Applied Machine Learning

Linear Regression

Siamak Ravanbakhsh

Learning objectives

- linear model
- evaluation criteria
- how to find the best fit
- geometric interpretation

Motivation

History: method of least squares was invented by **Legendre** and **Gauss** (1800's)

Gauss at age 24 used it to predict the future location of Ceres (largest astroid in the astroid belt)

source: http://chrisauld.com/2012/10/07/what-do-we-know-about-the-effect-of-income-inequality-on-health/

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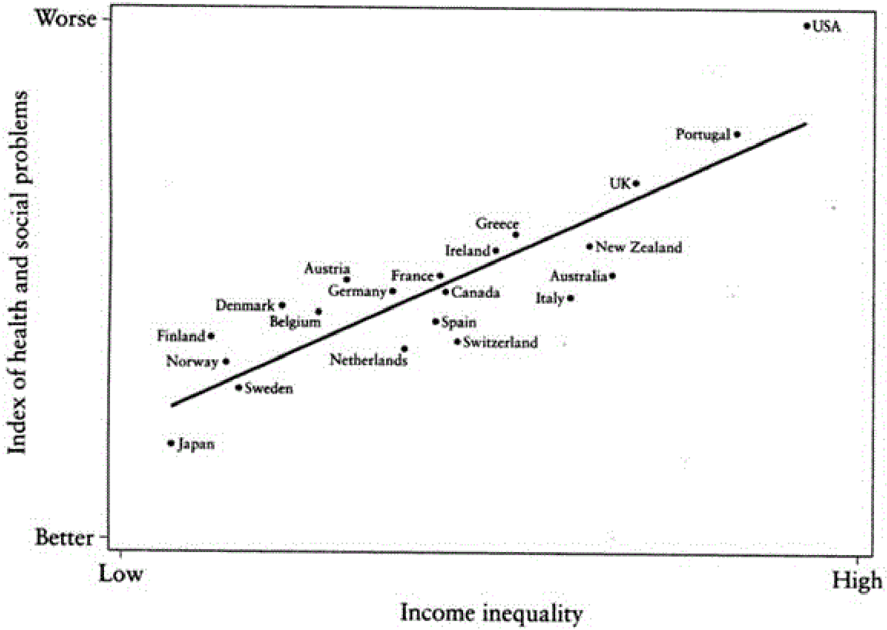
effect of income inequality on health and social problems



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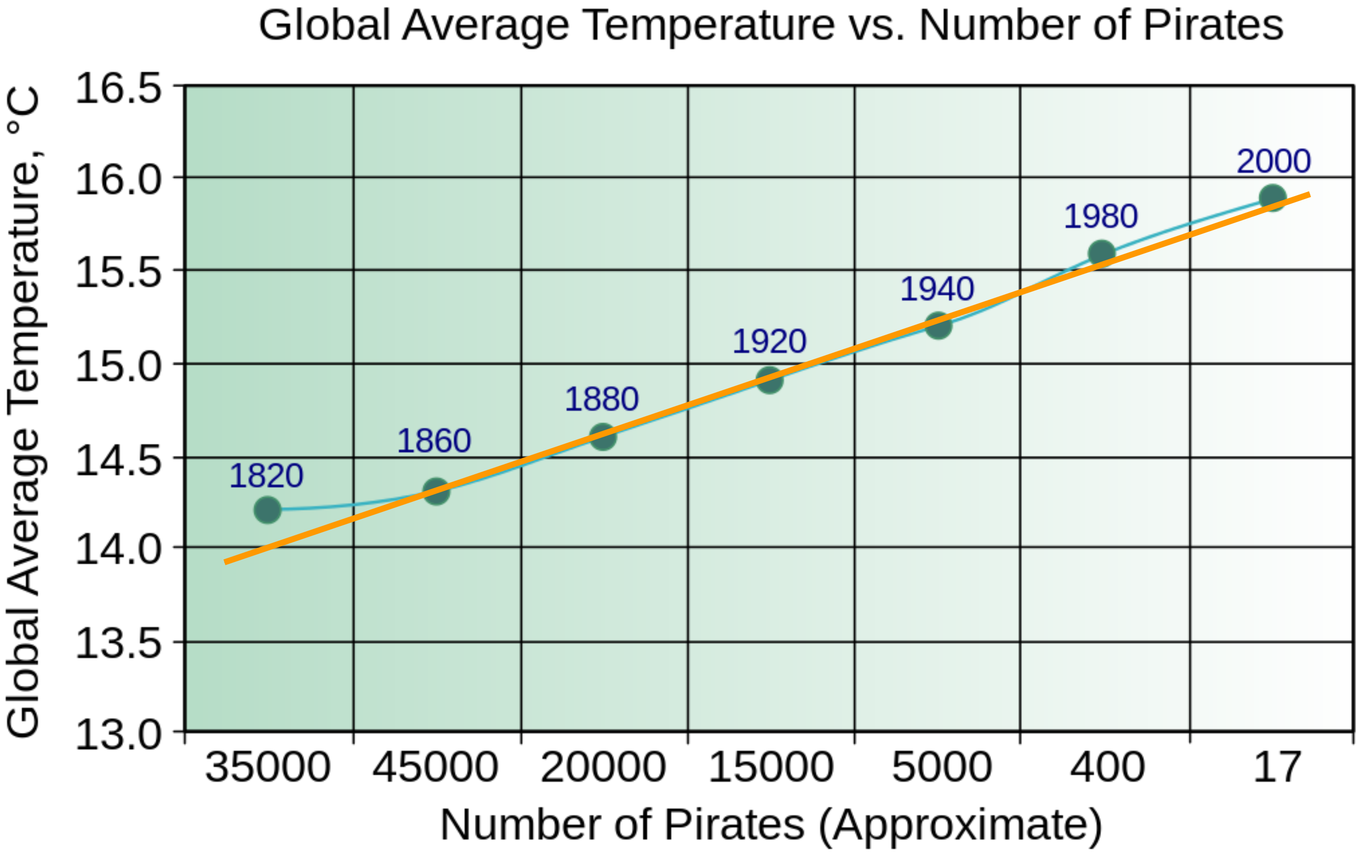
Motivation (?)


Global Average Temperature vs. Number of Pirates
Global Average Temperature, °C
16.5
16.0
15.5
15.0
14.5
14.0
13.5
13.0
1820
1860
1880
1920
1940
1980
2000
35000
45000
20000
15000
5000
400
17
Number of Pirates (Approximate)

Representing data

each instance: $\left| \begin{array}{l} x^{(n)} \in \mathbb{R}^D \\ y^{(n)} \in \mathbb{R} \end{array} \right.$

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vectors are assume to be column vectors $x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_D \end{bmatrix} = \begin{bmatrix} x_1, & x_2, & \dots, & x_D \end{bmatrix}^\top$

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we assume N instances in the dataset $\mathcal{D} = \{(x^{(n)}, y^{(n)})\}_{n=1}^N$

each instance has D features indexed by d

for example, $x_d^{(n)} \in \mathbb{R}$ is the feature d of instance n

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design matrix: *concatenate all instances*

- *each row is a datapoint, each column is a feature*

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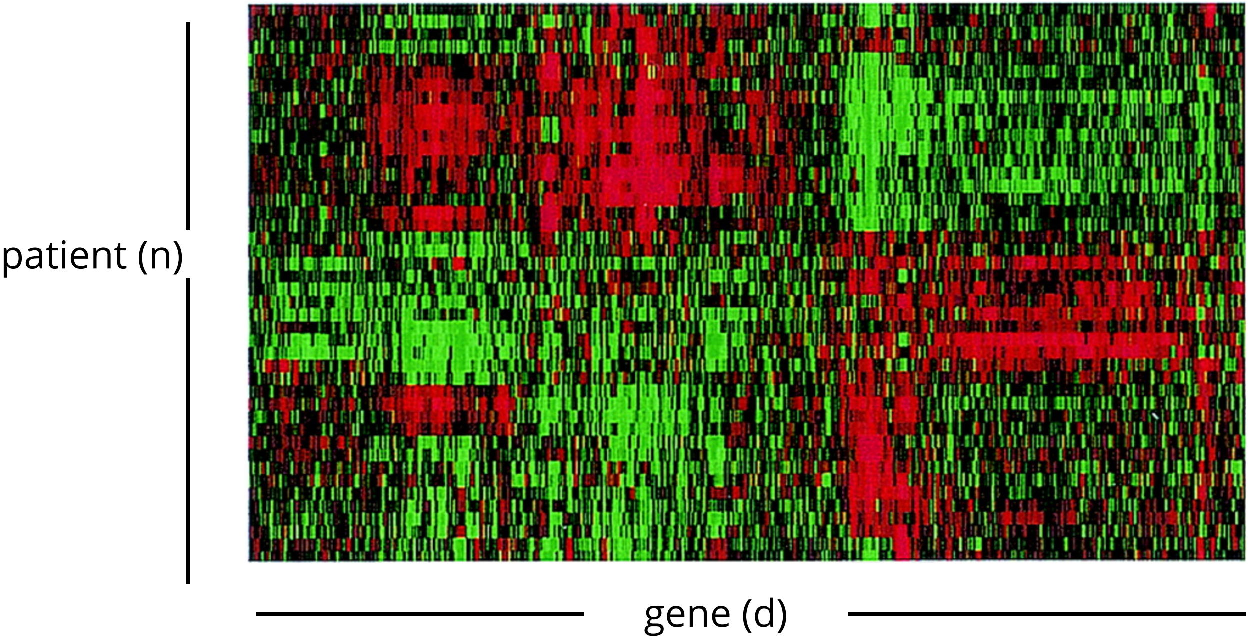
Representing data

Example:

Micro array data (X), contains gene expression levels
labels (y) can be {cancer/no cancer} label for each patient



$$\in \mathbb{R}^{N \times D}$$

Linear model

assuming a scalar output $f_w : \mathbb{R}^D \to \mathbb{R}$

will generalize to a vector later

$$f_w(x) = w_0 + w_1 x_1 + \ldots + w_D x_D$$

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simplification

concatenate a 1 to x $\longrightarrow$ $x = [1, x_1, \ldots, x_D]^\top$

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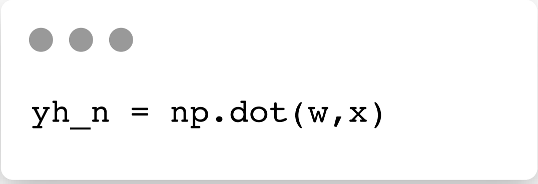

```
yh_n = np.dot(w,x)
```

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Loss function

objective: find parameters to fit the data $x^{(n)}, y^{(n)} \quad \forall n$

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square error **loss** (a.k.a. **L2** loss) $L(y, \hat{y}) \triangleq \frac{1}{2}(y - \hat{y})^2$

for a single instance (a function of labels)

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versus

for the whole dataset

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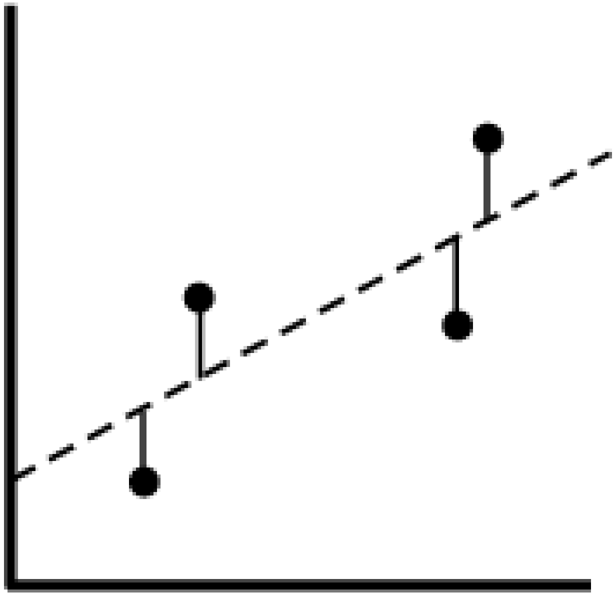
Example (D = 1) +bias (D=2)!



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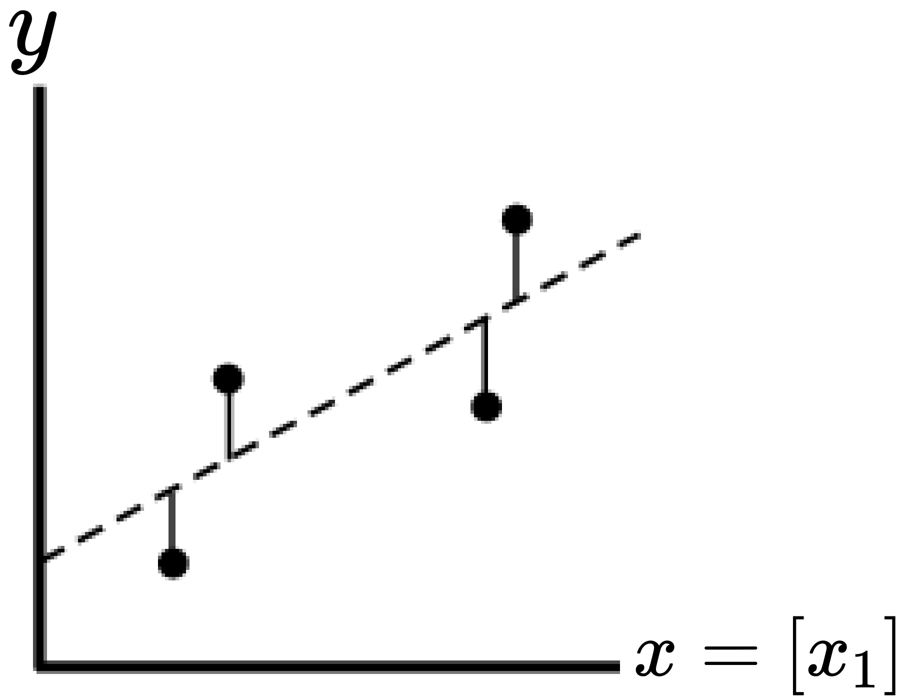

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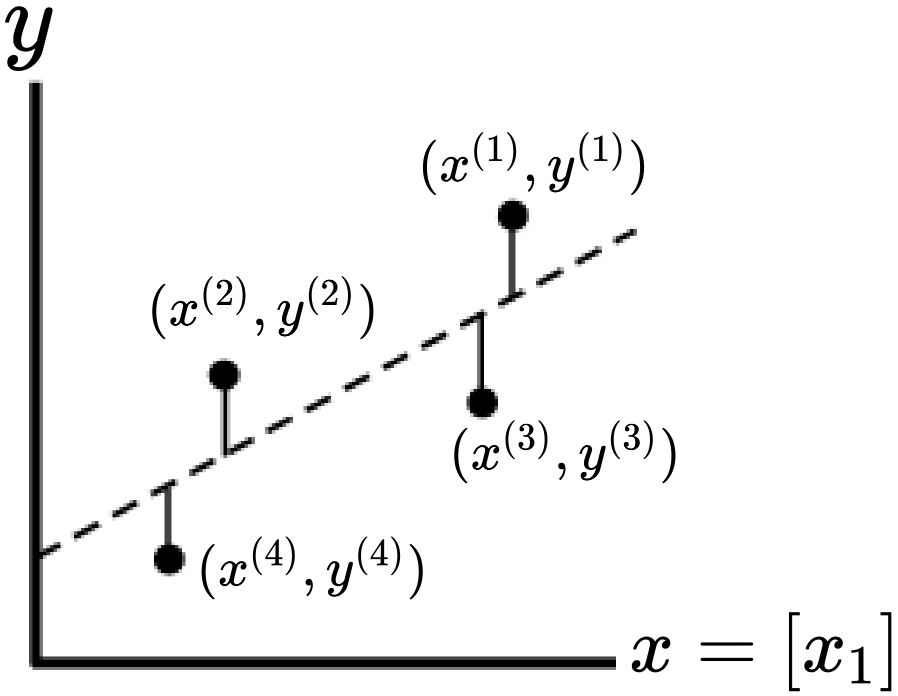

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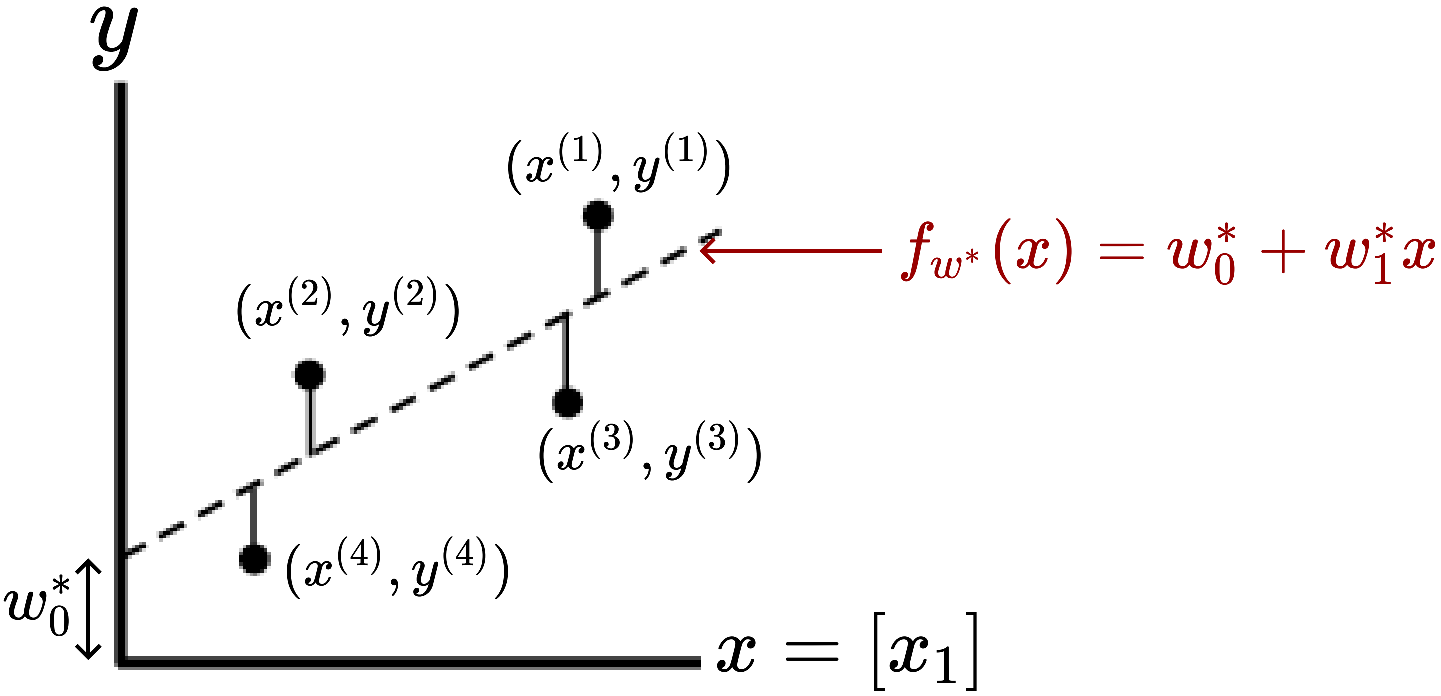

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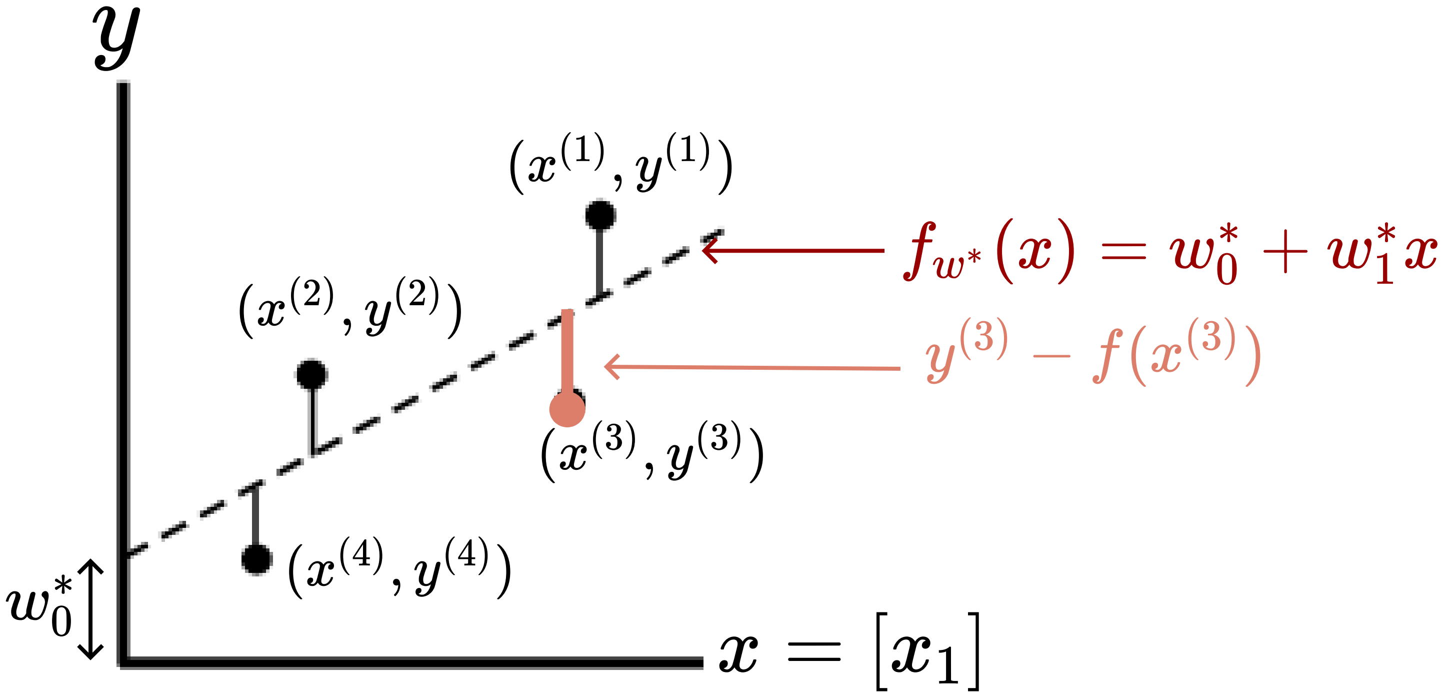

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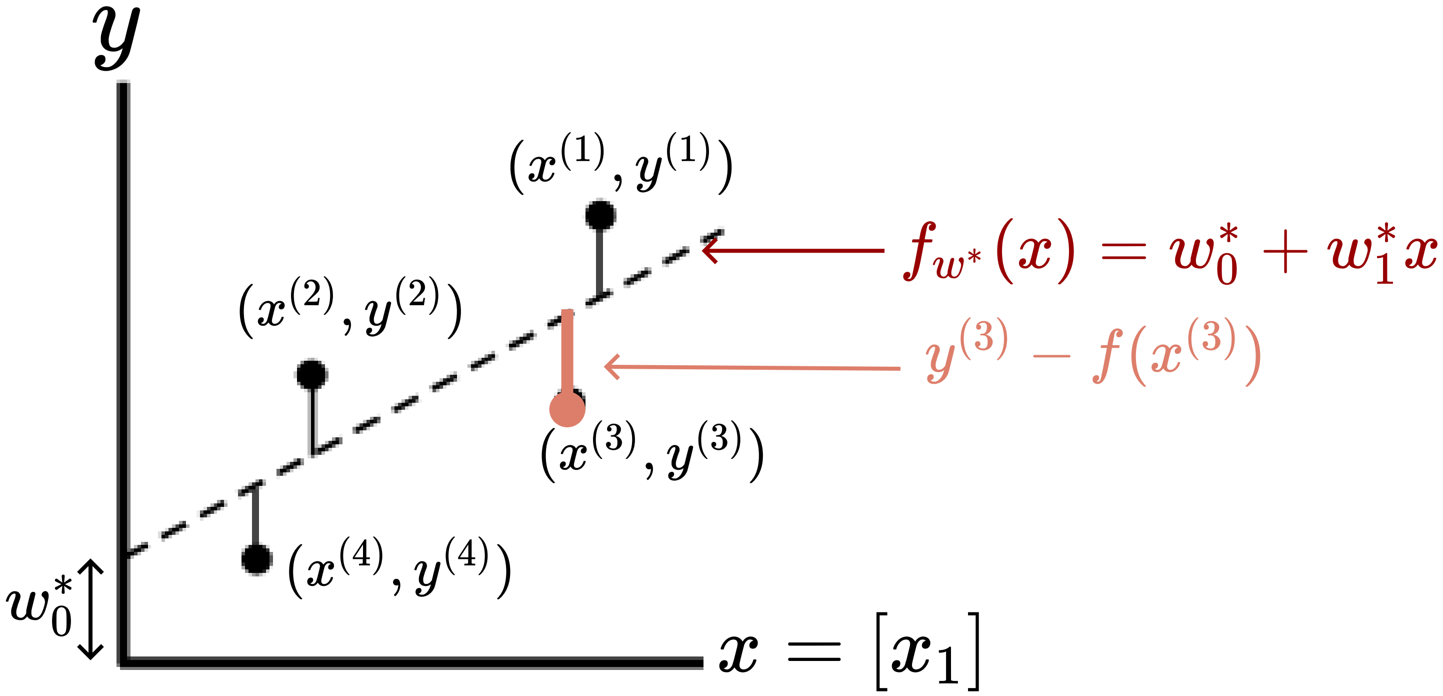
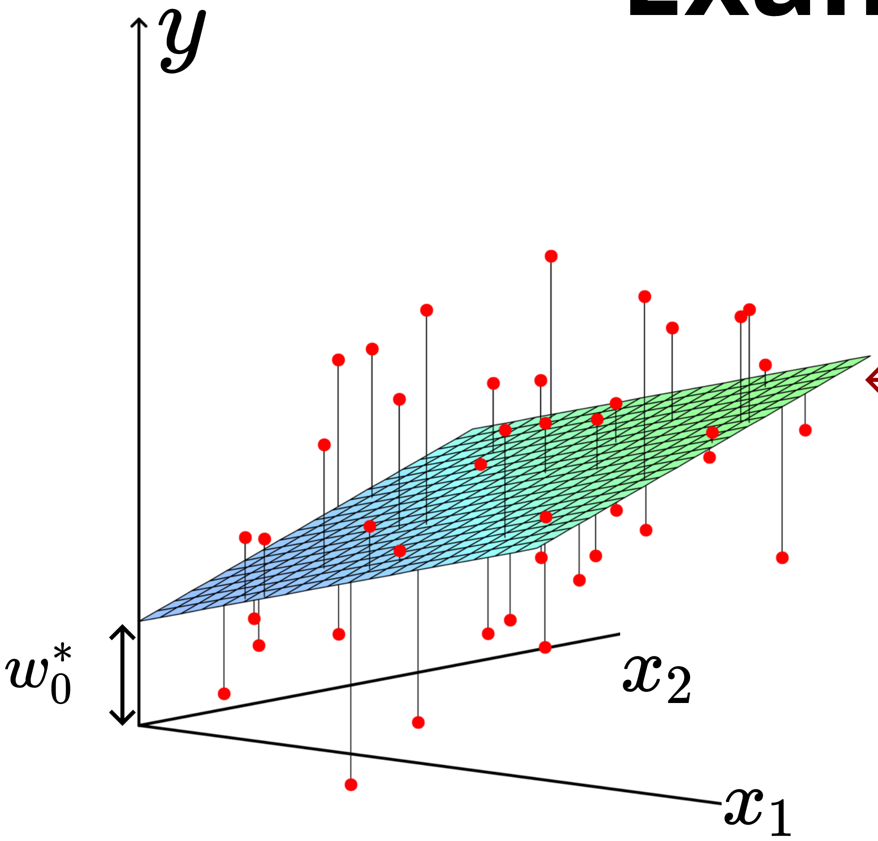


Linear Least Squares $\min_w \sum_n \left(y^{(n)} - w^T x^{(n)} \right)^2$

Example (D=2) +bias (D=3)!



$$f_{w^*}(x) = w_0^* + w_1^* x_1 + w_2^* x_2$$

Linear Least Squares $w^* = \arg\min_w \sum_n \left(y^{(n)} - w^T x^{(n)}\right)^2$

Matrix form

instead of $\underset{\in \mathbb{R}}{\hat{y}^{(n)}} = \underset{1 \times D}{w}^{\top} \underset{D \times 1}{x^{(n)}}$

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Linear least squares

$$\arg\min_w \frac{1}{2}||y - Xw||^2 = \frac{1}{2}(y - Xw)^\top (y - Xw)$$

squared L2 norm of the **residual** vector

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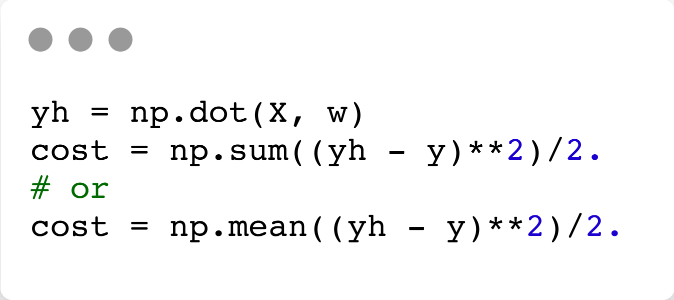

```
yh = np.dot(X, w)
cost = np.sum((yh - y)**2)/2.
# or
cost = np.mean((yh - y)**2)/2.
```

Minimizing the cost

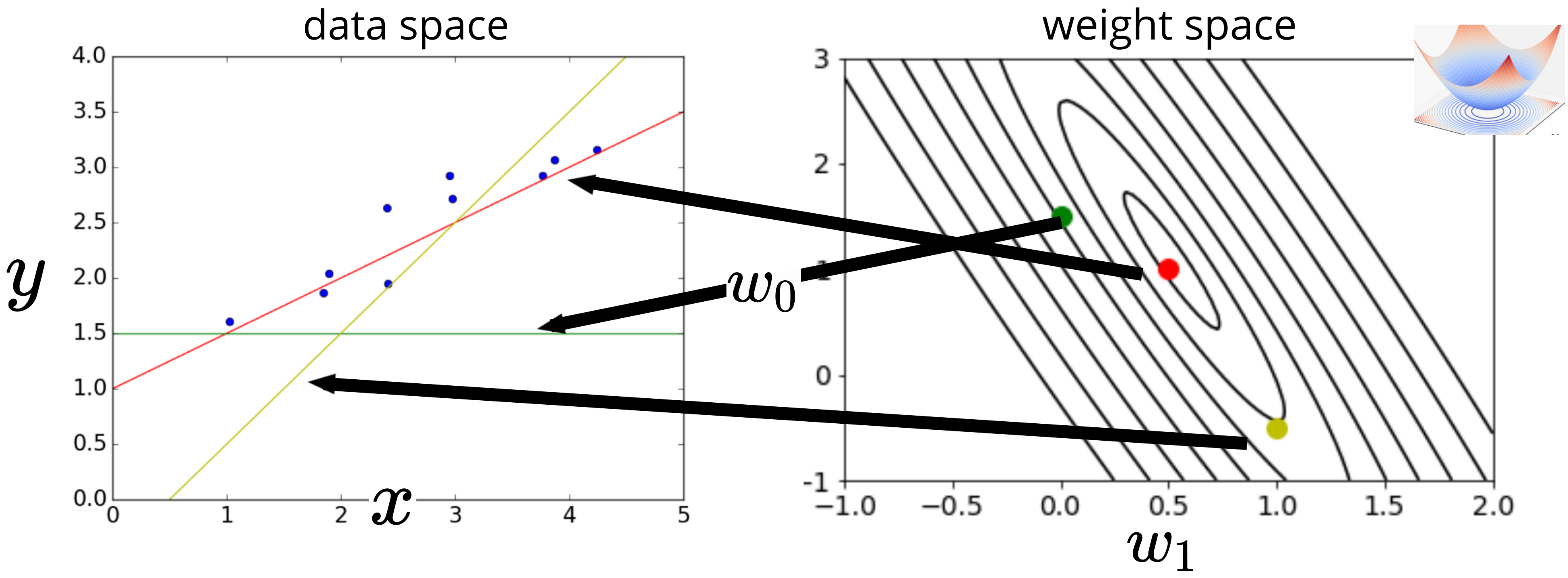

image: Grosse, Farahmand, Carrasquilla

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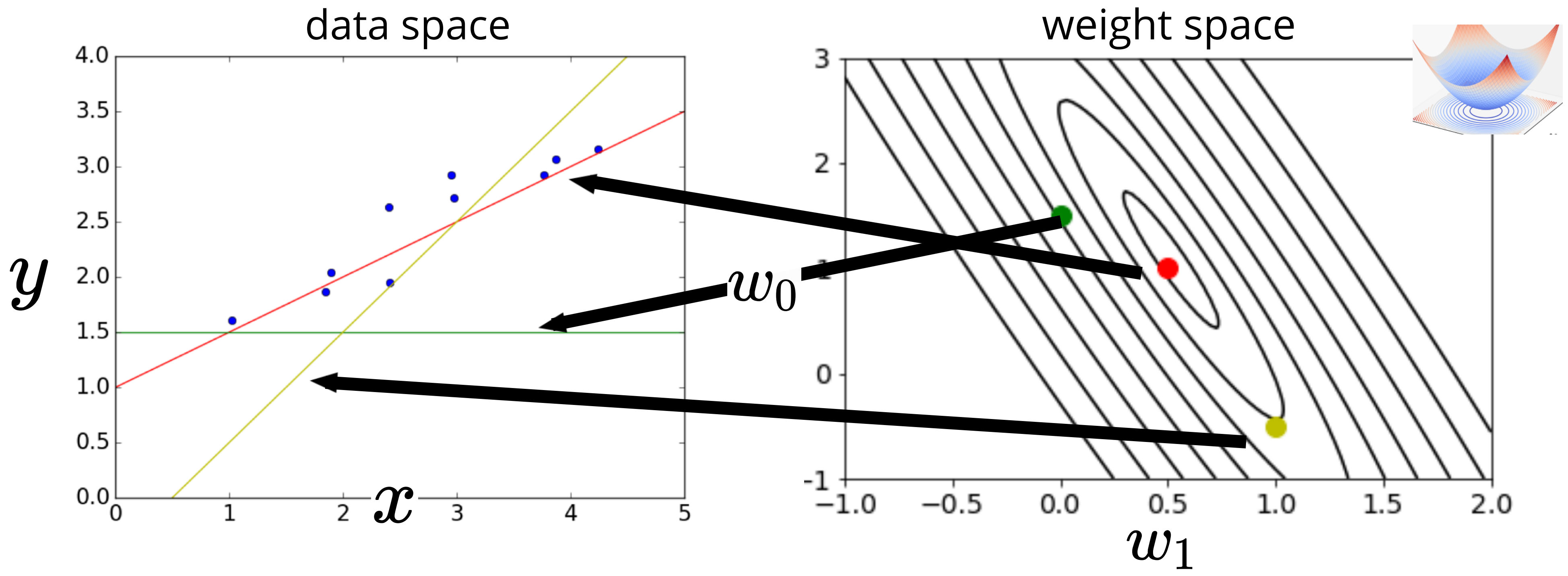

the objective is a smooth function of w

find minimum by setting partial derivatives to zero

image: Grosse, Farahmand, Carrasquilla

Simple case: D = 1

model $f_w(x) = \boxed{wx}$

both scalar

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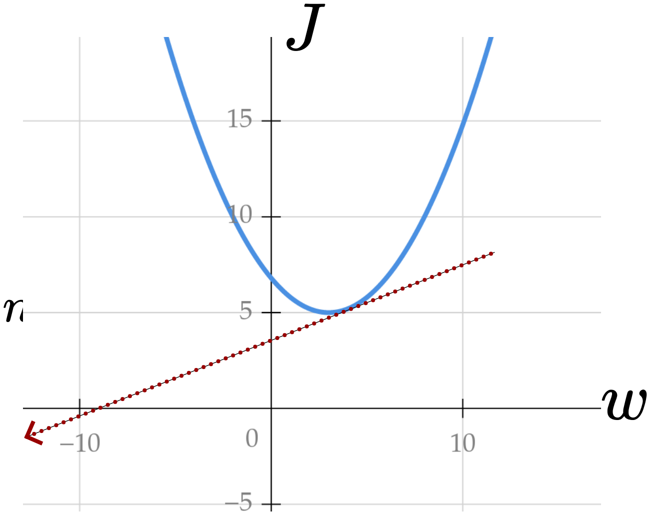

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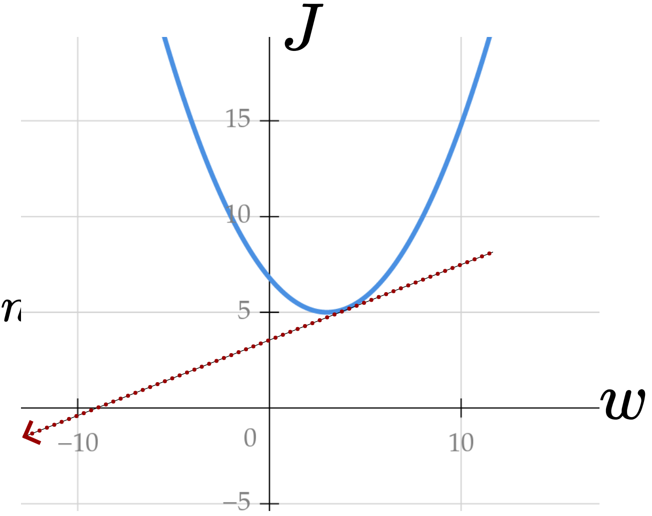

derivative $\frac{\mathrm{d}J}{\mathrm{d}w} = \sum_n x^{(n)}(wx^{(n)} - y^{(n)})$

setting the derivative to zero $w = \frac{\sum_n x^{(n)} y^{(n)}}{\sum_n {x^{(n)}}^2}$

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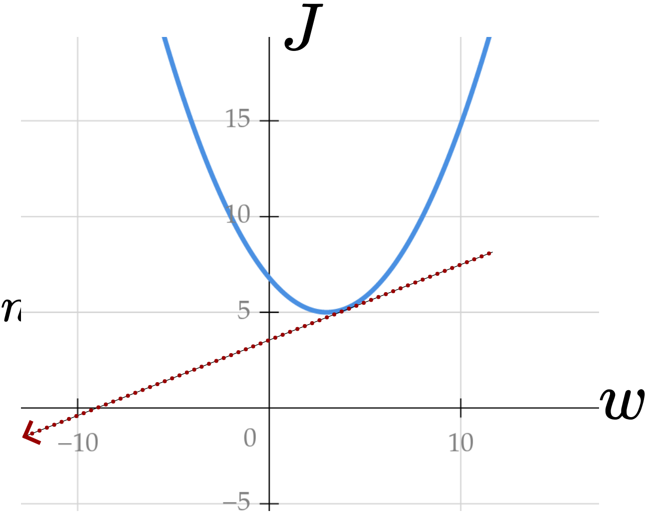

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global minimum because cost is smooth and *convex*

more on convexity layer

Gradient

for a multivariate function $J(w_0, w_1)$

partial derivatives instead of derivative

= derivative when other vars. are fixed

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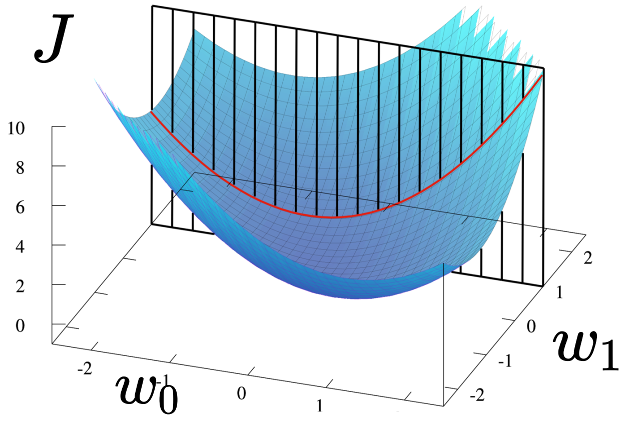
$$\frac{\partial}{\partial w_1} J(w_0, w_1) \triangleq \lim_{\epsilon \to 0} \frac{J(w_0, w_1+\epsilon) - J(w_0, w_1)}{\epsilon}$$



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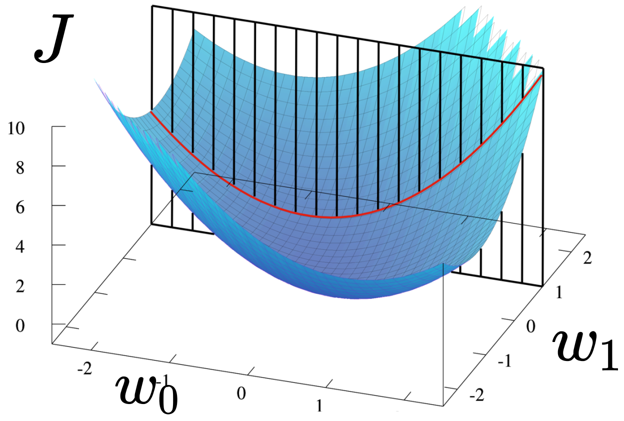

partial derivatives instead of derivative

= derivative when other vars. are fixed

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critical point: all partial derivatives are zero

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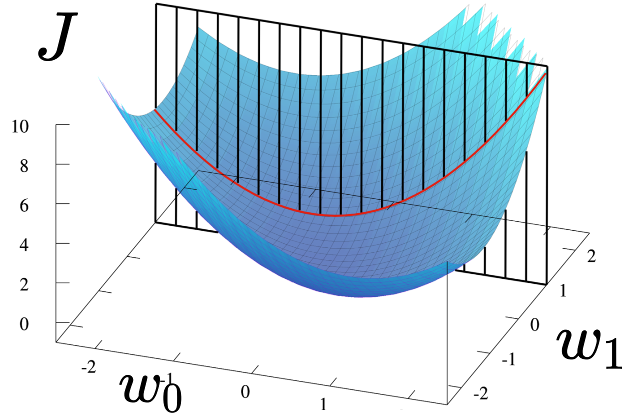
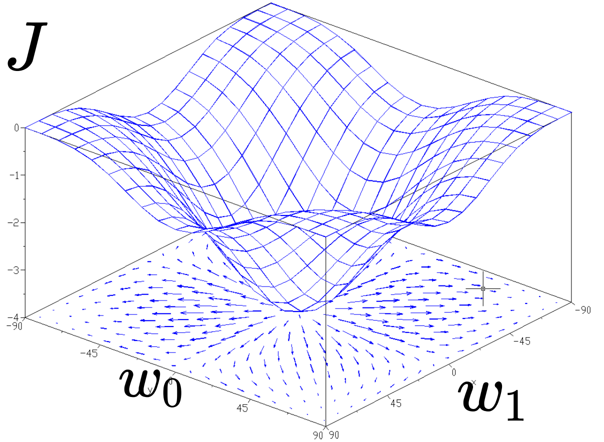
critical point: all partial derivatives are zero

gradient: vector of all partial derivatives

$$\nabla J(w) = [\frac{\partial}{\partial w_1} J(w), \cdots \frac{\partial}{\partial w_D} J(w)]^\top$$

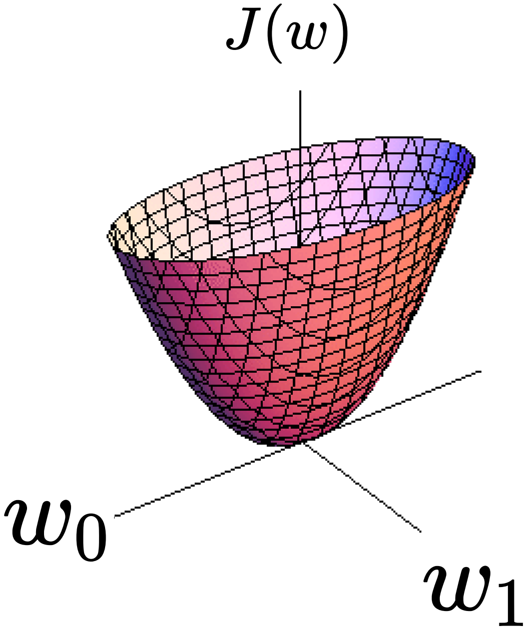




Finding w (any D)

setting $\frac{\partial}{\partial w_i} J(w) = 0$

$$\frac{\partial}{\partial w_i} \sum_n \frac{1}{2}(y^{(n)} - f_w(x^{(n)}))^2 = 0$$



cost is a smooth and convex function of w

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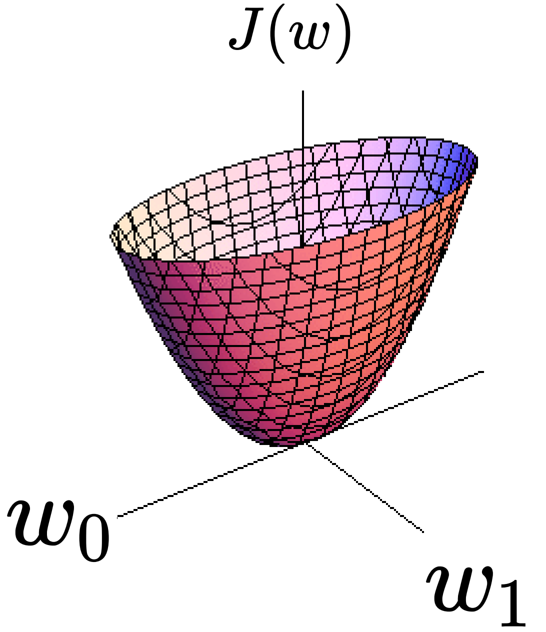

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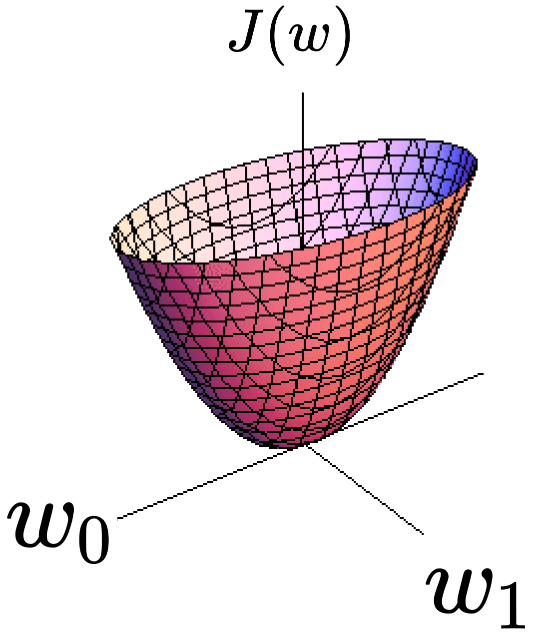

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using **chain rule**: $\frac{\partial J}{\partial w_i} = \frac{\mathrm{d}J}{\mathrm{d}f_w} \frac{\partial f_w}{\partial w_i}$

we get $\sum_n (w^\top x^{(n)} - y^{(n)}) x_d^{(n)} = 0 \quad \forall d \in \{1, \ldots, D\}$

Normal equation

system of D linear equations

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matrix form (using the design matrix)

each row enforces one of D equations

$$\overset{D \times N}{\overline{X^\top}} \overset{N \times 1}{\overline{(y - Xw)}} = \vec{0}$$

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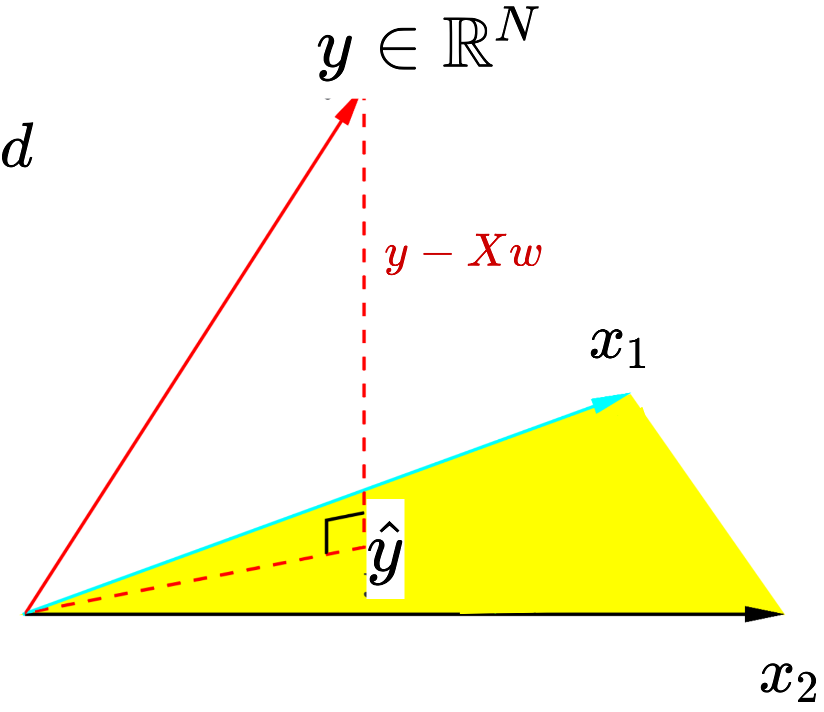

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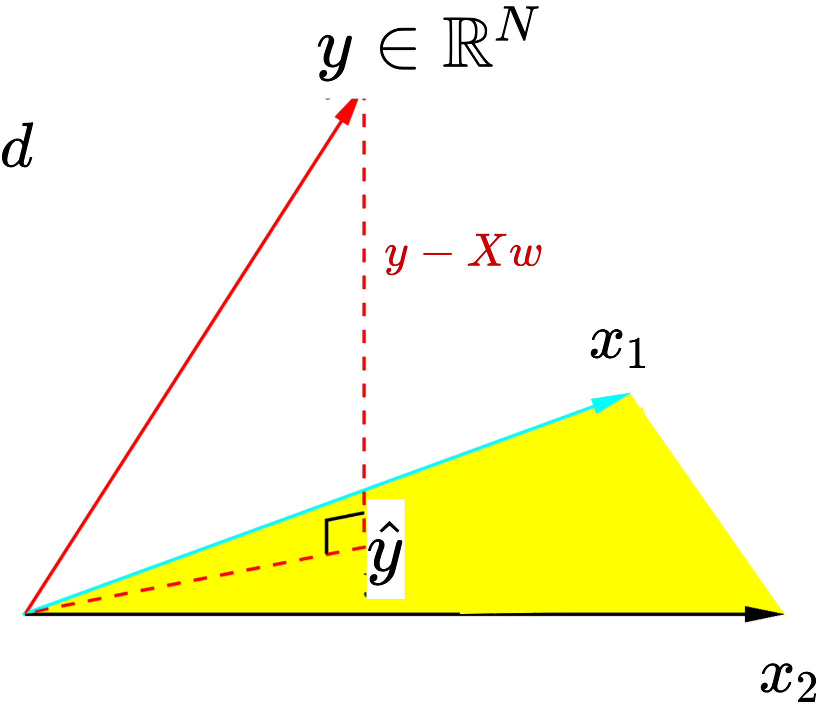
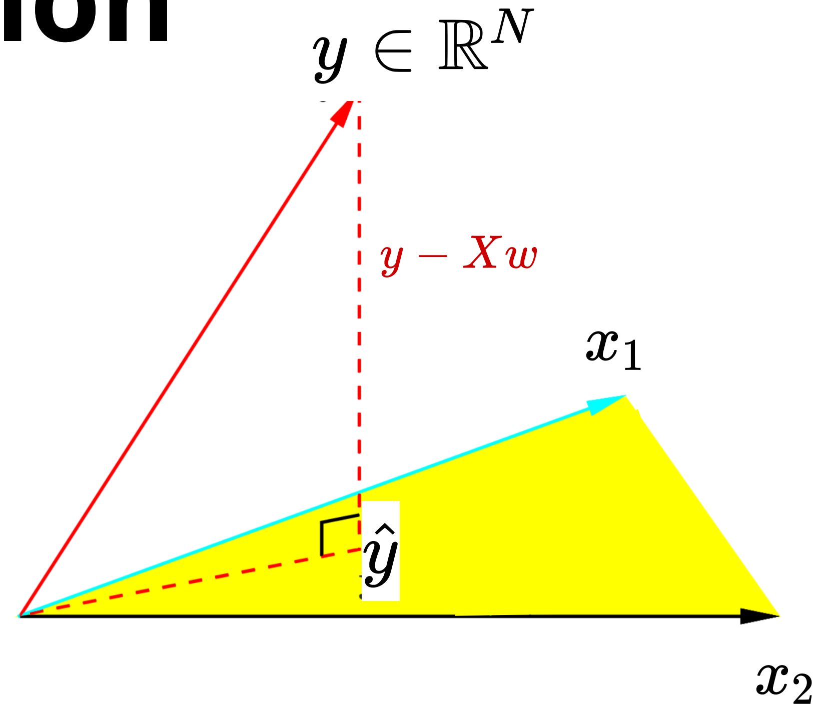


Normal equation: because for optimal w, the residual vector is normal to column space of the design matrix

Direct solution

we can get a closed form solution!



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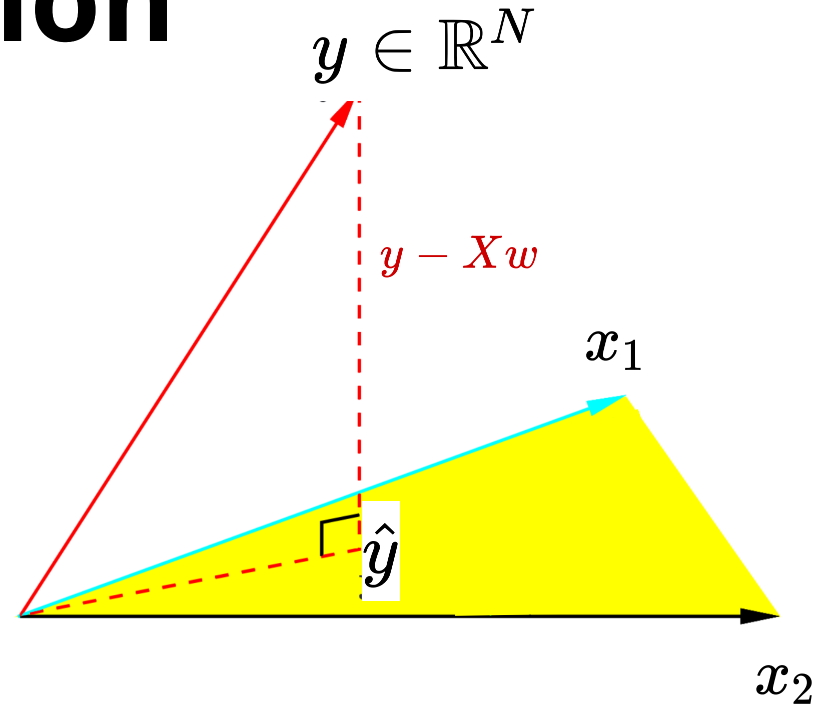

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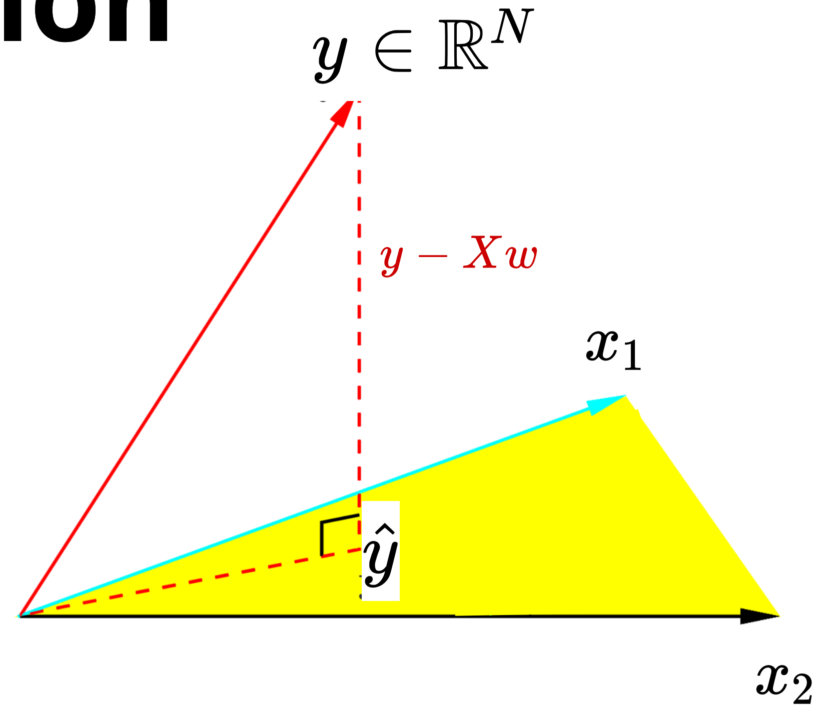

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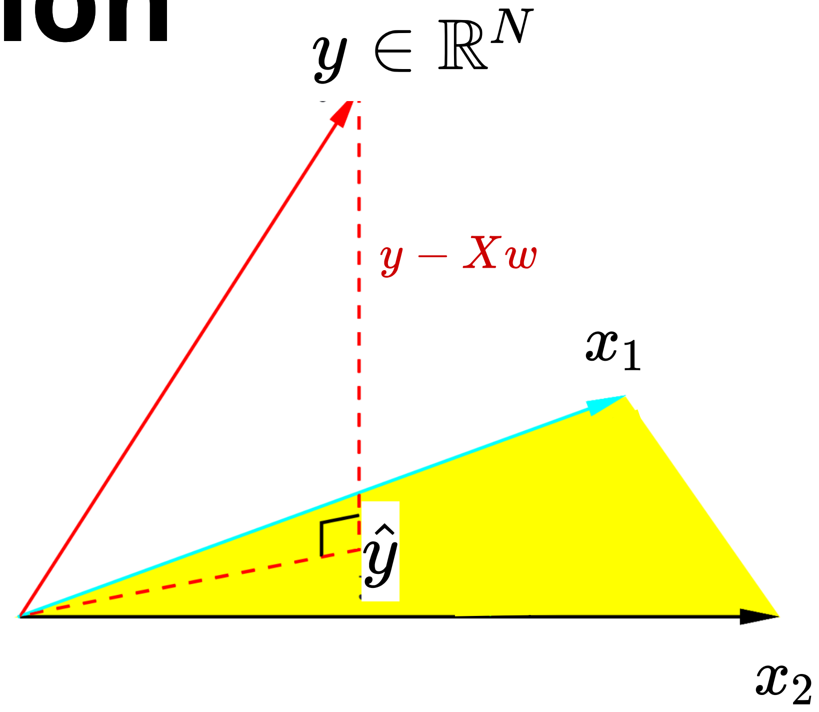

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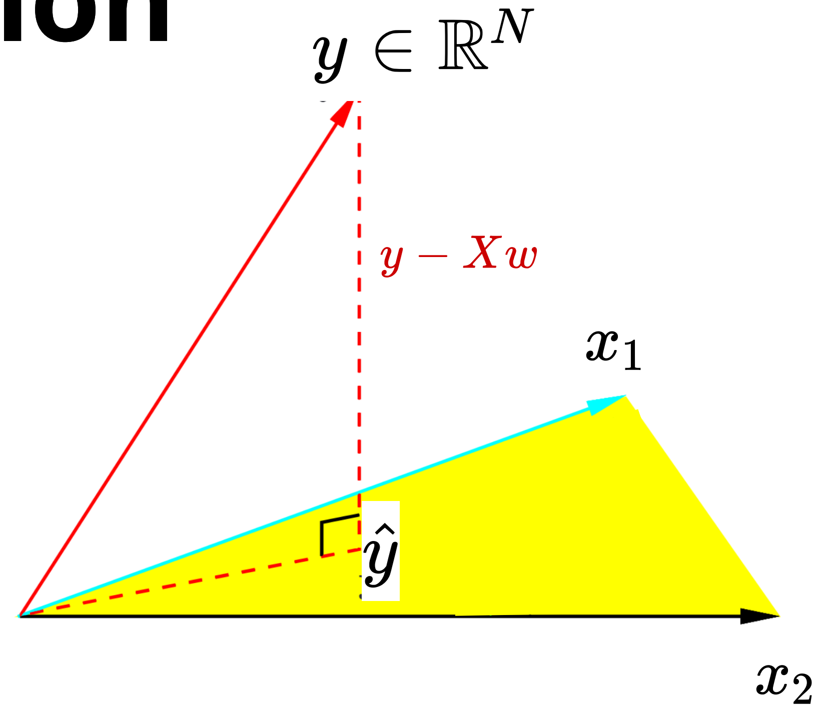

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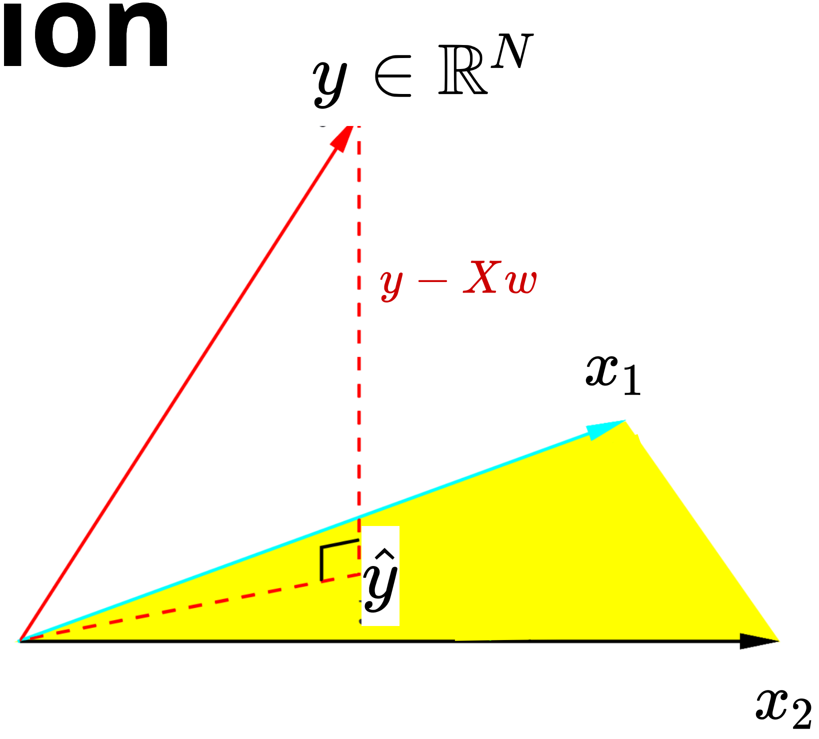

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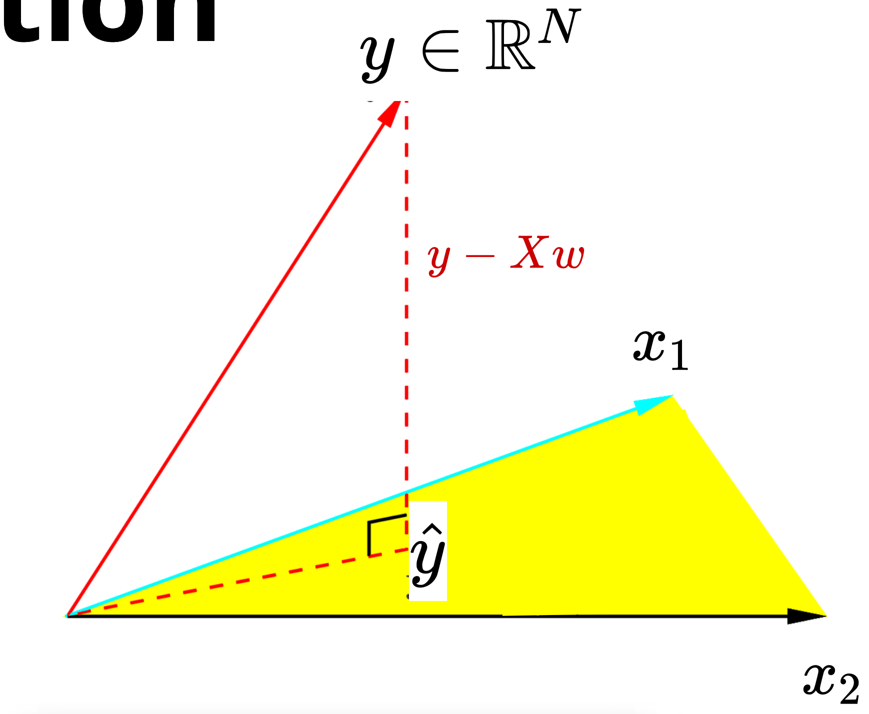

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total complexity for N > D is $\mathcal{O}(ND^2 + D^3)$

in practice we don't directly use matrix inversion (unstable)

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one instance

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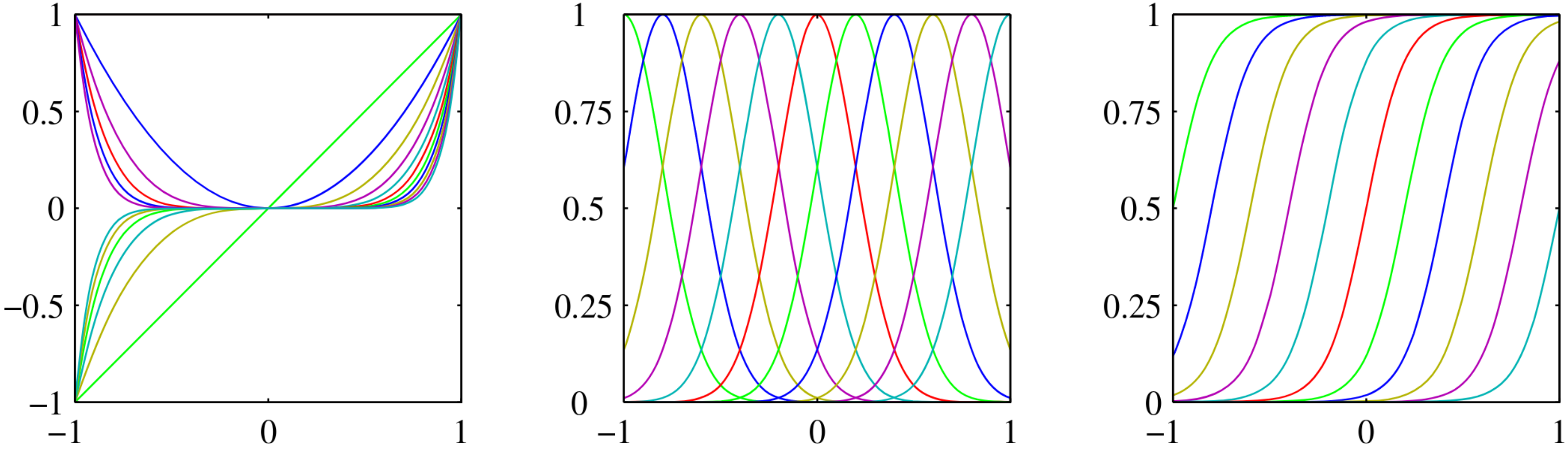

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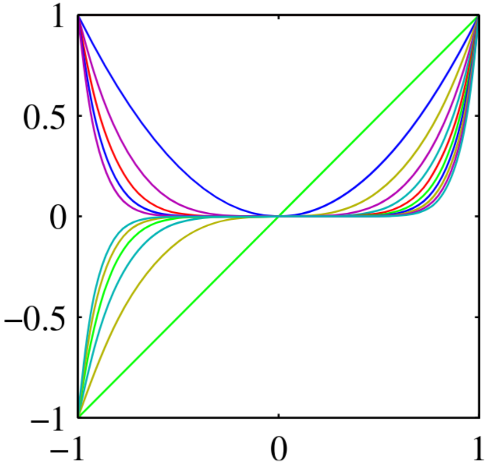

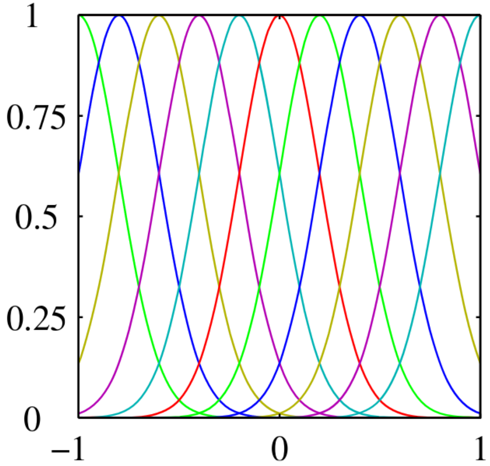

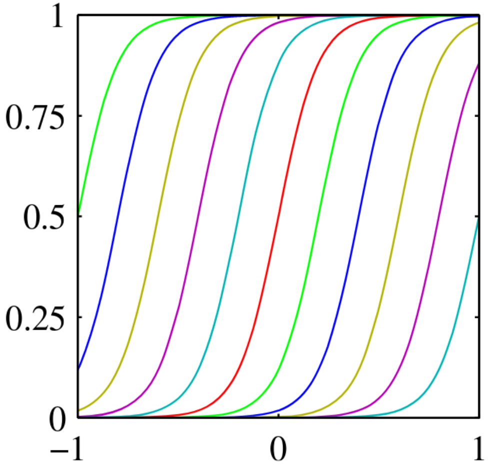

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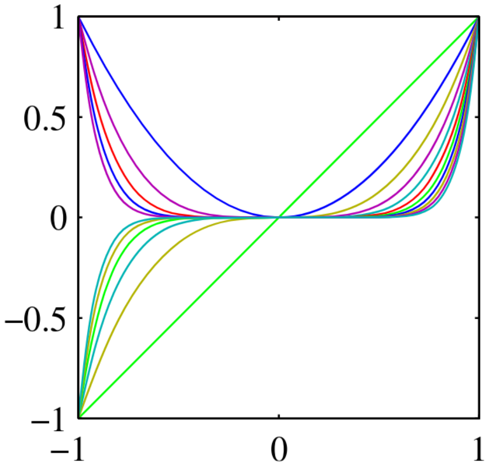

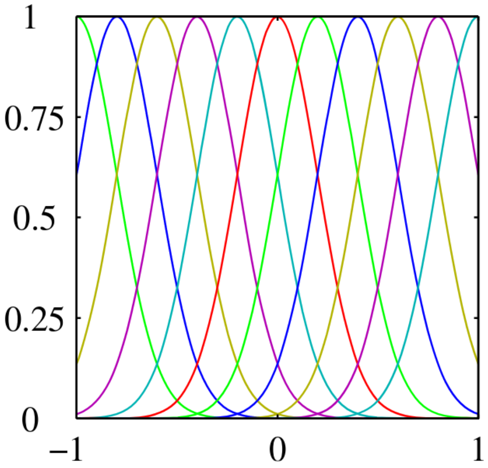

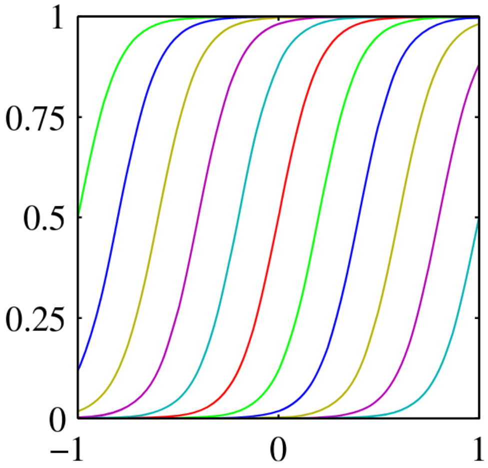

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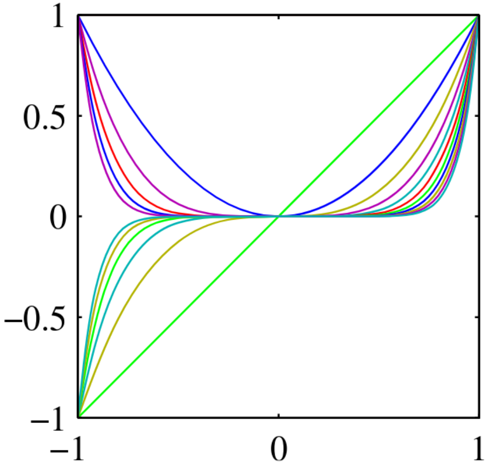

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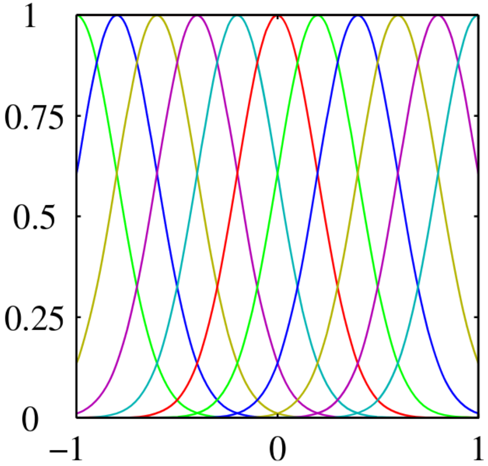

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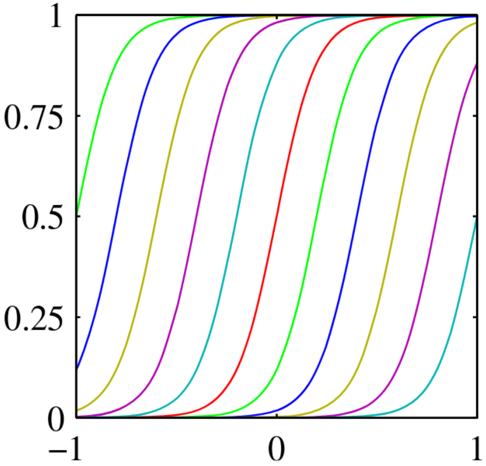

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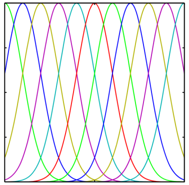

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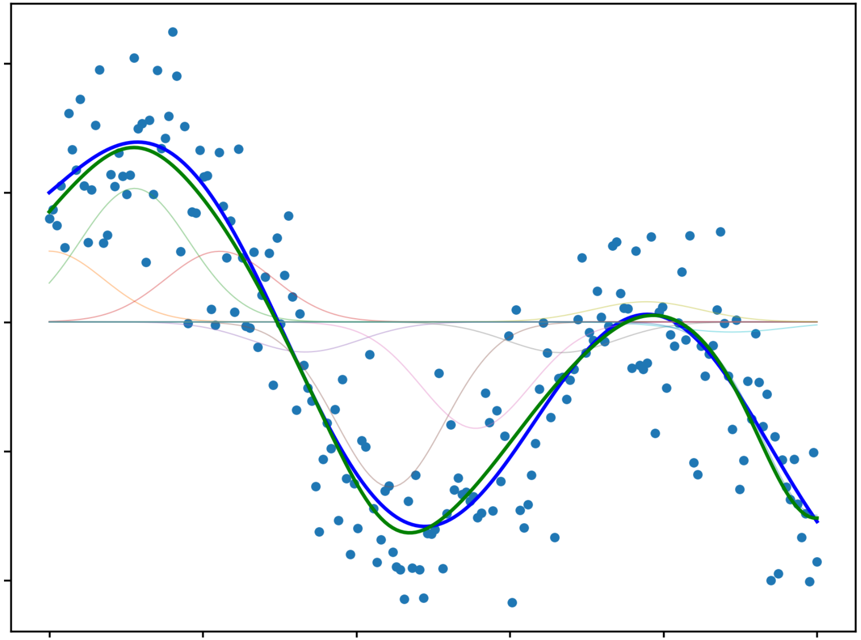

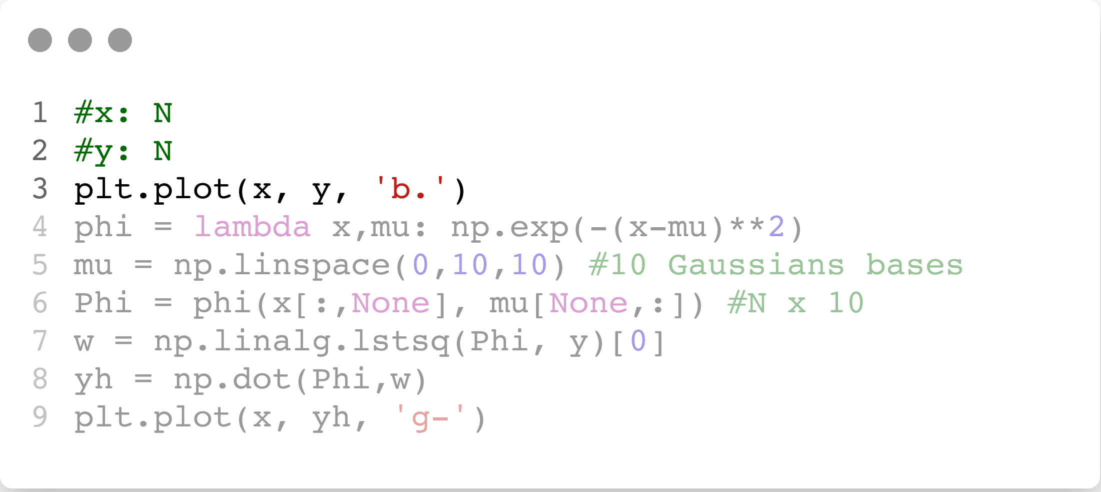

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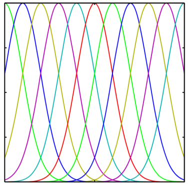

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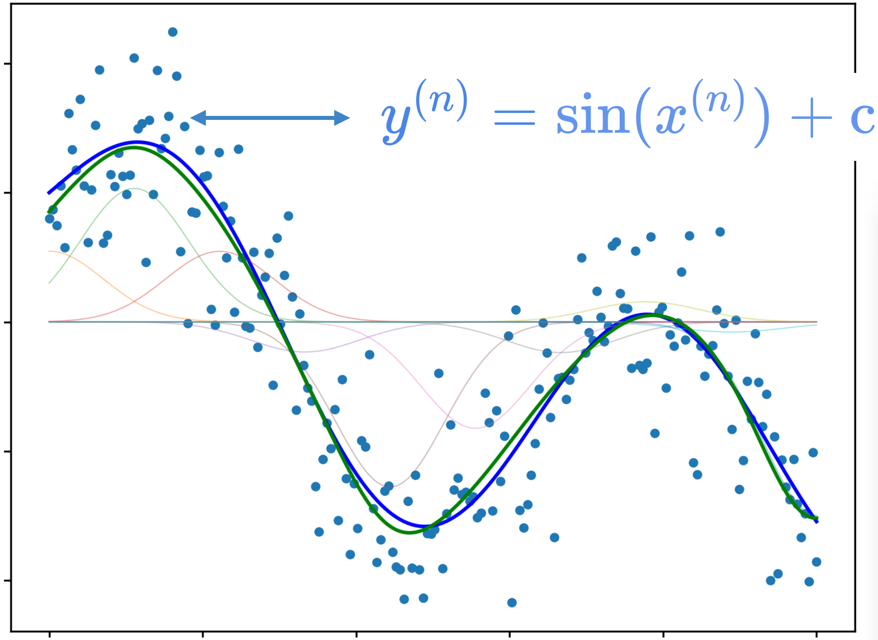

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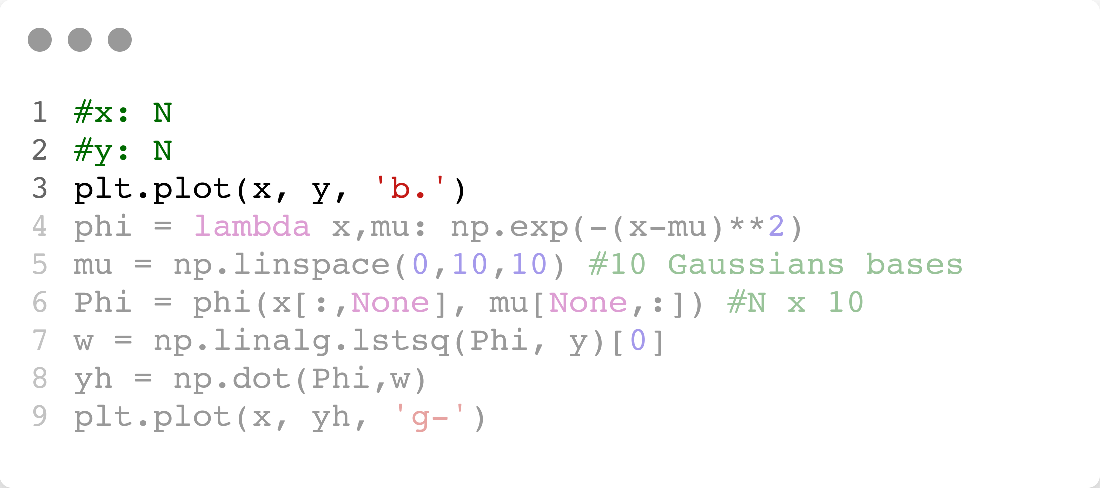

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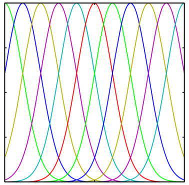

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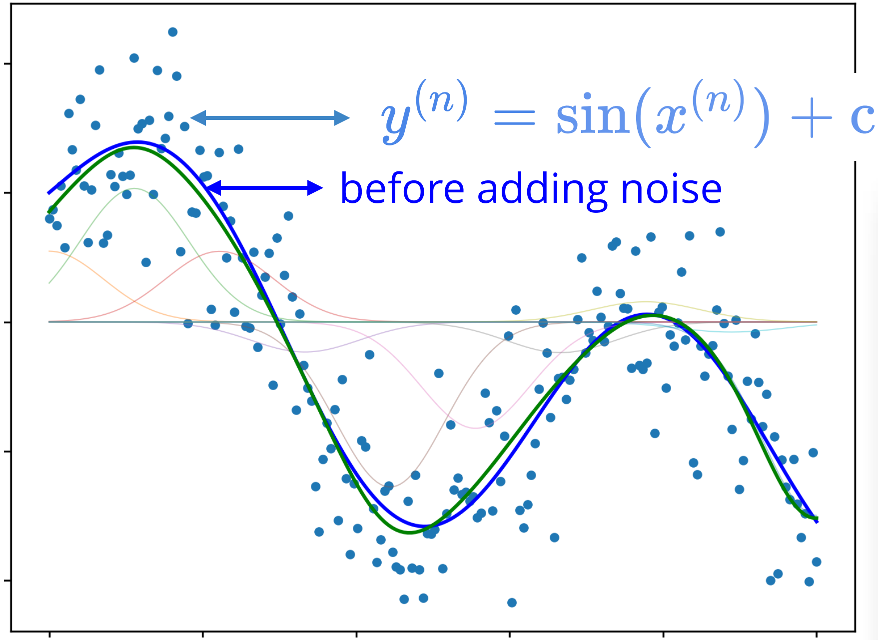

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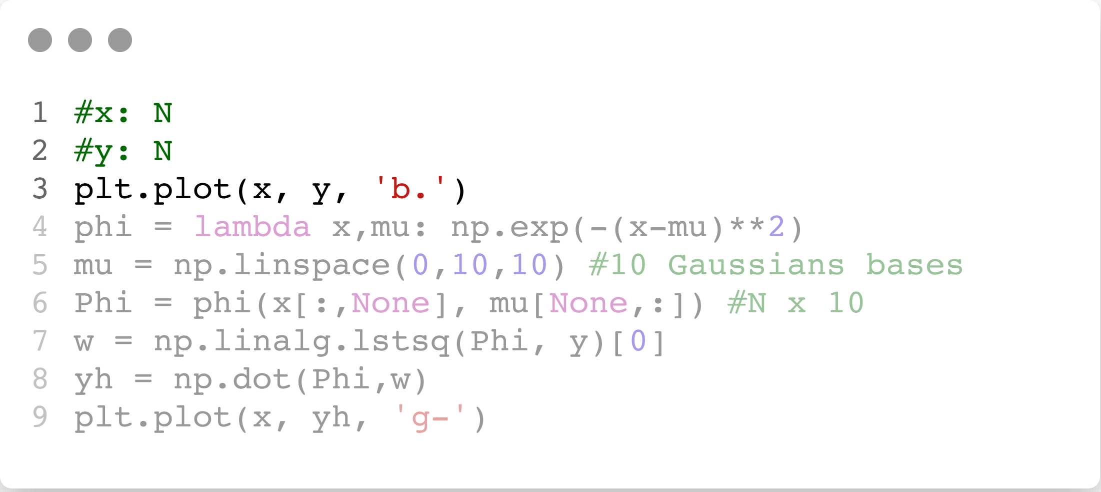

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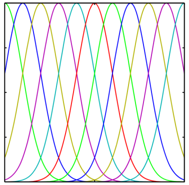

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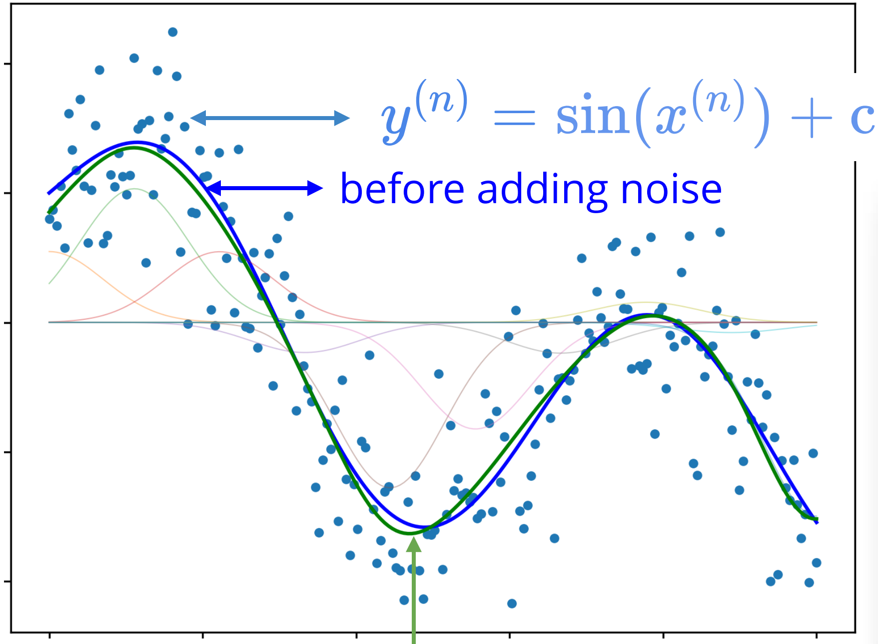

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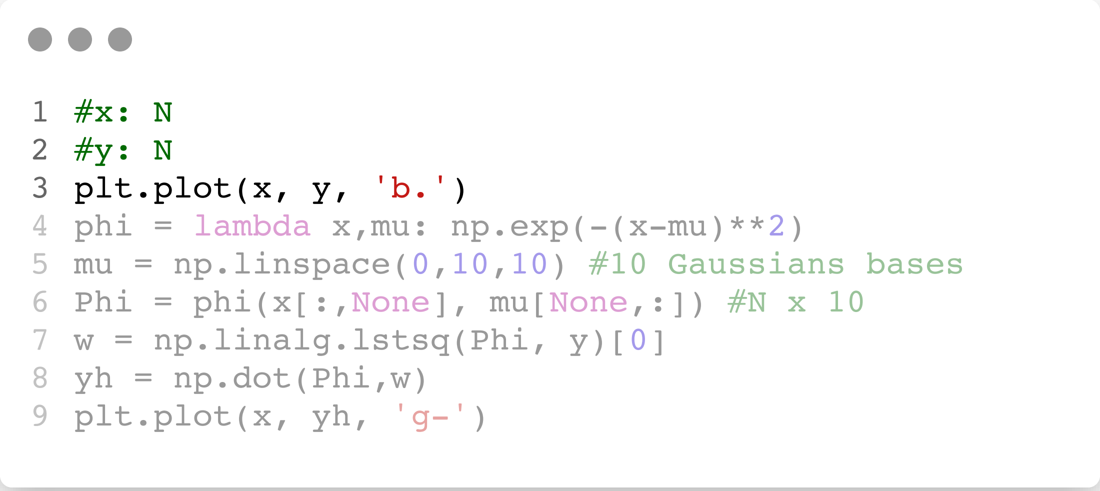

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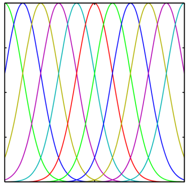

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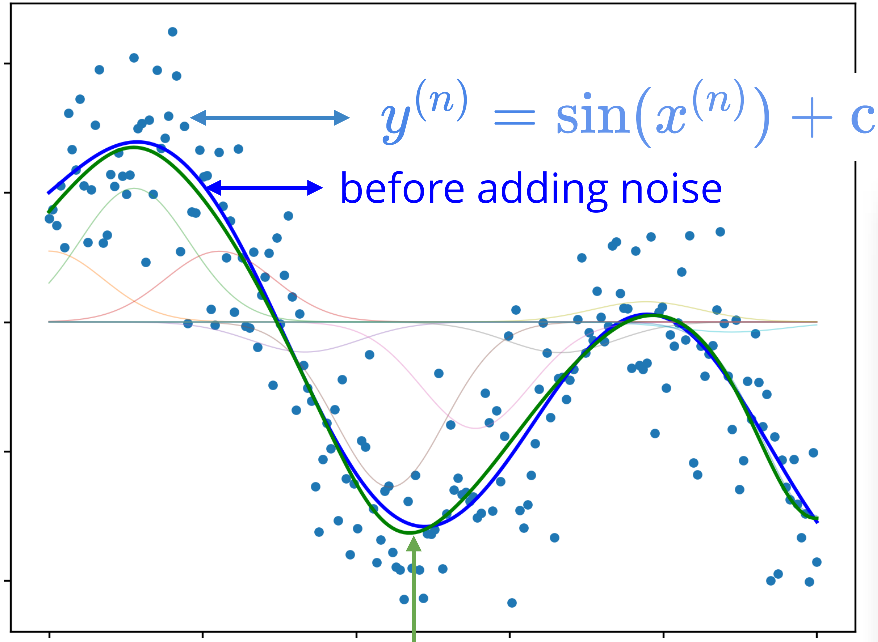

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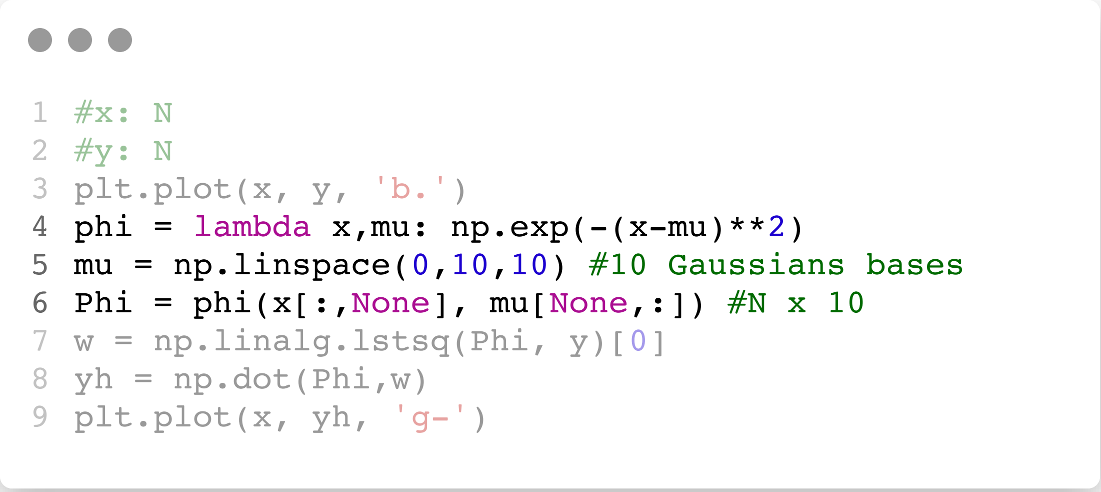

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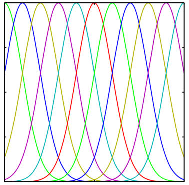

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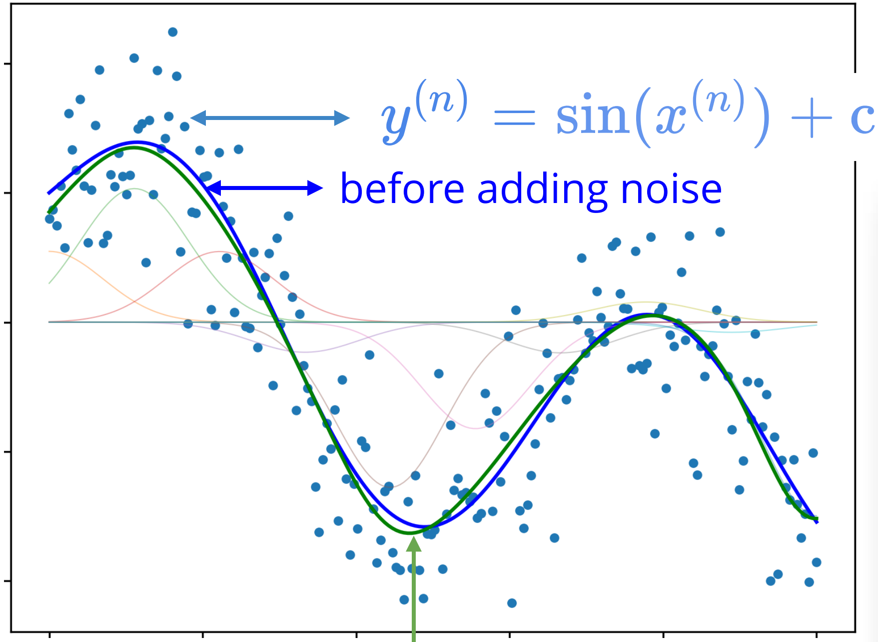

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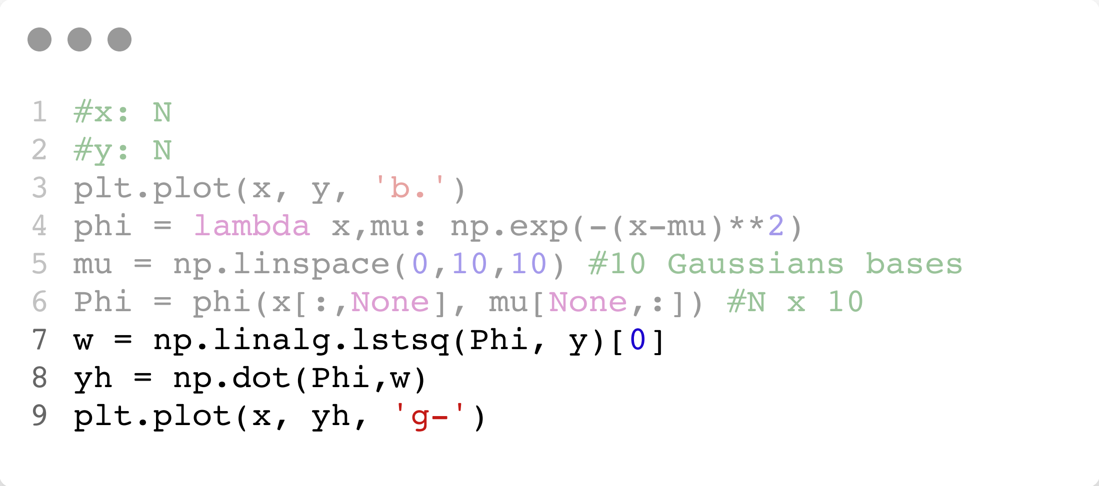

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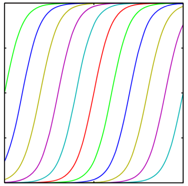

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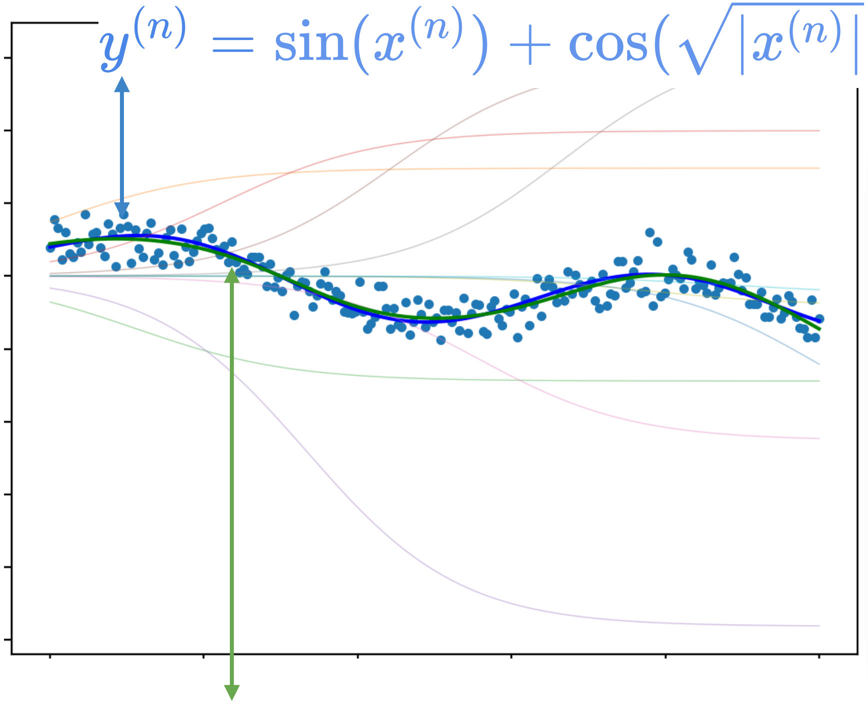

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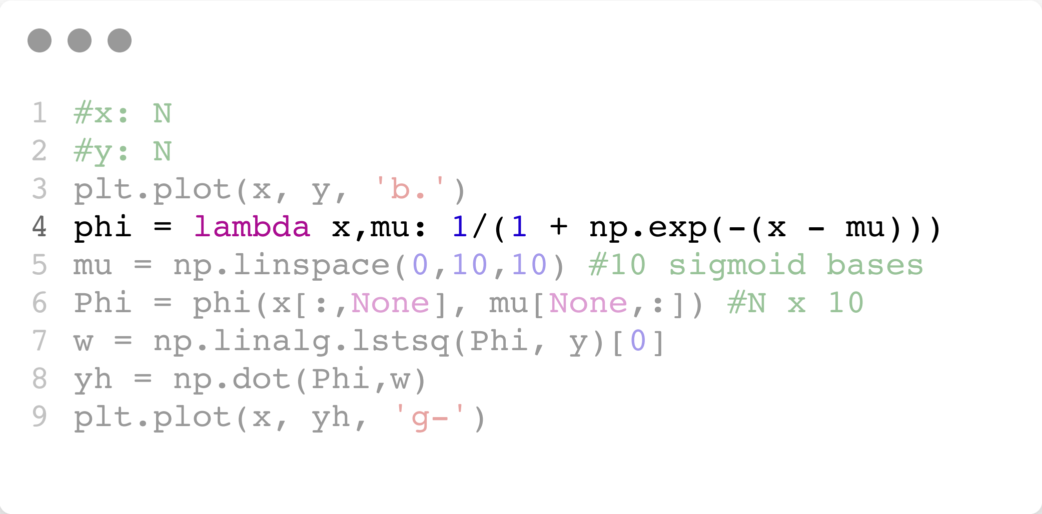

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plt.plot(x, y, 'b.')
phi = lambda x,mu: 1/(1 + np.exp(-(x - mu)))
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- W* is **not unique, make it unique** by
  - removing redundant features
  - regularization (later!)

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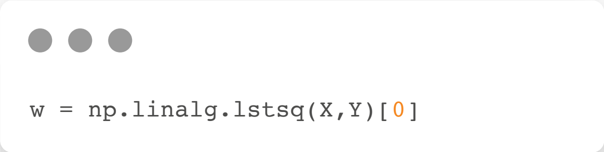
columns of X (features) are not linearly independent

(either redundant features or D > N)

- W* is **not unique, make it unique** by
  - removing redundant features
  - regularization (later!)

- **or find one** of the solutions
  - decomposition-based (not discussed) methods still work
  - use gradient descent (later!)



```
w = np.linalg.lstsq(X,Y)[0]
```

Summary

linear regression:

- models targets as a linear function of features
- fit the model by minimizing sum of squared errors
- has a direct solution with $\mathcal{O}(ND^2 + D^3)$ complexity
- gradient descent: future

we can build more expressive models:

- using any number of non-linear features
- ensure features are linearly independent