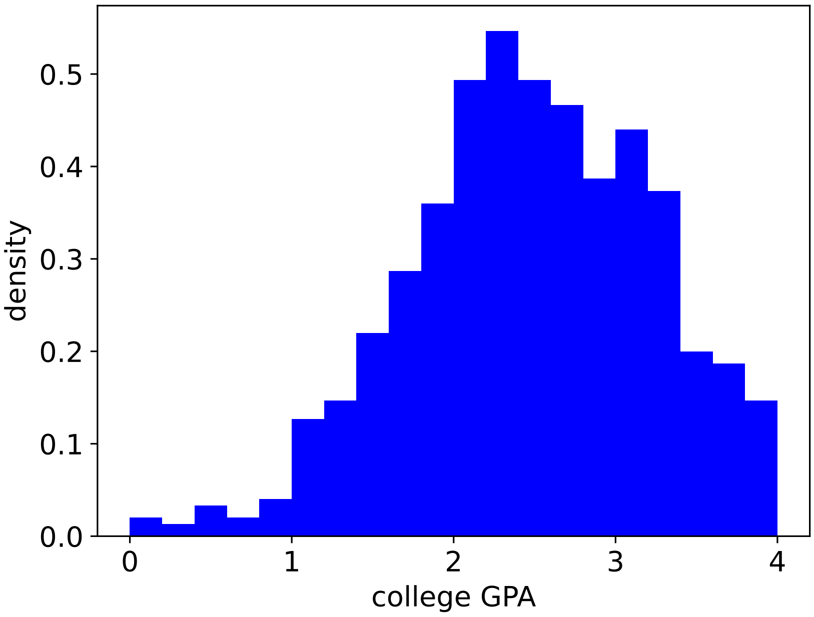
Linear regression

COMS 4771 Fall 2023

Dartmouth student dataset

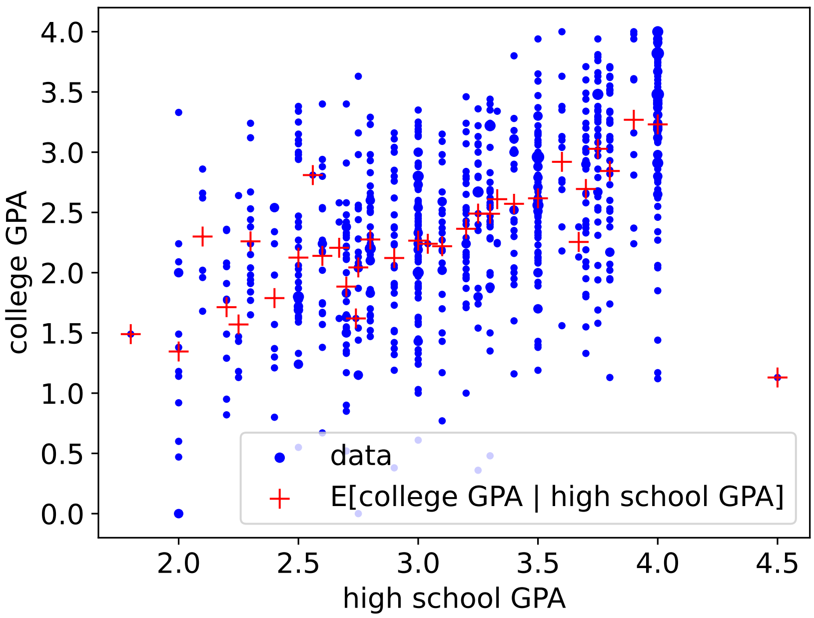
Dataset of 750 **Dartmouth students' (first-year) college GPA**[1]



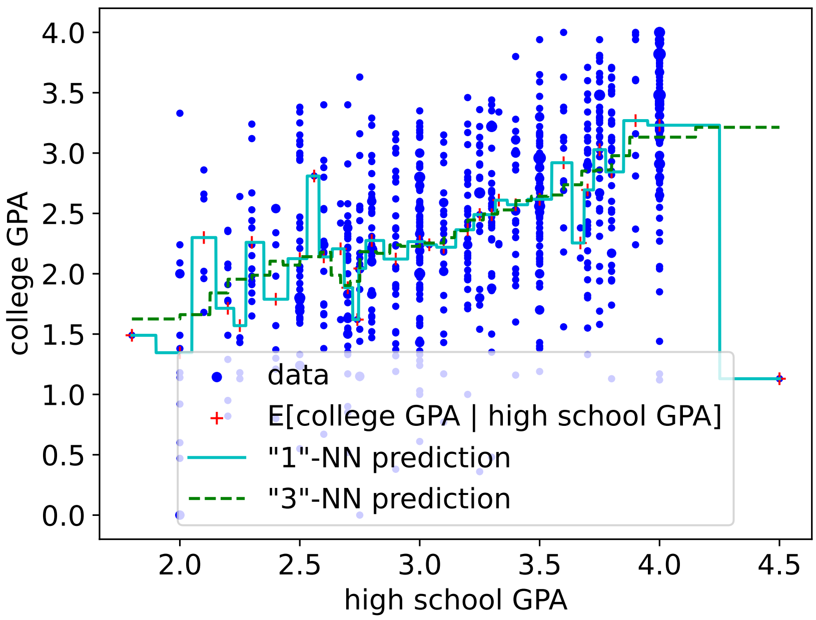
Mean 2.47
Standard deviation 0.75

[1] https://chance.dartmouth.edu/course/Syllabi/Princeton96/ETSValidation.html

Dartmouth dataset also has high school GPA of each student
Question: Is high school GPA predictive of college GPA?



Attempting to exploit "local regularity" using NN



Possible "global" modeling assumption:

- Increase in high school GPA by Δ should give an increase in (expected) college GPA by $\propto \Delta$

- In other words,

  $$\mathbb{E}[\text{college GPA} \mid \text{high school GPA}]$$

  is ________ function of high school GPA

Least squares linear regression

$f : \mathbb{R} \to \mathbb{R}$ is linear if it is of the form

$$f(x) = mx + b$$

for some parameters $m, b \in \mathbb{R}$

Problem: given a dataset $\mathcal{S}$ from $\mathbb{R} \times \mathbb{R}$, find (parameters of) a linear function $f(x) = mx + b$ of minimal sum of squared errors (SSE)

$$\mathrm{sse}[m, b] = \sum_{(x,y)\in\mathcal{S}} (mx + b - y)^2$$

Method of solution is called ordinary least squares (OLS)

Minimizers of SSE must be zeros of the two partial derivative functions:

$$\frac{\partial\,\mathrm{sse}}{\partial m}[m, b] = 2 \sum_{(x,y)\in\mathcal{S}} (mx + b - y)x = 0$$

$$\frac{\partial\,\mathrm{sse}}{\partial b}[m, b] = 2 \sum_{(x,y)\in\mathcal{S}} (mx + b - y) = 0$$

Two linear equations in two unknowns

Together, the equations are called the normal equations

Equivalent form:

$$\begin{aligned} \operatorname{avg}(x^2)\, m &+ \operatorname{avg}(x)\, b &= \operatorname{avg}(xy) \\ \operatorname{avg}(x)\, m &+ b &= \operatorname{avg}(y) \end{aligned}$$

where

$$\operatorname{avg}(x) = \frac{1}{|\mathcal{S}|} \sum_{(x,y)\in\mathcal{S}} x, \qquad \operatorname{avg}(x^2) = \frac{1}{|\mathcal{S}|} \sum_{(x,y)\in\mathcal{S}} x^2,$$

$$\operatorname{avg}(xy) = \frac{1}{|\mathcal{S}|} \sum_{(x,y)\in\mathcal{S}} xy, \qquad \operatorname{avg}(y) = \frac{1}{|\mathcal{S}|} \sum_{(x,y)\in\mathcal{S}} y$$

Solution to normal equations:

$$m = \frac{\operatorname{avg}(xy) - \operatorname{avg}(x) \cdot \operatorname{avg}(y)}{\operatorname{avg}(x^2) - \operatorname{avg}(x)^2},$$

$$b = \operatorname{avg}(y) - m \cdot \operatorname{avg}(x)$$

What if $\operatorname{avg}(x^2) = \operatorname{avg}(x)^2$?

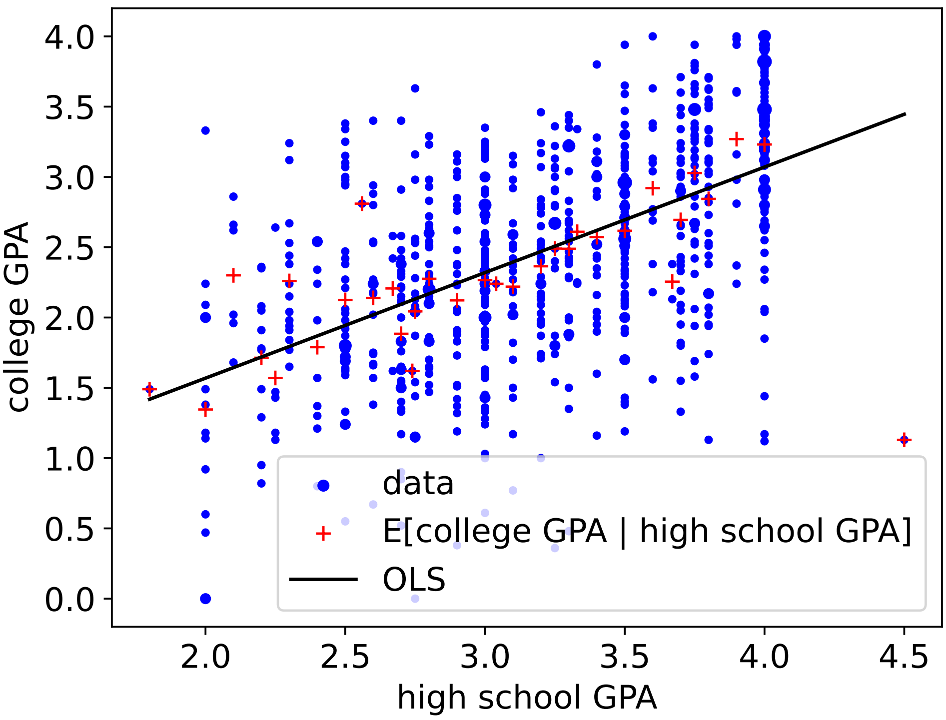
For Dartmouth dataset:

$$m = 0.751, \quad b = 0.067$$

RMSE:

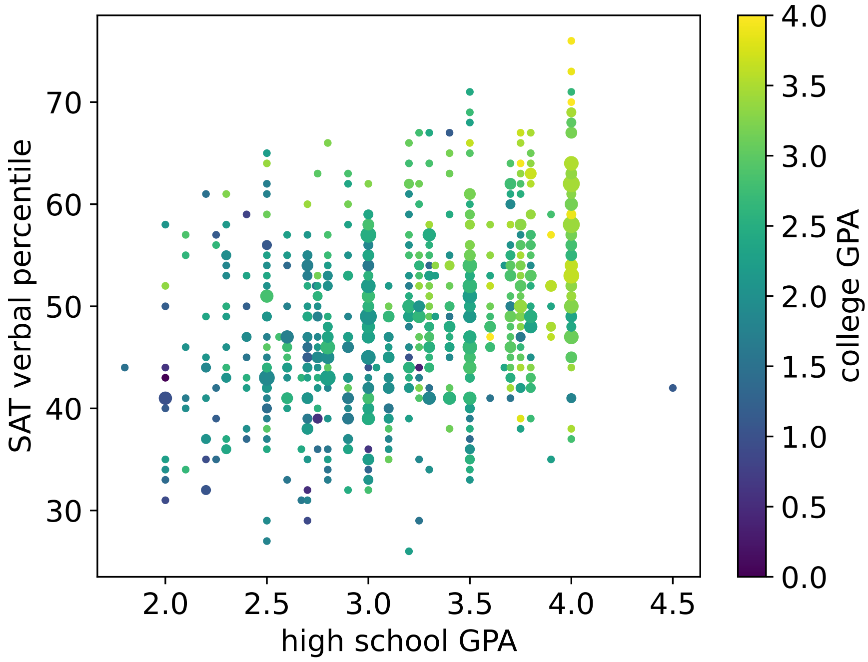
$$\sqrt{\frac{1}{|\mathcal{S}|}\operatorname{sse}[m, b; \mathcal{S}]} = 0.629$$

(Recall standard deviation of college GPA is 0.75)



Bivariate linear regression

Dartmouth dataset also includes SAT verbal percentiles



Linear function of two variables x_1 and x_2:

$$f(x_1, x_2) = m_1 x_1 + m_2 x_2 + b$$

Problem: given a dataset $\mathcal{S}$ from $\mathbb{R}^2 \times \mathbb{R}$, find (parameters of) a linear function $f(x_1, x_2) = m_1 x_1 + m_2 x_2 + b$ of minimal sum of squared errors

$$\mathrm{sse}[m, b; \mathcal{S}] = \sum_{(x_1, x_2, y) \in \mathcal{S}} (m_1 x_1 + m_2 x_2 + b - y)^2$$

Normal equations: three linear equations in three unknowns (m_1, m_2, b)

$$\begin{bmatrix} \mathrm{avg}(x_1^2) & \mathrm{avg}(x_1 x_2) & \mathrm{avg}(x_1) \\ \mathrm{avg}(x_2 x_1) & \mathrm{avg}(x_2^2) & \mathrm{avg}(x_2) \\ \mathrm{avg}(x_1) & \mathrm{avg}(x_2) & 1 \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \\ b \end{bmatrix} = \begin{bmatrix} \mathrm{avg}(x_1 y) \\ \mathrm{avg}(x_2 y) \\ \mathrm{avg}(y) \end{bmatrix}$$

Solve using elimination algorithm

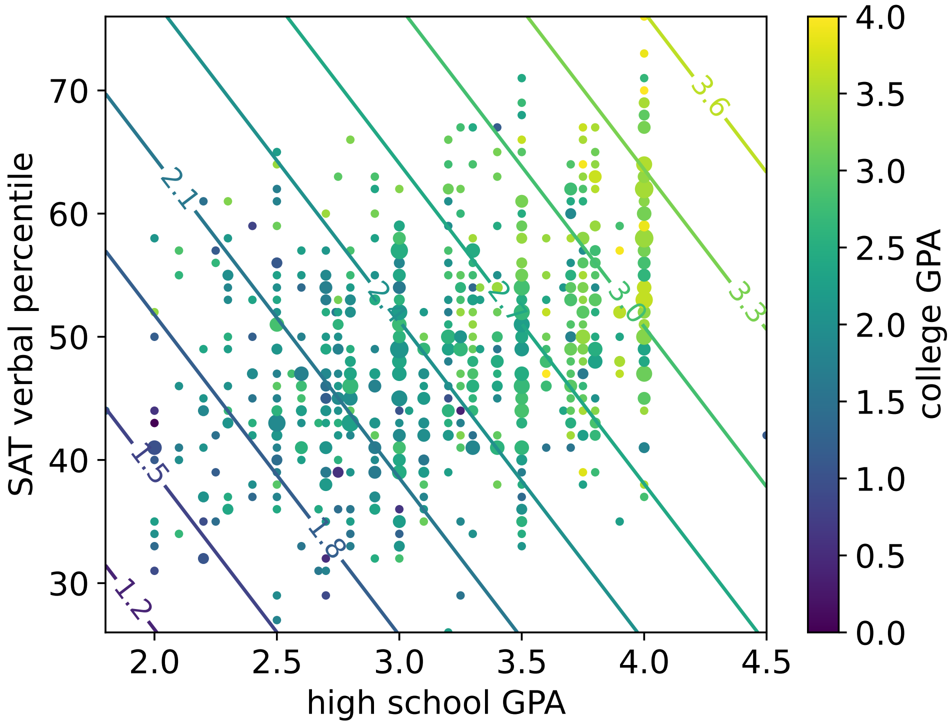
Dartmouth dataset: $x_1 =$ high school GPA, $x_2 =$ SAT verbal percentile

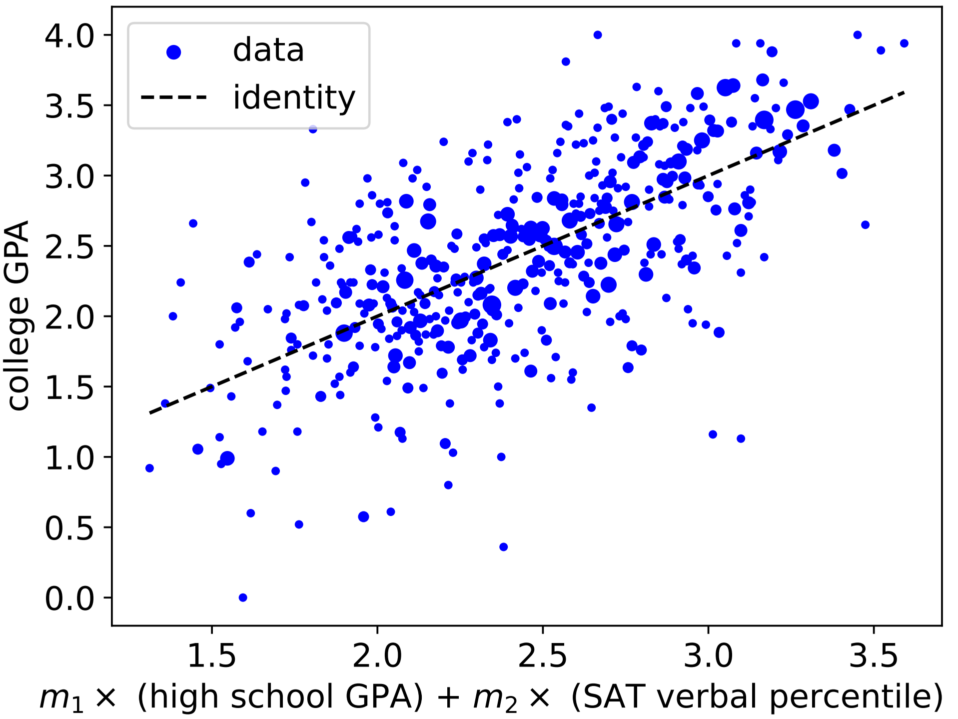
$$m_1 = 0.611, \quad m_2 = 0.024, \quad b = -0.639$$

RMSE:

$$\sqrt{\frac{1}{|\mathcal{S}|}\operatorname{sse}[m_1, m_2, b; \mathcal{S}]} = 0.603$$

(Recall standard deviation of college GPA is 0.75)





Linear algebra of ordinary least squares

(Homogeneous) linear function of d variables $x = (x_1, \ldots, x_d)$ is parameterize by d-dimensional weight vector $w = (w_1, \ldots, w_d)$:

$$f_w(x) = w^\mathsf{T} x$$

To handle inhomogeneous linear functions (i.e., affine functions), include an extra always-1 feature: $x_{d+1} = 1$

$$\begin{aligned} f_w(x) &= w^\mathsf{T} x \\ &= (w_1 x_1 + \cdots + w_d x_d) + \underline{\hspace{5em}} \end{aligned}$$

Problem: given a dataset $\mathcal{S}$ from $\mathbb{R}^d \times \mathbb{R}$, find $w \in \mathbb{R}^d$ of minimal sum of squared errors

$$\operatorname{sse}[w; \mathcal{S}] = \sum_{(x,y) \in \mathcal{S}} (w^\mathsf{T} x - y)^2$$

Method of solution: OLS

Matrix notation: let $\mathcal{S} = ((x^{(i)}, y^{(i)}))_{i=1}^{n}$, and put

$$A = \begin{bmatrix} \longleftarrow & (x^{(1)})^\intercal & \longrightarrow \\ & \vdots & \\ \longleftarrow & (x^{(n)})^\intercal & \longrightarrow \end{bmatrix}, \quad b = \begin{bmatrix} y^{(1)} \\ \vdots \\ y^{(n)} \end{bmatrix}$$

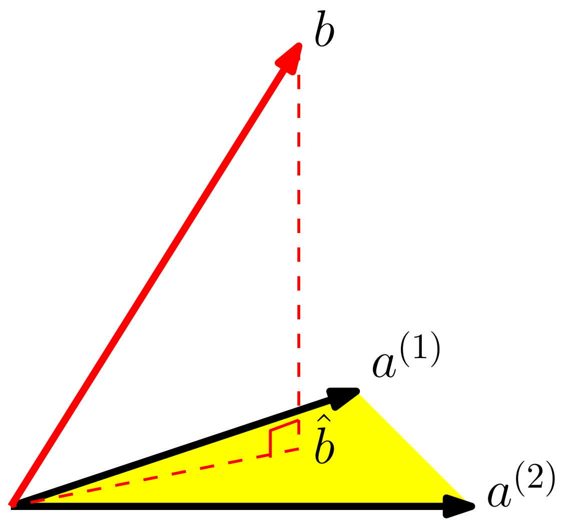
so

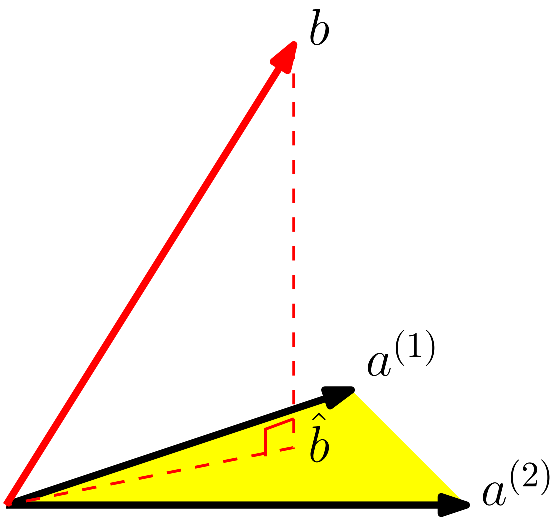
$$Aw = \begin{bmatrix} w^\intercal x^{(1)} \\ \vdots \\ w^\intercal x^{(n)} \end{bmatrix}, \quad Aw - b = \begin{bmatrix} w^\intercal x^{(1)} - y^{(1)} \\ \vdots \\ w^\intercal x^{(n)} - y^{(n)} \end{bmatrix}$$

Therefore

$$\|Aw - b\|^2 = \sum_{i=1}^{n} \underline{\hspace{4cm}}$$

$Aw \in \mathsf{CS}(A)$ for every $w \in \mathbb{R}^d$





How many ways to write $\hat{b}$ as a linear combination of the columns of A?

Normal equations in matrix notation

Key fact: CS(A) and NS($A^\intercal$) are orthogonal complements

Summary:

- Normal equations: $(A^\intercal A)w = A^\intercal b$
- If $\operatorname{rank}(A) = d$, then solution is unique
- Else, infinitely-many solutions
- Common choice for tie-breaking: minimum norm solution

$$\arg\min_{w \in \mathbb{R}^d} \|w\| \text{ s.t. } (A^\intercal A)w = A^\intercal b$$


```
def learn(train_x, train_y):
  return np.linalg.pinv(train_x).dot(train_y)

def predict(params, test_x):
  return test_x.dot(params)
```

Statistical view of ordinary least squares

Normal linear regression model: Conditional distribution of Y given $X = x$ is

$$\mathrm{N}(w^\intercal x, \sigma^2)$$

- w and σ^2 are parameters of the model
- In this model, best possible MSE is σ^2

MLE in normal linear regression model

- Likelihood of w and σ^2:

$$L(w, \sigma^2) = \prod_{(x,y) \in \mathcal{S}} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y - w^\intercal x)^2}{2\sigma^2}\right)$$

- Log-likelihood:

$$\ln L(w, \sigma^2) = -\frac{1}{2\sigma^2} \sum_{(x,y) \in \mathcal{S}} (y - w^\intercal x)^2 - \frac{|\mathcal{S}|}{2} \ln(2\pi\sigma^2)$$

- In terms of w, maximizing log-likelihood is same as minimizing SSE!

Statistical inference (example)

- Suppose you fit linear regression model to data, and find that $w \neq (0, \dots, 0)$

  How confident are you in this finding?

Generalization

- Suppose $\mathcal{S} \overset{\text{i.i.d.}}{\sim} (X, Y)$
- OLS gives minimizer of empirical risk (for square loss, among linear functions)

$$\widehat{\text{Risk}}[w] = \frac{1}{n} \sum_{(x,y) \in \mathcal{S}} \text{loss}_{\text{sq}}(w^{\top} x, y)$$

  But we actually care about the (true) risk

$$\text{Risk}[w] = \mathbb{E}[\text{loss}_{\text{sq}}(w^{\top} X, Y)]$$

- Is empirical risk a good estimate of (true) risk?
  - Usually only if $|\mathcal{S}|$ is sufficiently large

Extreme example: $d = 1$, $|\mathcal{S}| = 2$, $\widehat{\mathrm{Risk}}[w] = 0$