture 4

Generalized Linear Models, Kernel Methods

Junxian He
Sep 19, 2024

Announcement

HW1 is out, due on Oct 2nd, please start early

Recap: Exponential Family

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Rough Idea *"If P has a a special form, then inference and learning come for free"*

$$P(y; \eta) = b(y) \exp \left\{ \eta^T T(y) - a(\eta) \right\}.$$

Here y, $a(\eta)$, and $b(y)$ are scalars. $T(y)$ same dimension as η.

$T(y) = y$

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$$1 = \sum_y P(y;\eta) = e^{-a(\eta)} \sum_y b(y)\exp\left\{\eta^T T(y)\right\}$$

$$\implies a(\eta) = \log \sum_y b(y)\exp\left\{\eta^T T(y)\right\}$$

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Multiply out the square and group terms:

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In all the exponential family distribution we work with in the course, T(y) = y

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Is this true for general?

Log Partition Function

Yes! Recall that

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$$\nabla_\eta a(\eta) = \frac{\sum_y T(y) b(y) \exp\{\eta^T T(y)\}}{\sum_y b(y) \exp\{\eta^T T(y)\}} = \mathbb{E}[T(y); \eta]$$

prob(y) = P(y)

T(y) = y

$\nabla_\eta a(\eta) = E(y)$

Many Other Exponential Models

- There are many canonical exponential family models:
  - Binary $\mapsto$ Bernoulli
  - Multiple Classses $\mapsto$ Multinomial
  - Real $\mapsto$ Gaussian
  - Counts $\mapsto$ Poisson
  - $\mathbb{R}_+ \mapsto$ Gamma, Exponential
  - Distributions $\mapsto$ Dirichlet

Recap

- Linear Regression $h_\theta(x) = \theta^T x$

$y = \frac{1}{1+e^{-z}}$

- Logistic Regression $h_\theta(x) = g(\theta^T x)$
- Multi-class Classification Regression $h_\theta(x) = softmax(\theta_1^T x, \cdots, \theta_k^T x)$

Recap

LMS rule

- Linear Regression $h_\theta(x) = \theta^T x$ $\theta_j := \theta_j + \alpha \sum_{i=1}^{n} \left(y^{(i)} - h_\theta(x^{(i)})\right) x_j^{(i)}$

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Is this coincidence?

Generalized Linear Models

$x_0 = 1$

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We first we pick a distribution based on y's type.

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conditional distribution

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- Our model is *linear* beacuse we make the natural parameter $\eta = \theta^T x$ in which $\theta, x \in \mathbb{R}^{d+1}$.

$$\eta = \theta^T x$$

Generalized Linear Models

inference $h_\theta(x) = \mathbb{E}[y \mid x; \theta]$ is the **output**.

learn $\max_\theta \log p(y \mid x; \theta)$ by maximum likelihood.

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$T(y) = y$ for most of the examples you will see in this course

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algorithm: SGD $\theta^{(t+1)} = \theta^{(t)} + \alpha \left(y^{(i)} - h_{\theta^{(t)}}(x^{(i)}) \right) x^{(i)}$

Constructing GLMs

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- Pick an exponential family distribution given the type of y (Possion, Multinomial, Gaussian…)

$y = [0.1, 0.2, 0.7]$ Dirichlet

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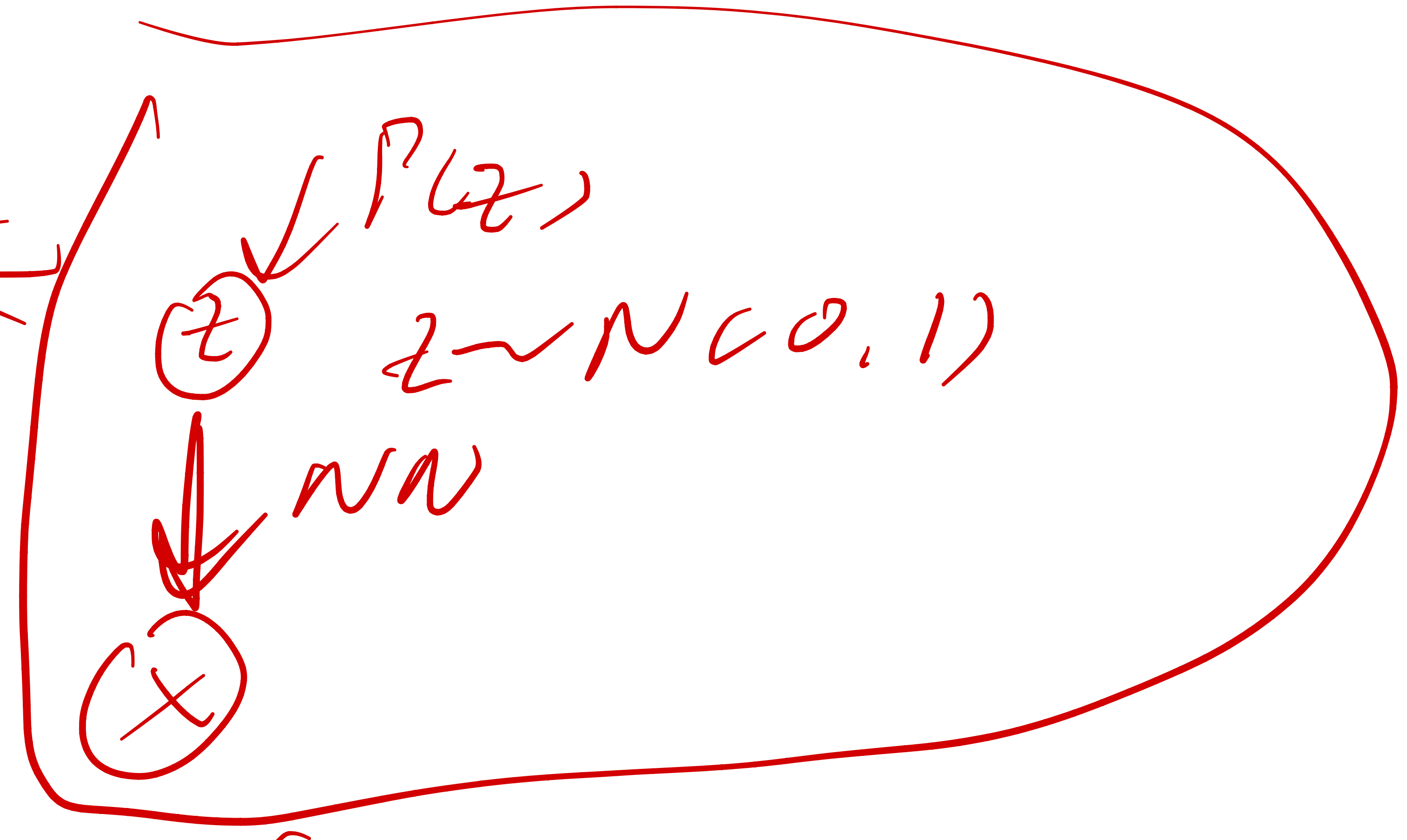
GANs



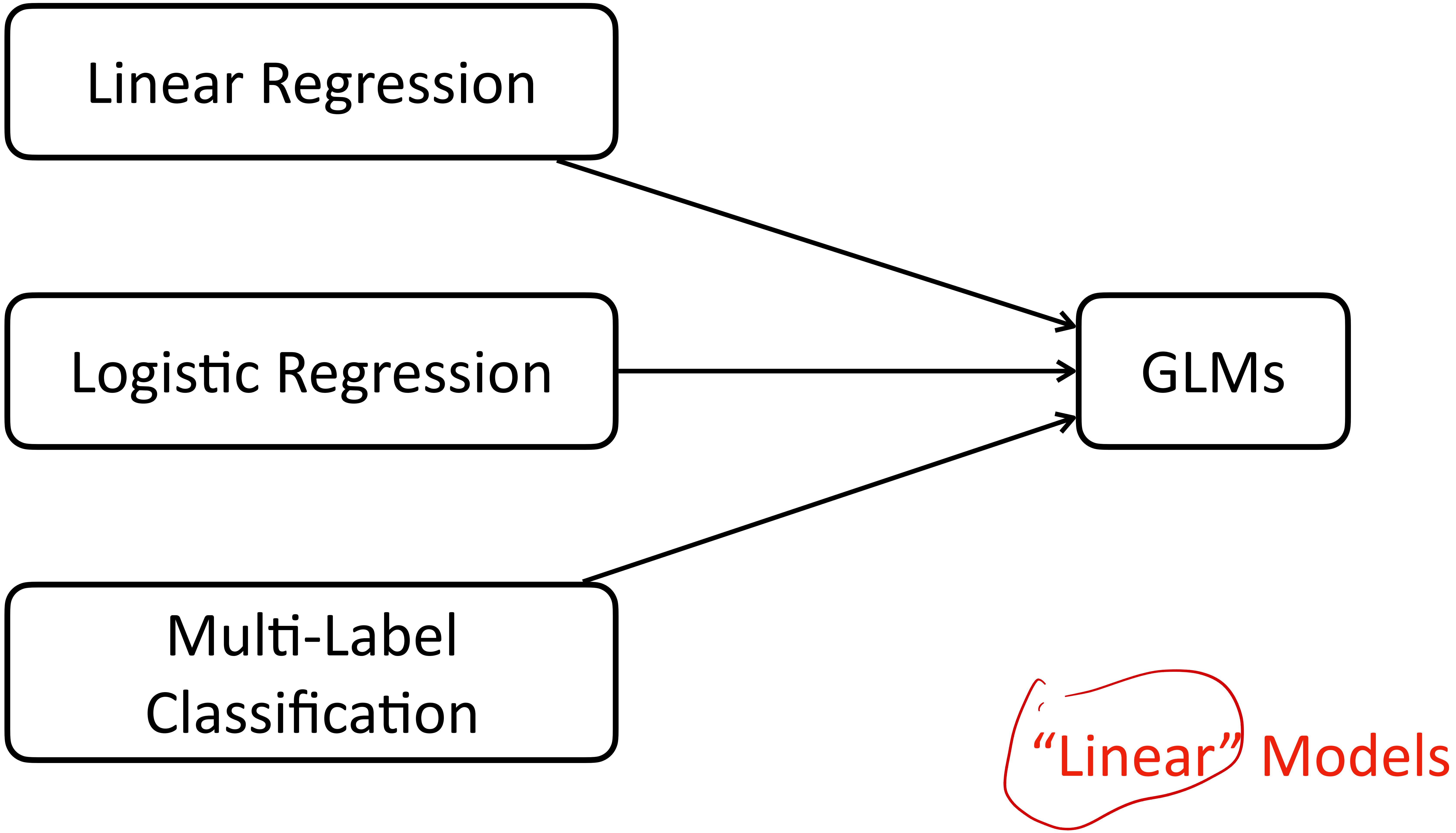
$P(x) = \int_z P(x, z)$

E(A)

Enjoy closed-form solution for various statistics

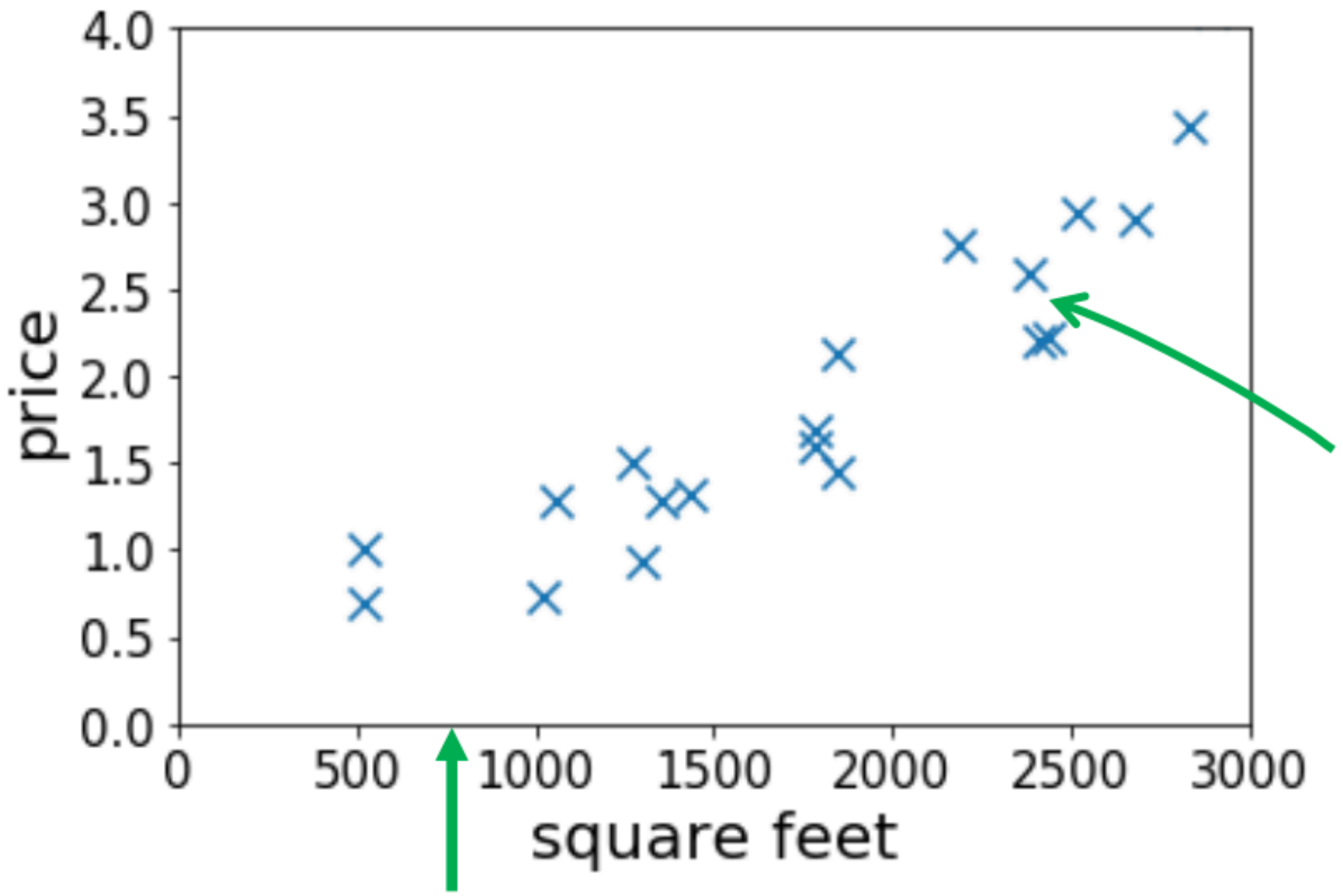
GLMs do not have local minimum

Generalized Linear Models



Kernel Methods

Feature Map

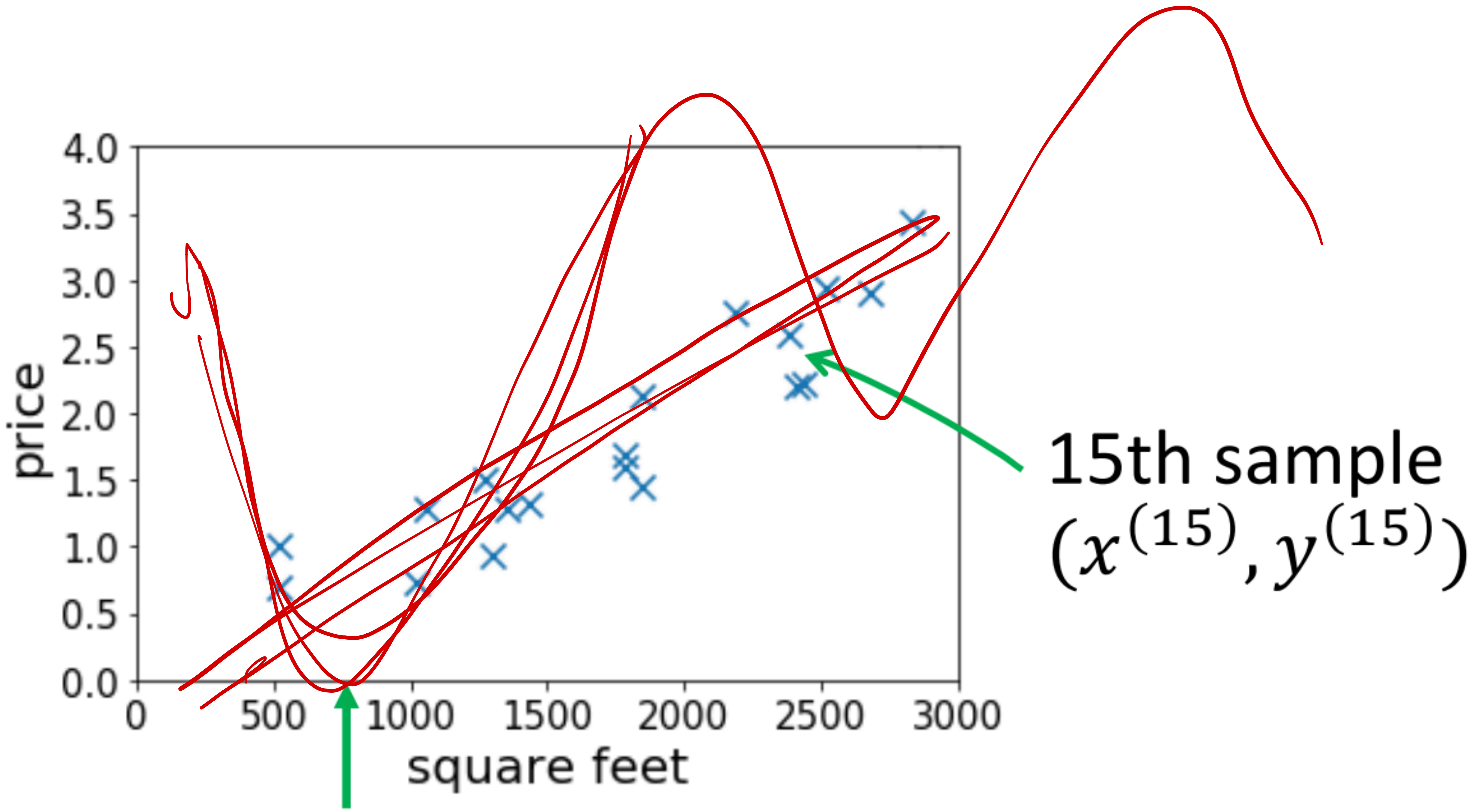


15th sample
$(x^{(15)}, y^{(15)})$

$x = 800$
$y = ?$

x

Feature Map



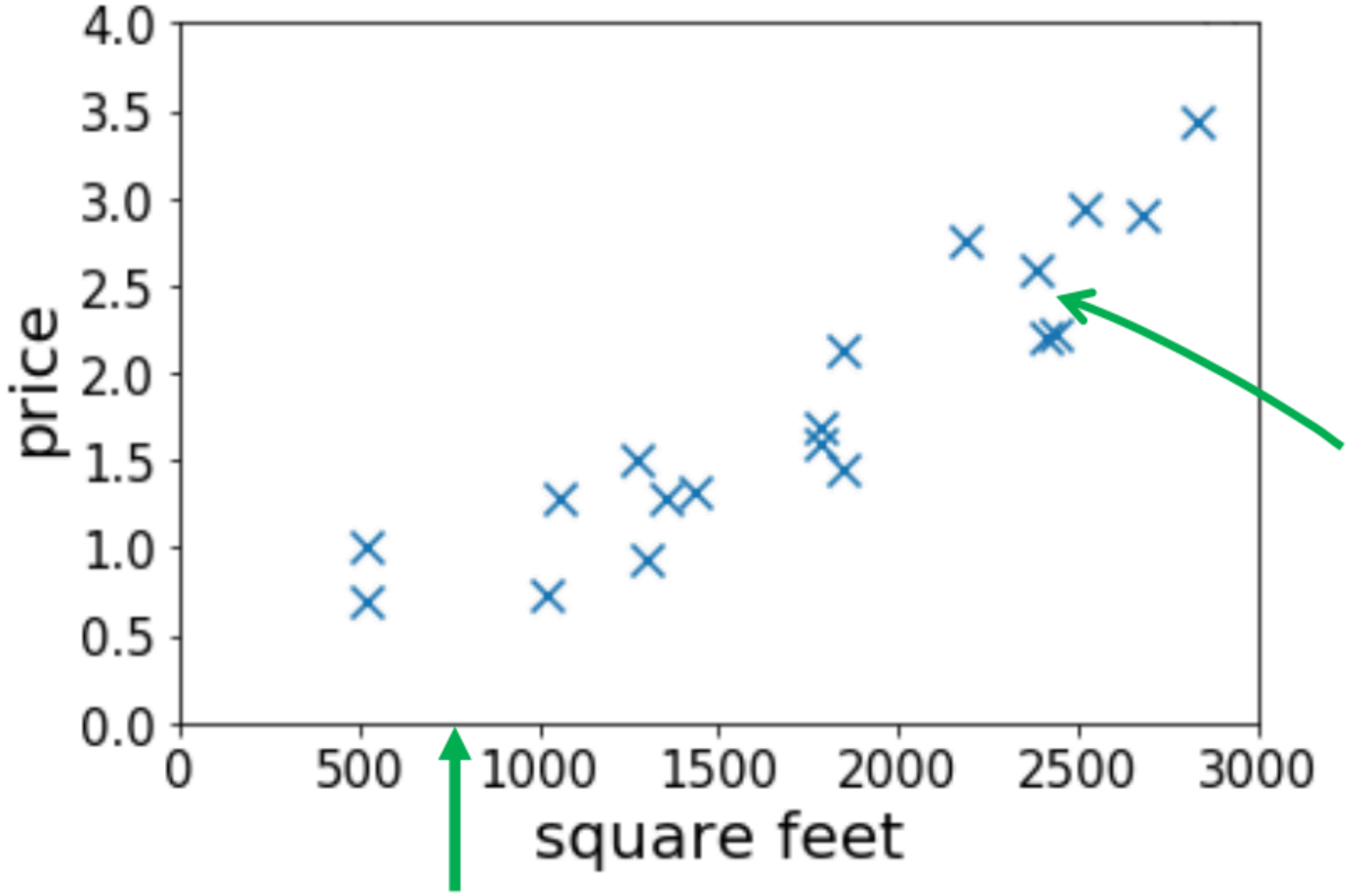
$x = 800$

$y = ?$

$$y = \theta x$$

$$y = \theta_1 x^2 + \theta_2 x + \theta_3 x^3$$

Feature Map



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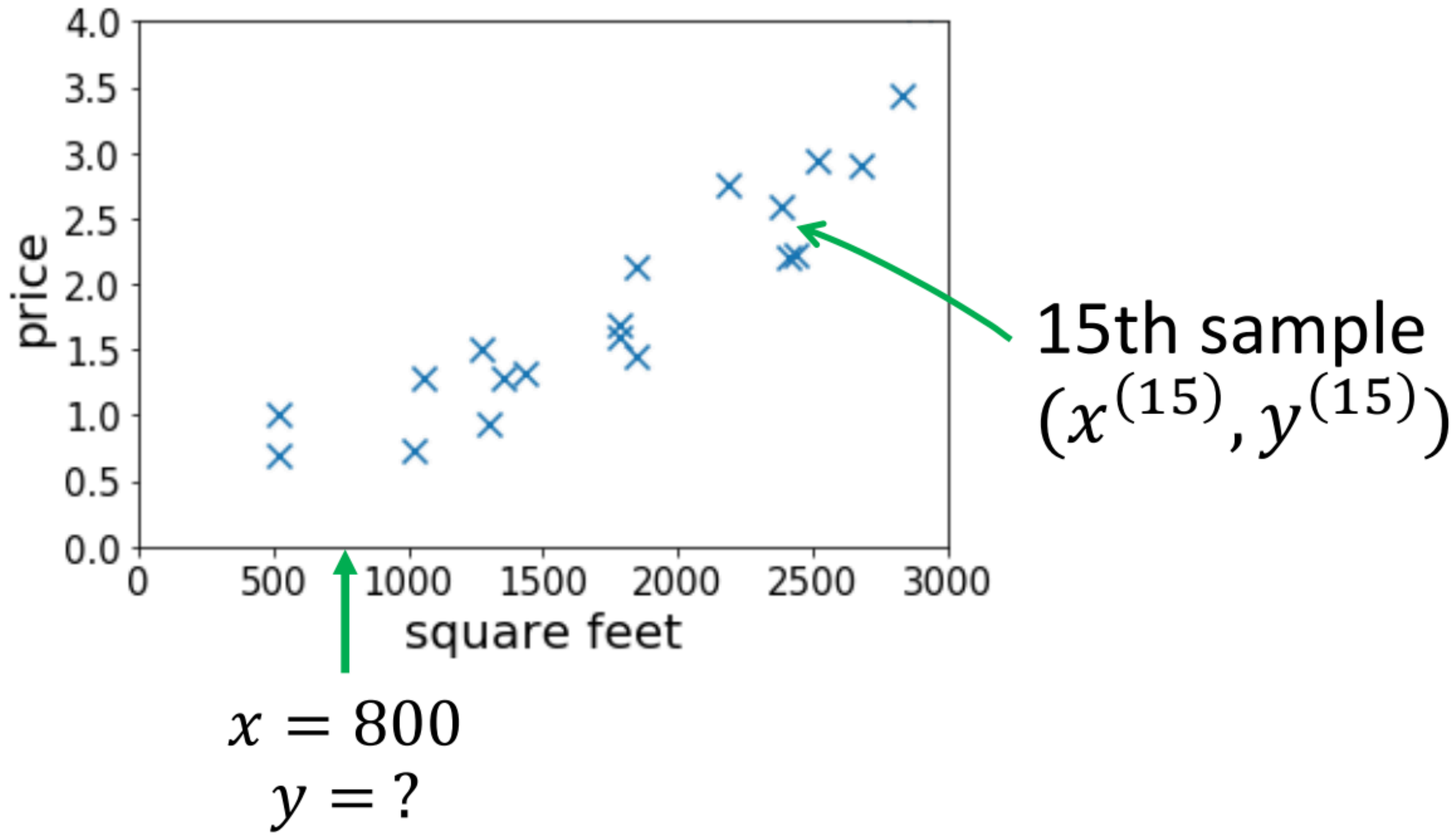

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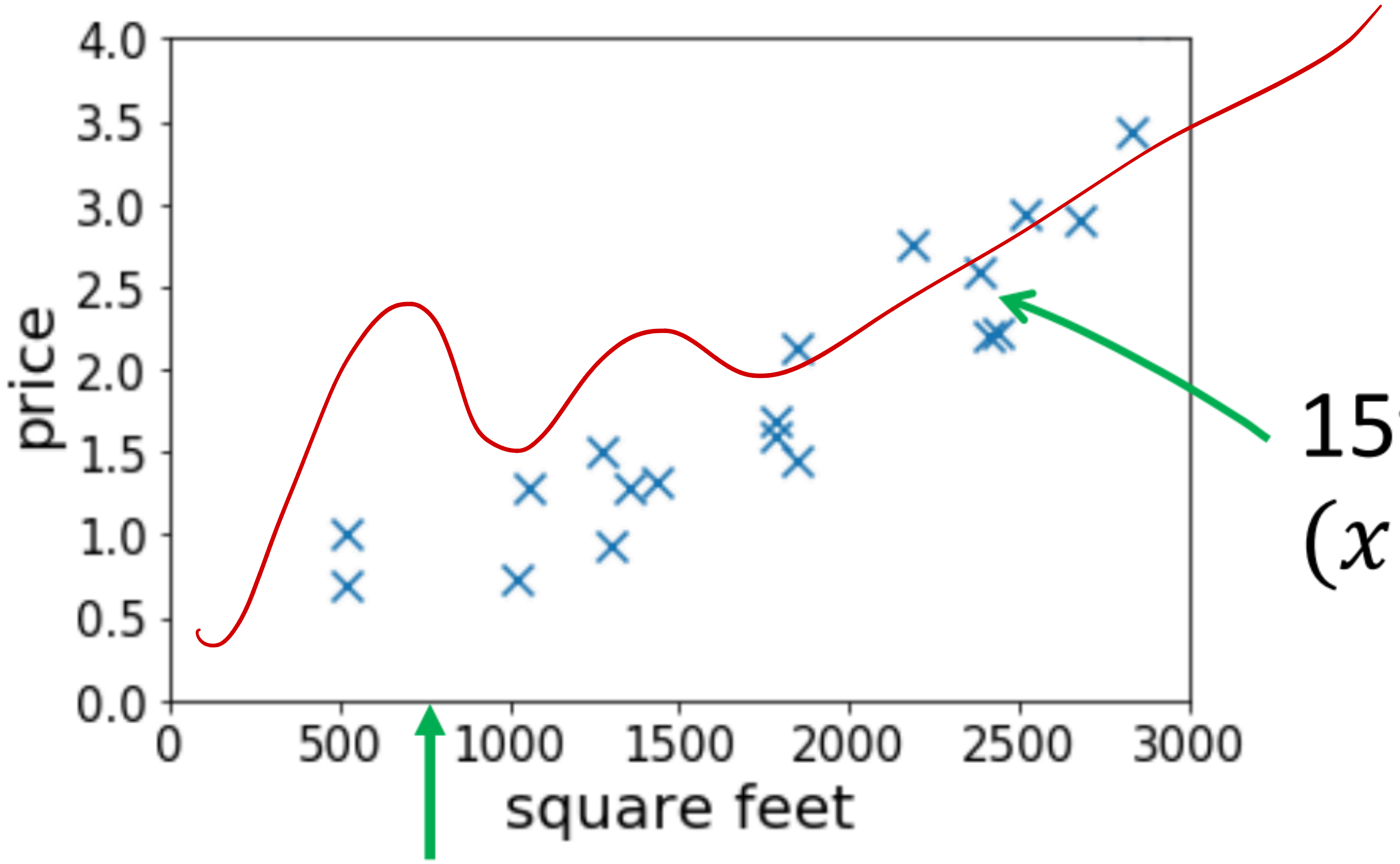

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no parameter

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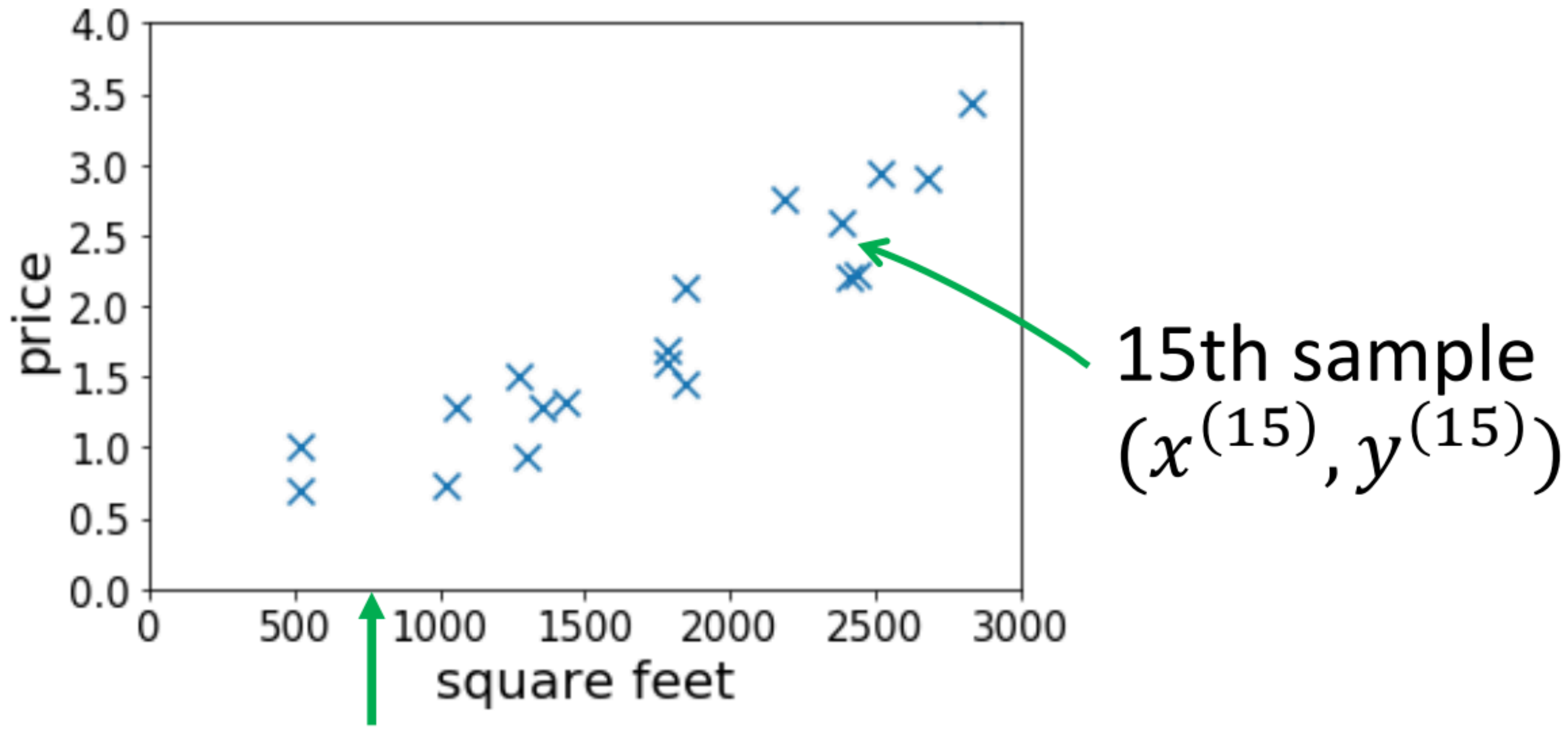
$$y = \theta^T \phi(x)$$

Feature Map



$x = 800$
$y = ?$

$d = 1$

$p = 4$

Feature map
$\phi : R^d \rightarrow R^p$

$$y = \theta x$$

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$$y = \theta^T \phi(x)$$

LMS Update Rule with Features

Linear Regression:

$$\theta := \theta + \alpha \sum_{i=1}^{n} \left(y^{(i)} - h_\theta(x^{(i)})\right) x^{(i)}$$

$$:= \theta + \alpha \sum_{i=1}^{n} \left(y^{(i)} - \theta^T x^{(i)}\right) x^{(i)}.$$

With Features:

LMS Update Rule with Features

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With Features:

$$\theta := \theta + \alpha \sum_{i=1}^{n} \left(y^{(i)} - \theta^T \phi(x^{(i)})\right) \phi(x^{(i)})$$

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How about Generalized Linear Models with Features?

New Feature Vector Can Be Very High-Dimensional

$$\phi(x) = \begin{bmatrix} 1 \\ x_1 \\ x_2 \\ \vdots \\ x_1^2 \\ x_1 x_2 \\ x_1 x_3 \\ \vdots \\ x_2 x_1 \\ \vdots \\ x_1^3 \\ x_1^2 x_2 \\ \vdots \end{bmatrix}$$

Computationally expensive

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Computationally expensive

Is the computation evitable given $\theta \in R^p$?

Kernel Trick

- If θ is initialized as 0, then at any step of the gradient descent:

$$\theta = \sum_{i=1}^{n} \beta_i \phi(x^{(i)}) \qquad \beta_i \in R$$

θ initialized as 0

$$\theta := \theta + \alpha \sum_{i=1}^{n} (y^{(i)} - \theta^T \phi(x^{(i)})) \phi(x^{(i)})$$

constant

$$= \sum_{i=1}^{n} \beta_i^{old} \phi(x^{(i)}) + \alpha \sum_{i=1}^{n} (y^{(i)} - \theta^T \phi(x^{(i)})) \phi(x^{(i)})$$

$$= \sum_{i=1}^{n} (\beta_i + \alpha (y^{(i)} - \theta^T \phi(x^{(i)}))) \phi(x^{(i)})$$

$$\parallel$$

$$\beta_i^{new}$$

$$\theta = \sum_i \beta_i \phi(x^{(i)})$$ ϕ is constant

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Kernel Trick

$$\beta_i := \beta_i + \alpha \left(y^{(i)} - \sum_{j=1}^{n} \beta_j \phi(x^{(j)})^T \phi(x^{(i)}) \right)$$

Rewrite $\phi(x^{(j)})^T \phi(x^{(i)}) = < \phi(x^{(j)}), \phi(x^{(i)}) >$ $\in R$

We can precompute all pairwise $< \phi(x^{(j)}), \phi(x^{(i)}) >$ beforehand, and reuse it for every gradient descent update

expensive $\theta = \sum_{i=1}^{n} \beta_i \phi(x^{(i)})$, $\in R^p$

$y^{(i)} = h_\theta(\theta^T \phi(x^{(i)}))$

n: # data samples

Kernel Trick

$$\beta_i := \beta_i + \alpha \left(y^{(i)} - \sum_{j=1}^{n} \beta_j \phi(x^{(j)})^T \phi(x^{(i)}) \right)$$

Kernel $K(x, z)$ $\quad \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ $\quad \mathcal{X}$ is the space of the input

$$K(x, z) \triangleq \langle \phi(x), \phi(z) \rangle$$

The Algorithm

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- Compute $K(\phi(x^{(i)}), \phi(x^{(j)})) = <\phi(x^{(i)}), \phi(x^{(j)})>$ for all i, j

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- Loop $$\beta_i := \beta_i + \alpha \left(y^{(i)} - \sum_{j=1}^{n} \beta_j K(x^{(i)}, x^{(j)}) \right) \quad \forall i \in \{1, \ldots, n\}$$

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Recall that n is the number of data samples

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Recall that n is the number of data samples

Or in vector notation, letting K be the $n \times n$ matrix with $K_{ij} = K(x^{(i)}, x^{(j)})$, we have

$$\beta := \beta + \alpha(\vec{y} - K\beta)$$

Inference

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We do not need to explicitly compute θ !

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$$\theta^T \phi(x) = \sum_{i=1}^{n} \beta_i \phi(x^{(i)})^T \phi(x) = \sum_{i=1}^{n} \beta_i K(x^{(i)}, x)$$

$K(x^{(i)}, x) =$

Inference

We do not need to explicitly compute θ !

$$\theta^T \phi(x) = \sum_{i=1}^{n} \beta_i \phi(x^{(i)})^T \phi(x) = \sum_{i=1}^{n} \beta_i K(x^{(i)}, x)$$

The Kernel function is all we need for training and inference!

x is new

$K(x^{(i)}, x) = \langle \phi(x^{(i)}), \phi(x) \rangle$

Implicit Feature Map

Do we still need to define feature maps?

$$K(x, z) \triangleq \langle \phi(x), \phi(z) \rangle$$

$K(x, z) = (x^T z)^2 \stackrel{?}{=} \langle \phi(x), \phi(z) \rangle$

valid kernal function?

cheap, $x, z \in \mathbb{R}^d$ low-dim

$\phi(x) \in \mathbb{R}^p$ high-dim

Implicit Feature Map

Do we still need to define feature maps?

$$K(x, z) \triangleq \langle \phi(x), \phi(z) \rangle$$

What kinds of kernel functions K() can correspond to some feature map ϕ

Example

valid, $\phi(x)$?

$$K(x,z) = (x^T z)^2 \qquad x, z \in \mathbb{R}^d$$

explicit : $\phi(x) \longrightarrow K(x,z)$

implicit : $K(x,z) \overset{?}{\longrightarrow} \phi(x)$

Example

$$K(x, z) = (x^T z)^2 \qquad x, z \in \mathbb{R}^d$$

What is the feature map to make K a valid kernel function?

Example

$$K(x,z) = (x^T z)^2 \qquad x, z \in \mathbb{R}^d$$

What is the feature map to make K a valid kernel function?

$$\begin{aligned} K(x,z) &= \left(\sum_{i=1}^{d} x_i z_i\right)\left(\sum_{j=1}^{d} x_j z_j\right) \\ &= \sum_{i=1}^{d}\sum_{j=1}^{d} x_i x_j z_i z_j \\ &= \sum_{i,j=1}^{d} (x_i x_j)(z_i z_j) \end{aligned}$$

$\phi(x)$

$\langle \phi(x), \phi(z) \rangle$

$= \phi(x)^T \phi(z)$

Example

Valid

$$K(x, z) = (x^T z)^2 \qquad x, z \in \mathbb{R}^d$$

d=3

What is the feature map to make K a valid kernel function?

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$$\phi(x) = \begin{bmatrix} x_1x_1 \\ x_1x_2 \\ x_1x_3 \\ x_2x_1 \\ x_2x_2 \\ x_2x_3 \\ x_3x_1 \\ x_3x_2 \\ x_3x_3 \end{bmatrix}$$

$\phi(x)^T \phi(z)$

Example

complexity O(d)

$$K(x,z) = (x^T z)^2 \qquad x, z \in \mathbb{R}^d$$

What is the feature map to make K a valid kernel function?

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Requires O(d^2) compute for feature mapping

Example

Gaussian kernel

$K(x,t) = \exp(\quad)$

⇓

infinite-dim feature map

valid

$$K(x, z) = (x^T z)^2 \qquad x, z \in \mathbb{R}^d$$

What is the feature map to make K a valid kernel function?

$$K(x,z) = \left(\sum_{i=1}^{d} x_i z_i\right)\left(\sum_{j=1}^{d} x_j z_j\right)$$

$$= \sum_{i=1}^{d}\sum_{j=1}^{d} x_i x_j z_i z_j$$

$$= \sum_{i,j=1}^{d} (x_i x_j)(z_i z_j)$$

$$\phi(x) = \begin{bmatrix} x_1x_1 \\ x_1x_2 \\ x_1x_3 \\ x_2x_1 \\ x_2x_2 \\ x_2x_3 \\ x_3x_1 \\ x_3x_2 \\ x_3x_3 \end{bmatrix}$$

O(d^3)

Requires O(d^2) compute for feature mapping

Requires O(d) compute for Kernel function

Next Lecture

criterions

- What kinds of functions would make a kernel function?
- Infinite dimensions of feature mapping?
- Support Vector Machines

Thank You!
Q & A