# Reinforcement Learning
# Intelligent Systems Series

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# Lecture 1: Supervised learning Regression

- Linear Regression
- Regularization
- Model Evaluation and Model Selection
- Nonlinear Regression
- Robust Regression

Given this data:

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| **value** | 5.88 | 8.28 | 2.91 | 0.87 | 10.72 | 6.16 | 7.64 | 3.46 | 1.23 | 1.36 |
| **outcome** | 3.35 | 8.30 | 1.52 | 1.43 | 7.81 | 4.64 | 7.27 | 4.26 | 3.85 | 0.10 |

How to fit a model that can predict future outcomes?

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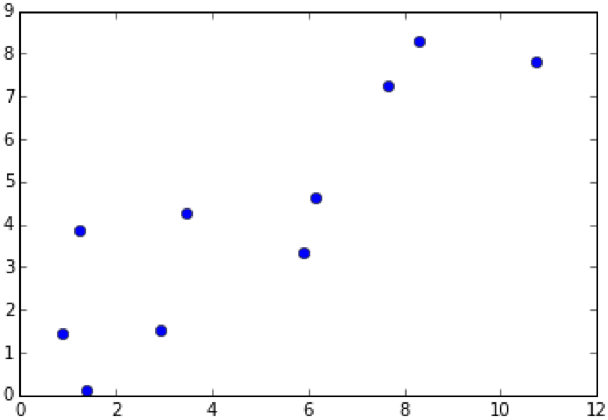


Looks more or less straight...

Data: *black board*

| $x_i$ | 5.88 | 8.28 | 2.91 | 0.87 | 10.72 | 6.16 | 7.64 | 3.46 | 1.23 | 1.36 |
|---|---|---|---|---|---|---|---|---|---|---|
| $y_i$ | 3.35 | 8.30 | 1.52 | 1.43 | 7.81 | 4.64 | 7.27 | 4.26 | 3.85 | 0.10 |

Let's fit a linear model: $f(x) = ax$ for unknown $a \in \mathbb{R}$.

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How to choose $a$? Least squares criterion: $\mathbf{min}_{a \in \mathbb{R}} \sum_{i=1}^{n} (ax_i - y_i)^2$

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| $x_i$ | 5.88 | 8.28 | 2.91 | 0.87 | 10.72 | 6.16 | 7.64 | 3.46 | 1.23 | 1.36 |
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To find minimum, compute derivative:

$$\frac{d}{da}\sum_{i=1}^{n}(ax_i - y_i)^2 = 2\sum_i x_i(ax_i - y_i) = 2a\sum_i (x_i)^2 - 2\sum_i x_i y_i$$

Set derivative to $0$ and solve for $a$:

$$a = \frac{\sum_i x_i y_i}{\sum_i (x_i)^2} = \frac{281.56}{339.06} = 0.83 \qquad \rightarrow \qquad f(x) = 0.83x$$

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| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| $x_i$ | 5.88 | 8.28 | 2.91 | 0.87 | 10.72 | 6.16 | 7.64 | 3.46 | 1.23 | 1.36 |
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What else could we have done?

Since we want $f(x) \approx y$ for $f(x) = ax$. Since $a = \frac{f(x)}{x}$, how about

$$\min_a \sum_{i=1}^{n} \left(a - \frac{y_i}{x_i}\right)^2$$

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|---|---|---|---|---|---|---|---|---|---|---|
| $y_i$ | 3.35 | 8.30 | 1.52 | 1.43 | 7.81 | 4.64 | 7.27 | 4.26 | 3.85 | 0.10 |
| $y_i/x_i$ | 0.57 | 1.00 | 0.52 | 1.64 | 0.73 | 0.75 | 0.95 | 1.23 | 3.12 | 0.07 |

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Arithmetic mean of ratios? Maybe rather geometric mean:

$$a = \sqrt[n]{\prod_i \frac{y_i}{x_i}} \quad = 0.77$$

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Arithmetic mean of ratios? Maybe rather geometric mean:

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Something completely different: piecewise linear?

Data:

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
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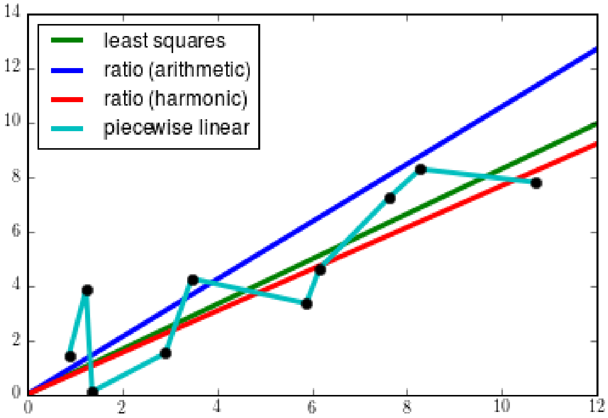

Data:

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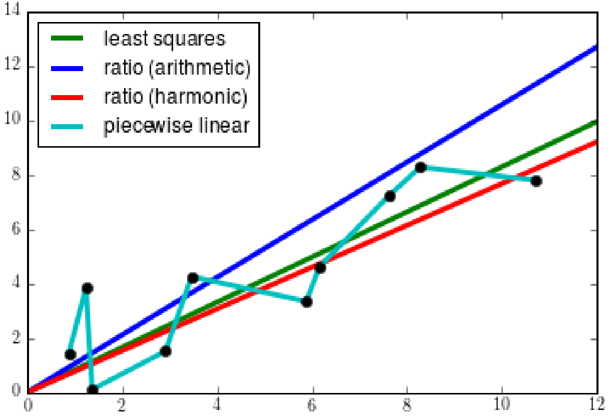


Visual inspection: least squares (green) might be best...

# Real data is large and high-dimensional: Boston housing dataset

| $x \in \mathbb{R}^{13}$ | | | | | | | | | | | | | $y$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0.01 | 18.00 | 2.31 | 0.00 | 0.54 | 6.58 | 65.20 | 4.09 | 1.00 | 296.00 | 15.30 | 396.90 | 4.98 | 24.00 |
| 0.03 | 0.00 | 7.07 | 0.00 | 0.47 | 6.42 | 78.90 | 4.97 | 2.00 | 242.00 | 17.80 | 396.90 | 9.14 | 21.60 |
| 0.03 | 0.00 | 7.07 | 0.00 | 0.47 | 7.18 | 61.10 | 4.97 | 2.00 | 242.00 | 17.80 | 392.83 | 4.03 | 34.70 |
| 0.03 | 0.00 | 2.18 | 0.00 | 0.46 | 7.00 | 45.80 | 6.06 | 3.00 | 222.00 | 18.70 | 394.63 | 2.94 | 33.40 |
| 0.07 | 0.00 | 2.18 | 0.00 | 0.46 | 7.15 | 54.20 | 6.06 | 3.00 | 222.00 | 18.70 | 396.90 | 5.33 | 36.20 |
| 0.03 | 0.00 | 2.18 | 0.00 | 0.46 | 6.43 | 58.70 | 6.06 | 3.00 | 222.00 | 18.70 | 394.12 | 5.21 | 28.70 |
| 0.09 | 12.50 | 7.87 | 0.00 | 0.52 | 6.01 | 66.60 | 5.56 | 5.00 | 311.00 | 15.20 | 395.60 | 12.43 | 22.90 |
| 0.14 | 12.50 | 7.87 | 0.00 | 0.52 | 6.17 | 96.10 | 5.95 | 5.00 | 311.00 | 15.20 | 396.90 | 19.15 | 27.10 |
| 0.21 | 12.50 | 7.87 | 0.00 | 0.52 | 5.63 | 100.00 | 6.08 | 5.00 | 311.00 | 15.20 | 386.63 | 29.93 | 16.50 |
| 0.17 | 12.50 | 7.87 | 0.00 | 0.52 | 6.00 | 85.90 | 6.59 | 5.00 | 311.00 | 15.20 | 386.71 | 17.10 | 18.90 |
| 0.22 | 12.50 | 7.87 | 0.00 | 0.52 | 6.38 | 94.30 | 6.35 | 5.00 | 311.00 | 15.20 | 392.52 | 20.45 | 15.00 |
| 0.12 | 12.50 | 7.87 | 0.00 | 0.52 | 6.01 | 82.90 | 6.23 | 5.00 | 311.00 | 15.20 | 396.90 | 13.27 | 18.90 |
| 0.09 | 12.50 | 7.87 | 0.00 | 0.52 | 5.89 | 39.00 | 5.45 | 5.00 | 311.00 | 15.20 | 390.50 | 15.71 | 21.70 |
| 0.63 | 0.00 | 8.14 | 0.00 | 0.54 | 5.95 | 61.80 | 4.71 | 4.00 | 307.00 | 21.00 | 396.90 | 8.26 | 20.40 |
| 0.64 | 0.00 | 8.14 | 0.00 | 0.54 | 6.10 | 84.50 | 4.46 | 4.00 | 307.00 | 21.00 | 380.02 | 10.26 | 18.20 |
| 0.63 | 0.00 | 8.14 | 0.00 | 0.54 | 5.83 | 56.50 | 4.50 | 4.00 | 307.00 | 21.00 | 395.62 | 8.47 | 19.90 |
| 1.05 | 0.00 | 8.14 | 0.00 | 0.54 | 5.93 | 29.30 | 4.50 | 4.00 | 307.00 | 21.00 | 386.85 | 6.58 | 23.10 |
| 0.78 | 0.00 | 8.14 | 0.00 | 0.54 | 5.99 | 81.70 | 4.26 | 4.00 | 307.00 | 21.00 | 386.75 | 14.67 | 17.50 |
| 0.80 | 0.00 | 8.14 | 0.00 | 0.54 | 5.46 | 36.60 | 3.80 | 4.00 | 307.00 | 21.00 | 288.99 | 11.69 | 20.20 |
| 0.73 | 0.00 | 8.14 | 0.00 | 0.54 | 5.73 | 69.50 | 3.80 | 4.00 | 307.00 | 21.00 | 390.95 | 11.28 | 18.20 |
| 1.25 | 0.00 | 8.14 | 0.00 | 0.54 | 5.57 | 98.10 | 3.80 | 4.00 | 307.00 | 21.00 | 376.57 | 21.02 | 13.60 |
| 0.85 | 0.00 | 8.14 | 0.00 | 0.54 | 5.96 | 89.20 | 4.01 | 4.00 | 307.00 | 21.00 | 392.53 | 13.83 | 19.60 |
| 1.23 | 0.00 | 8.14 | 0.00 | 0.54 | 6.14 | 91.70 | 3.98 | 4.00 | 307.00 | 21.00 | 396.90 | 18.72 | 15.20 |
| 0.99 | 0.00 | 8.14 | 0.00 | 0.54 | 5.81 | 100.00 | 4.10 | 4.00 | 307.00 | 21.00 | 394.54 | 19.88 | 14.50 |
| 0.75 | 0.00 | 8.14 | 0.00 | 0.54 | 5.92 | 94.10 | 4.40 | 4.00 | 307.00 | 21.00 | 394.33 | 16.30 | 15.60 |
| 0.84 | 0.00 | 8.14 | 0.00 | 0.54 | 5.60 | 85.70 | 4.45 | 4.00 | 307.00 | 21.00 | 303.42 | 16.51 | 13.90 |
| 0.67 | 0.00 | 8.14 | 0.00 | 0.54 | 5.81 | 90.30 | 4.68 | 4.00 | 307.00 | 21.00 | 376.88 | 14.81 | 16.60 |
| 0.96 | 0.00 | 8.14 | 0.00 | 0.54 | 6.05 | 88.80 | 4.45 | 4.00 | 307.00 | 21.00 | 306.38 | 17.28 | 14.80 |
| 0.77 | 0.00 | 8.14 | 0.00 | 0.54 | 6.50 | 94.40 | 4.45 | 4.00 | 307.00 | 21.00 | 387.94 | 12.80 | 18.40 |
| 1.00 | 0.00 | 8.14 | 0.00 | 0.54 | 6.67 | 87.30 | 4.24 | 4.00 | 307.00 | 21.00 | 380.23 | 11.98 | 21.00 |
| 1.13 | 0.00 | 8.14 | 0.00 | 0.54 | 5.71 | 94.10 | 4.23 | 4.00 | 307.00 | 21.00 | 360.17 | 22.60 | 12.70 |
| 1.35 | 0.00 | 8.14 | 0.00 | 0.54 | 6.07 | 100.00 | 4.17 | 4.00 | 307.00 | 21.00 | 376.73 | 13.04 | 14.50 |
| 1.39 | 0.00 | 8.14 | 0.00 | 0.54 | 5.95 | 82.00 | 3.99 | 4.00 | 307.00 | 21.00 | 232.60 | 27.71 | 13.20 |
| 1.15 | 0.00 | 8.14 | 0.00 | 0.54 | 5.70 | 95.00 | 3.79 | 4.00 | 307.00 | 21.00 | 358.77 | 18.35 | 13.10 |
| 1.61 | 0.00 | 8.14 | 0.00 | 0.54 | 6.10 | 96.90 | 3.76 | 4.00 | 307.00 | 21.00 | 248.31 | 20.34 | 13.50 |
| | | | | | | | ⋮ | | | | | | |
| 0.08 | 0.00 | 5.96 | 0.00 | 0.50 | 5.85 | 41.50 | 3.93 | 5.00 | 279.00 | 19.20 | 396.90 | 8.77 | 11.90 |

Given $(x_1, y_1), \dots, (x_n, y_n)$ with $x_i = (x_i^1, \dots, x_i^d) \in \mathbb{R}^d$ and $y_i \in \mathbb{R}$.*black board*

Linear model: $f(x) = w^\top x$ for $w^\top x = \sum_{j=1}^{d} w^j x^j$

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$$\text{Least squares:} \quad \min_{w \in \mathbb{R}^d} \mathcal{L}(w) \quad \text{with } \mathcal{L}(w) = \sum_i (w^\top x_i - y_i)^2$$

Given $(x_1, y_1), \dots, (x_n, y_n)$ with $x_i = (x_i^1, \dots, x_i^d) \in \mathbb{R}^d$ and $y_i \in \mathbb{R}$.*black board*

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$$\text{Least squares:} \quad \min_{w \in \mathbb{R}^d} \mathcal{L}(w) \quad \text{with } \mathcal{L}(w) = \sum_i (w^\top x_i - y_i)^2$$

$$\nabla_w \mathcal{L}(w) = 2 \sum_i x_i ({x_i}^\top w - y_i) = 2 \sum_i x_i {x_i}^\top w - 2 \sum_i x_i y_i$$

Setting the gradient to zero:

$$\underbrace{\sum_i x_i {x_i}^\top}_{\in \mathbb{R}^{d \times d}} w = \sum_i x_i y_i$$

We can solve for $w$ if $\sum_i x_i x_i$ is full rank (at least: $n \geq d$),

$$w = \Big( \sum_i x_i {x_i}^\top \Big)^{-1} \sum_i x_i y_i$$

In matrix notation: $X = \big(x_1|x_2|\dots|x_n\big) \in \mathbb{R}^{d\times n}$, $Y \in \mathbb{R}^n$, $w \in \mathbb{R}^d$.

Least squares: $\min\limits_{w\in\mathbb{R}^d} \mathcal{L}(w)$ with $\mathcal{L}(w) = \|X^\top w - Y\|^2$

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Least squares: $\min\limits_{w\in\mathbb{R}^d} \mathcal{L}(w)$ with $\mathcal{L}(w) = \|X^\top w - Y\|^2$

$$\nabla_w \mathcal{L}(w) = \nabla_w \big(w^\top X X^\top w - Y^\top X^\top w - w^\top X Y + Y^\top Y\big) = 2XX^\top w - 2XY$$

---

Very useful to memorize: matrix calculus

$$\nabla_x a = 0 \qquad \nabla_x\ c^\top x = c \qquad \nabla_x\ x^\top c = c \qquad \nabla_x\ x^\top A x = (A^\top + A)x$$

In matrix notation: $X = \big(x_1|x_2|\dots|x_n\big) \in \mathbb{R}^{d\times n}$, $Y \in \mathbb{R}^n$, $w \in \mathbb{R}^d$.

Least squares: $\min\limits_{w\in\mathbb{R}^d} \mathcal{L}(w)$ with $\mathcal{L}(w) = \|X^\top w - Y\|^2$

$$\nabla_w \mathcal{L}(w) = \nabla_w \big(w^\top X X^\top w - Y^\top X^\top w - w^\top X Y + Y^\top Y\big) = 2XX^\top w - 2XY$$

Setting the gradient to zero:

$$XX^\top w = XY$$

If $XX^\top$ is full rank, we can solve for $w$:

$$w = \big(XX^\top\big)^{-1} XY$$

or

```
lhs = dot(X, X.T)
rhs = dot(X, Y)
w = solve(lhs, rhs)
```

---

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$\nabla_x a = 0 \qquad \nabla_x\ c^\top x = c \qquad \nabla_x\ x^\top c = c \qquad \nabla_x\ x^\top A x = (A^\top + A)x$

# Boston housing dataset

| | | | | | | $x \in \mathbb{R}^{13}$ | | | | | | | $y$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0.01 | 18.00 | 2.31 | 0.00 | 0.54 | 6.58 | 65.20 | 4.09 | 1.00 | 296.00 | 15.30 | 396.90 | 4.98 | 24.00 |
| 0.03 | 0.00 | 7.07 | 0.00 | 0.47 | 6.42 | 78.90 | 4.97 | 2.00 | 242.00 | 17.80 | 396.90 | 9.14 | 21.60 |
| 0.03 | 0.00 | 7.07 | 0.00 | 0.47 | 7.18 | 61.10 | 4.97 | 2.00 | 242.00 | 17.80 | 392.83 | 4.03 | 34.70 |
| 0.03 | 0.00 | 2.18 | 0.00 | 0.46 | 7.00 | 45.80 | 6.06 | 3.00 | 222.00 | 18.70 | 394.63 | 2.94 | 33.40 |
| 0.07 | 0.00 | 2.18 | 0.00 | 0.46 | 7.15 | 54.20 | 6.06 | 3.00 | 222.00 | 18.70 | 396.90 | 5.33 | 36.20 |
| 0.03 | 0.00 | 2.18 | 0.00 | 0.46 | 6.43 | 58.70 | 6.06 | 3.00 | 222.00 | 18.70 | 394.12 | 5.21 | 28.70 |
| 0.09 | 12.50 | 7.87 | 0.00 | 0.52 | 6.01 | 66.60 | 5.56 | 5.00 | 311.00 | 15.20 | 395.60 | 12.43 | 22.90 |
| 0.14 | 12.50 | 7.87 | 0.00 | 0.52 | 6.17 | 96.10 | 5.95 | 5.00 | 311.00 | 15.20 | 396.90 | 19.15 | 27.10 |
| 0.21 | 12.50 | 7.87 | 0.00 | 0.52 | 5.63 | 100.00 | 6.08 | 5.00 | 311.00 | 15.20 | 386.63 | 29.93 | 16.50 |
| 0.17 | 12.50 | 7.87 | 0.00 | 0.52 | 6.00 | 85.90 | 6.59 | 5.00 | 311.00 | 15.20 | 386.71 | 17.10 | 18.90 |
| 0.22 | 12.50 | 7.87 | 0.00 | 0.52 | 6.38 | 94.30 | 6.35 | 5.00 | 311.00 | 15.20 | 392.52 | 20.45 | 15.00 |
| 0.12 | 12.50 | 7.87 | 0.00 | 0.52 | 6.01 | 82.90 | 6.23 | 5.00 | 311.00 | 15.20 | 396.90 | 13.27 | 18.90 |
| 0.09 | 12.50 | 7.87 | 0.00 | 0.52 | 5.89 | 39.00 | 5.45 | 5.00 | 311.00 | 15.20 | 390.50 | 15.71 | 21.70 |
| 0.63 | 0.00 | 8.14 | 0.00 | 0.54 | 5.95 | 61.80 | 4.71 | 4.00 | 307.00 | 21.00 | 396.90 | 8.26 | 20.40 |
| 0.64 | 0.00 | 8.14 | 0.00 | 0.54 | 6.10 | 84.50 | 4.46 | 4.00 | 307.00 | 21.00 | 380.02 | 10.26 | 18.20 |
| 0.63 | 0.00 | 8.14 | 0.00 | 0.54 | 5.83 | 56.50 | 4.50 | 4.00 | 307.00 | 21.00 | 395.62 | 8.47 | 19.90 |
| | | | | | | | ⋮ | | | | | | |
| 0.08 | 0.00 | 5.96 | 0.00 | 0.50 | 5.85 | 41.50 | 3.93 | 5.00 | 279.00 | 19.20 | 396.90 | 8.77 | 11.90 |

Learned linear least-square model:

$$f(x) = w^\top x$$

for

$$w = (0.11, 0.02, 0.08, -0.96, 19.2, -2.9, 0.09, 0.63, -0.07, 0, 0.64, 0)^\top$$

# Boston housing dataset

| | | | | | | $x \in \mathbb{R}^{13}$ | | | | | | | $y$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0.01 | 18.00 | 2.31 | 0.00 | 0.54 | 6.58 | 65.20 | 4.09 | 1.00 | 296.00 | 15.30 | 396.90 | 4.98 | 24.00 |
| 0.03 | 0.00 | 7.07 | 0.00 | 0.47 | 6.42 | 78.90 | 4.97 | 2.00 | 242.00 | 17.80 | 396.90 | 9.14 | 21.60 |
| 0.03 | 0.00 | 7.07 | 0.00 | 0.47 | 7.18 | 61.10 | 4.97 | 2.00 | 242.00 | 17.80 | 392.83 | 4.03 | 34.70 |
| 0.03 | 0.00 | 2.18 | 0.00 | 0.46 | 7.00 | 45.80 | 6.06 | 3.00 | 222.00 | 18.70 | 394.63 | 2.94 | 33.40 |
| 0.07 | 0.00 | 2.18 | 0.00 | 0.46 | 7.15 | 54.20 | 6.06 | 3.00 | 222.00 | 18.70 | 396.90 | 5.33 | 36.20 |
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| 0.09 | 12.50 | 7.87 | 0.00 | 0.52 | 6.01 | 66.60 | 5.56 | 5.00 | 311.00 | 15.20 | 395.60 | 12.43 | 22.90 |
| 0.14 | 12.50 | 7.87 | 0.00 | 0.52 | 6.17 | 96.10 | 5.95 | 5.00 | 311.00 | 15.20 | 396.90 | 19.15 | 27.10 |
| 0.21 | 12.50 | 7.87 | 0.00 | 0.52 | 5.63 | 100.00 | 6.08 | 5.00 | 311.00 | 15.20 | 386.63 | 29.93 | 16.50 |
| 0.17 | 12.50 | 7.87 | 0.00 | 0.52 | 6.00 | 85.90 | 6.59 | 5.00 | 311.00 | 15.20 | 386.71 | 17.10 | 18.90 |
| 0.22 | 12.50 | 7.87 | 0.00 | 0.52 | 6.38 | 94.30 | 6.35 | 5.00 | 311.00 | 15.20 | 392.52 | 20.45 | 15.00 |
| 0.12 | 12.50 | 7.87 | 0.00 | 0.52 | 6.01 | 82.90 | 6.23 | 5.00 | 311.00 | 15.20 | 396.90 | 13.27 | 18.90 |
| 0.09 | 12.50 | 7.87 | 0.00 | 0.52 | 5.89 | 39.00 | 5.45 | 5.00 | 311.00 | 15.20 | 390.50 | 15.71 | 21.70 |
| 0.63 | 0.00 | 8.14 | 0.00 | 0.54 | 5.95 | 61.80 | 4.71 | 4.00 | 307.00 | 21.00 | 396.90 | 8.26 | 20.40 |
| 0.64 | 0.00 | 8.14 | 0.00 | 0.54 | 6.10 | 84.50 | 4.46 | 4.00 | 307.00 | 21.00 | 380.02 | 10.26 | 18.20 |
| 0.63 | 0.00 | 8.14 | 0.00 | 0.54 | 5.83 | 56.50 | 4.50 | 4.00 | 307.00 | 21.00 | 395.62 | 8.47 | 19.90 |
| | | | | | | | $\vdots$ | | | | | | |
| 0.08 | 0.00 | 5.96 | 0.00 | 0.50 | 5.85 | 41.50 | 3.93 | 5.00 | 279.00 | 19.20 | 396.90 | 8.77 | 11.90 |

Learned linear least-square model:

$$f(x) = w^\top x$$

for

$$w = (0.11, 0.02, 0.08, -0.96, 19.2, -2.9, 0.09, 0.63, -0.07, 0, 0.64, 0)^\top$$

**Is this a good model? What else could we do?**

**Linear model with bias term (= "intercept"):**

$$f(x) = w^\top x + b \text{ for } w \in \mathbb{R}^d, b \in \mathbb{R}$$

Least squares: $\displaystyle \min_{w \in \mathbb{R}^d, b \in \mathbb{R}} \mathcal{L}(w, b)$ with $\mathcal{L}(w, b) = \sum_i (w^\top x_i + b - y_i)^2$

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$$0 = \nabla_b \mathcal{L}(w, b) = 2 \sum_i ({x_i}^\top w + b - y_i) \quad \rightarrow \quad b^{\text{opt}} = \bar{y} - \bar{x}^\top w$$

for $\bar{x} = \frac{1}{n} \sum_i x_i$ and $\bar{y} = \frac{1}{n} \sum_i y_i$.

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for $\bar{x} = \frac{1}{n}\sum_i x_i$ and $\bar{y} = \frac{1}{n}\sum_i y_i$.

$$\bar{\mathcal{L}}(w) = \bar{\mathcal{L}}(w, b^{\text{opt}}) = \sum_i \Big( (x_i - \bar{x})^\top w - (y_i - \bar{y}) \Big)^2$$

$$0 = \nabla_w \bar{\mathcal{L}}(w) = 2\sum_i \Big( (x_i - \bar{x})(x_i - \bar{x})^\top w - (y_i - \bar{y}) \Big)$$

Solve for $w$ (if possible):

$$w = \underbrace{\Big(\sum_i (x_i - \bar{x})(x_i - \bar{x})^\top\Big)^{-1}}_{= n\mathrm{Cov}(x_1,\dots,x_n)} \underbrace{\sum_i (x_i - \bar{x})(y_i - \bar{y})}_{= n\mathrm{Cov}(x_1,\dots,x_n; y_1,,\dots,y_n)}$$

$$= \mathrm{Cov}(X)^{-1}\mathrm{Cov}(X,Y)$$

## Observation: centered data

If the training data is centered, i.e. $\frac{1}{n}\sum_i x_i = 0$, $\frac{1}{n}\sum_i y_i = 0$, we don't need a bias term $\rightarrow$ we can reuse code for linear regression without bias.

## Alternative trick: feature augmentation

Adding a constant feature allows us to avoid models with explicit bias term:

- instead of $x = (x^1, \dots, x^d) \in \mathbb{R}^d$, use $\tilde{x} = (x^1, \dots, x^d, 1) \in \mathbb{R}^{d+1}$
- for any $\tilde{w} \in \mathbb{R}^{d+1}$, think $\tilde{w} = (w, b)$ with $w \in \mathbb{R}^d$ and $b \in \mathbb{R}$

Linear model in $\mathbb{R}^{d+1}$:

$$f(\tilde{x}) = \tilde{w}^\top \tilde{x} = \sum_{i=1}^{d+1} \tilde{w}_i \tilde{x}_i = \sum_{i=1}^{d} \tilde{w}_i \tilde{x}_i + \tilde{w}_{d+1}\tilde{x}_{d+1} = w^\top x + b$$

Linear model with bias term in $\mathbb{R}^d$ $\quad\equiv\quad$ linear model with no bias term in $\mathbb{R}^{d+1}$

Boston housing dataset

| $x \in \mathbb{R}^{13}$ | | | | | | | | | | | | | $y$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0.01 | 18.00 | 2.31 | 0.00 | 0.54 | 6.58 | 65.20 | 4.09 | 1.00 | 296.00 | 15.30 | 396.90 | 4.98 | 24.00 |
| 0.03 | 0.00 | 7.07 | 0.00 | 0.47 | 6.42 | 78.90 | 4.97 | 2.00 | 242.00 | 17.80 | 396.90 | 9.14 | 21.60 |
| 0.03 | 0.00 | 7.07 | 0.00 | 0.47 | 7.18 | 61.10 | 4.97 | 2.00 | 242.00 | 17.80 | 392.83 | 4.03 | 34.70 |
| 0.03 | 0.00 | 2.18 | 0.00 | 0.46 | 7.00 | 45.80 | 6.06 | 3.00 | 222.00 | 18.70 | 394.63 | 2.94 | 33.40 |
| 0.07 | 0.00 | 2.18 | 0.00 | 0.46 | 7.15 | 54.20 | 6.06 | 3.00 | 222.00 | 18.70 | 396.90 | 5.33 | 36.20 |
| 0.03 | 0.00 | 2.18 | 0.00 | 0.46 | 6.43 | 58.70 | 6.06 | 3.00 | 222.00 | 18.70 | 394.12 | 5.21 | 28.70 |
| 0.09 | 12.50 | 7.87 | 0.00 | 0.52 | 6.01 | 66.60 | 5.56 | 5.00 | 311.00 | 15.20 | 395.60 | 12.43 | 22.90 |
| 0.14 | 12.50 | 7.87 | 0.00 | 0.52 | 6.17 | 96.10 | 5.95 | 5.00 | 311.00 | 15.20 | 396.90 | 19.15 | 27.10 |
| 0.21 | 12.50 | 7.87 | 0.00 | 0.52 | 5.63 | 100.00 | 6.08 | 5.00 | 311.00 | 15.20 | 386.63 | 29.93 | 16.50 |
| 0.17 | 12.50 | 7.87 | 0.00 | 0.52 | 6.00 | 85.90 | 6.59 | 5.00 | 311.00 | 15.20 | 386.71 | 17.10 | 18.90 |
| 0.22 | 12.50 | 7.87 | 0.00 | 0.52 | 6.38 | 94.30 | 6.35 | 5.00 | 311.00 | 15.20 | 392.52 | 20.45 | 15.00 |
| 0.12 | 12.50 | 7.87 | 0.00 | 0.52 | 6.01 | 82.90 | 6.23 | 5.00 | 311.00 | 15.20 | 396.90 | 13.27 | 18.90 |
| 0.09 | 12.50 | 7.87 | 0.00 | 0.52 | 5.89 | 39.00 | 5.45 | 5.00 | 311.00 | 15.20 | 390.50 | 15.71 | 21.70 |
| 0.63 | 0.00 | 8.14 | 0.00 | 0.54 | 5.95 | 61.80 | 4.71 | 4.00 | 307.00 | 21.00 | 396.90 | 8.26 | 20.40 |
| 0.64 | 0.00 | 8.14 | 0.00 | 0.54 | 6.10 | 84.50 | 4.46 | 4.00 | 307.00 | 21.00 | 380.02 | 10.26 | 18.20 |
| 0.63 | 0.00 | 8.14 | 0.00 | 0.54 | 5.83 | 56.50 | 4.50 | 4.00 | 307.00 | 21.00 | 395.62 | 8.47 | 19.90 |
| | | | | | | | ⋮ | | | | | | |
| 0.08 | 0.00 | 5.96 | 0.00 | 0.50 | 5.85 | 41.50 | 3.93 | 5.00 | 279.00 | 19.20 | 396.90 | 8.77 | 11.90 |

Learned linear least-square model: $f(x) = w^{\top}x + b$

for $w = (0.10, 0.01, 0.01, -1.02, 5.20, -4.41, 0.09, 0.15, 0.05, 0, -0.12, 0)$
$b = 30.15$

Boston housing dataset

| | | | | | | $x \in \mathbb{R}^{13}$ | | | | | | | $y$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0.01 | 18.00 | 2.31 | 0.00 | 0.54 | 6.58 | 65.20 | 4.09 | 1.00 | 296.00 | 15.30 | 396.90 | 4.98 | 24.00 |
| 0.03 | 0.00 | 7.07 | 0.00 | 0.47 | 6.42 | 78.90 | 4.97 | 2.00 | 242.00 | 17.80 | 396.90 | 9.14 | 21.60 |
| 0.03 | 0.00 | 7.07 | 0.00 | 0.47 | 7.18 | 61.10 | 4.97 | 2.00 | 242.00 | 17.80 | 392.83 | 4.03 | 34.70 |
| 0.03 | 0.00 | 2.18 | 0.00 | 0.46 | 7.00 | 45.80 | 6.06 | 3.00 | 222.00 | 18.70 | 394.63 | 2.94 | 33.40 |
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$b = 30.15$

**Is this model better than the one without bias term?**

## Understanding model quality

**So you've trained a model. How good it is?**

**You've trained multiple models. Which one to choose?**

**Is the model 'good enough'? What would be the best possible model?**

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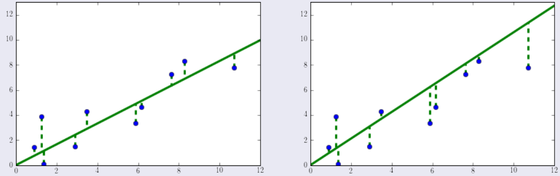
### Wrong approach to evaluate predictive models: explained variance

Evaluate model error by checking how well it fits the training data.



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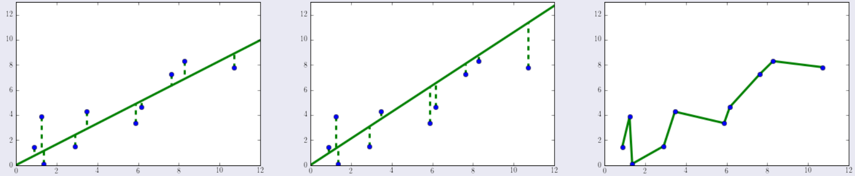



Explained variance prefers complex models over simple ones (always!)

The model is *not for you*, it's send out to be used by a *user*.

**You: train the model on your data**

**input** training data $\mathcal{D}_{trn}$

$f \hookleftarrow$ some procedure using $\mathcal{D}_{trn}$

**output** predictive model $f : \mathcal{X} \to \mathbb{R}$

**The user: make predictions on his/her own data**

**input** trained predictive model $f : \mathcal{X} \to \mathbb{R}$

**input** new data $\mathcal{D}_{tst}$

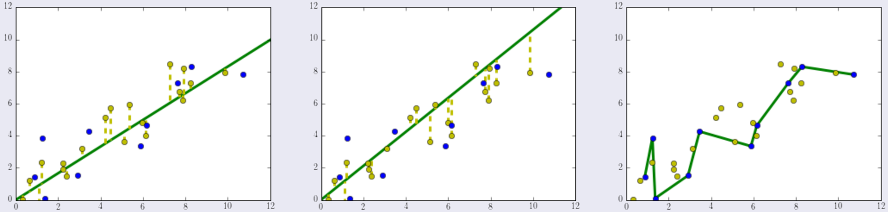
use $f$ to make predictions on $\mathcal{D}_{tst}$

**output** happy face or lawsuit

What matters isn't how good the model is on the training set, but on **new data**.

## Evaluate predictive models: generalization performance

Evaluate model error on data that has not been used for training.




For trained model $f$ and new data $\mathcal{D}_{tst} = \{(x'_1, y'_1), \ldots, (x'_m, y'_m)\}$,

$$E(f) = \frac{1}{m} \sum_{i=1}^{m} \left(f(x'_i) - y'_i\right)^2$$

**Observation**: A model can be perfect on training data (blue), but still not do great on new data (yellow).

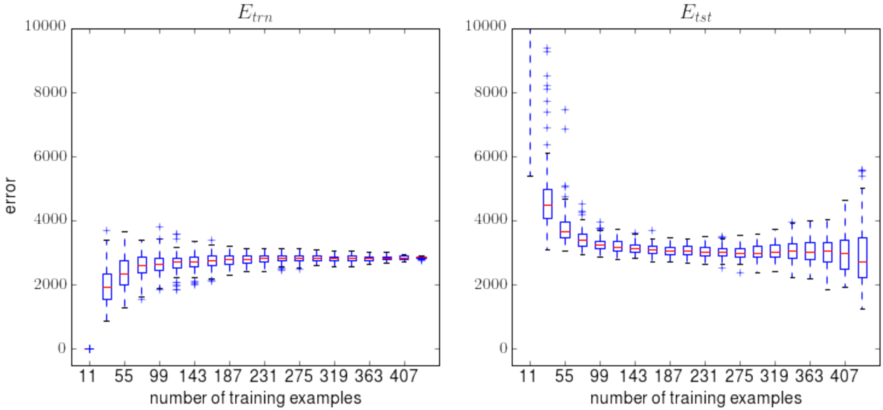
# Model evaluation

In practice, we don't get "new" data. We'll have to use the available data both for training and for evaluation.

## Model Training and Evaluation

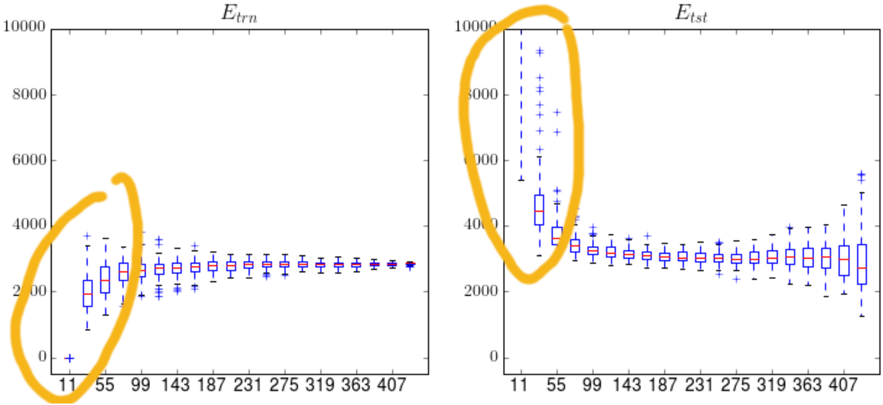
**input** data $\mathcal{D}$
**input** learning method $A$
  randomly split $\mathcal{D} = \mathcal{D}_{trn} \,\dot{\cup}\, \mathcal{D}_{tst}$ disjointly
  set aside $\mathcal{D}_{tst}$ to a safe place // do not look at it!
  $f \leftarrow A[\mathcal{D}_{trn}]$ // i.e. train model on training set
  $E(f) \leftarrow$ performance of $f$ on $\mathcal{D}_{tst}$
**output** trained model $f$, performance estimate $E(f)$

- Do not use $\mathcal{D}_{tst}$ for anything except the very last step.
- Do not look at $\mathcal{D}_{tst}$! Even if the learning algorithm doesn't see it, you looking at it can and will influence your model design or parameter selection (human overfitting).

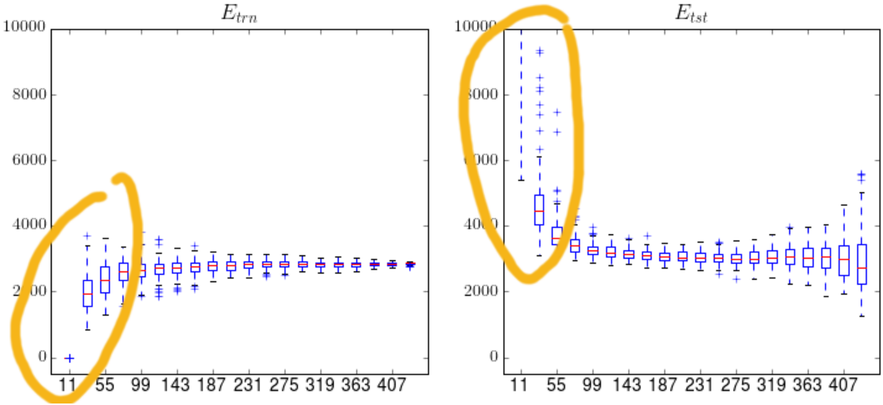



**Fact 1:** Predictive models tend to get better when trained on more data.
**Fact 2:** A too small test set makes the quality estimate unreliable.

**Guideline:** $\mathcal{D}_{trn}$ should be as big as possible, but $\mathcal{D}_{tst}$ must be large enough to be convincing.




**Fact 3:** With very little training data, the training error is very small, but the test error is very large.




**Fact 3:** With very little training data, the training error is very small, but the test error is very large.

**OVERFITTING!**

The model has learned to reproduce idiosyncracies/noise. On new data, this causes a large error.

**Observation:** Least squares regression overfits if the number of example is not much bigger than the number of data dimensions.

**How to avoid overfitting?**

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**How to avoid overfitting?**

### Feature Selection

**Idea:** reduce the dimensionality of the data by dropping some dimensions

**Problems:** 1) which ones? 2) simply throwing away data is rarely a good idea

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### Dimensionality Reduction

**Idea:** reduce data dimensionality differently, e.g. Principal Component Analysis.

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### Dimensionality Reduction

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### Regularization

**Idea:** prevent the model from overfitting by making it **robust**

**Problems:** almost none. This is actually a good idea.

## What do we mean by robustness?

### Robustness of model parameters

How robust are the linear least squares model parameters

$$w = (XX^\top)^{-1}XY$$

against small changes in the training data $X$?

### Robustness of predictions

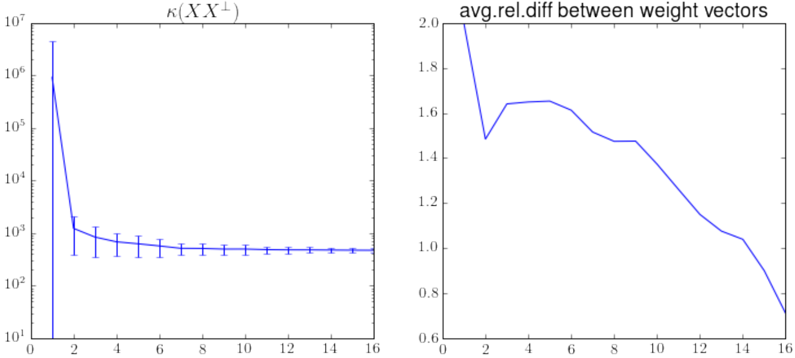
How robust are the predictions

$$f(x) = w^\top x$$

against small changes of $x$ ?

Robustness of the parameter vector $w = (XX^\top)^{-1}XY$ is determined by the **condition number** of the matrix $XX^\top$:

$$\kappa = \frac{\sigma_{\text{max}}(XX^\top)}{\sigma_{\text{min}}(XX^\top)}.$$




- for real data, $\kappa$ is often large unless $n$ is much larger than $d$
  $\rightarrow$ randomness in $X$ can have large impact on $w$

*black board*

For any linear model, the robustness of the predictions $f(x) = w^\top x$ is determined by the **norm** of the weight vector $\|w\|$:

$$\frac{f(x+\epsilon) - f(x)}{\|\epsilon\|} = \frac{\langle w, x+\epsilon\rangle - \langle w, x\rangle}{\|\epsilon\|} = \frac{\langle w, \epsilon\rangle}{\|\epsilon\|} \leq \frac{\|w\|\|\epsilon\|}{\|\epsilon\|} = \|w\|$$

**Insight:**

- if many different $w$ work well on the training data, prefer the one with small $\|w\|$
- maybe even: allows for higher $E_{\text{trn}}$ to avoid models with very large $\|w\|$

So far:

- learn model parameters by minimizing error on training set

Now:

- take *robustness* into account as well when learning parameters

### Regularized Least Squared Regression (= Ridge Regression)

For some $\lambda \geq 0$ (=regularization parameter), solve

$$\min_{w \in \mathbb{R}^d} \quad \sum_i (w^\top x_i - y_i)^2 + \lambda \quad \|w\|^2$$

# Regularization

So far:

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## Regularized Least Squared Regression (= Ridge Regression)

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**Regularized Least Squared Regression (= Ridge Regression)**

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$$\min_{w \in \mathbb{R}^d} \underbrace{\sum_i (w^\top x_i - y_i)^2}_{\text{training error}} + \lambda \underbrace{\|w\|^2}_{\text{"regularizer"}}$$

Observation:

- the bigger $\lambda$, the more emphasis we put on *robustness* versus *training error*
- $\lambda = 0 \quad \rightarrow$ no regularization, original least squares regression
- $\lambda \rightarrow \infty \quad \rightarrow$ training error ignored ($w \rightarrow 0$), but perfectly robust

Open question: what's the best value for $\lambda$?

# Ridge Regression

Ridge regression is as easy to learn as least squares: *black board*

$$\min_{w\in\mathbb{R}^d} \ \mathcal{L}(w) + \lambda\Omega(w)$$

for $\mathcal{L}(w) = \sum_i (w^\top x_i - y_i)^2$ and $\Omega(w) = \|w\|^2$.

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$$\nabla_w \Big[\mathcal{L}(w) + \lambda\Omega(w)\Big] = 2\sum_i x_i x_i^\top w - 2\sum_i x_i y_i + 2\lambda w$$

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$$\min_{w\in\mathbb{R}^d} \; \mathcal{L}(w) + \lambda\Omega(w)$$

for $\mathcal{L}(w) = \sum_i (w^\top x_i - y_i)^2$ and $\Omega(w) = \|w\|^2$.

$$\nabla_w\Big[\mathcal{L}(w) + \lambda\Omega(w)\Big] = 2\sum_i x_i {x_i}^\top w - 2\sum_i x_i y_i + 2\lambda w$$

Set gradient to zero:

$$\sum_i x_i {x_i}^\top w + \lambda w \quad = \sum_i x_i y_i$$

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$$\min_{w \in \mathbb{R}^d} \ \mathcal{L}(w) + \lambda \Omega(w)$$

for $\mathcal{L}(w) = \sum_i (w^\top x_i - y_i)^2$ and $\Omega(w) = \|w\|^2$.

$$\nabla_w \Big[ \mathcal{L}(w) + \lambda \Omega(w) \Big] = 2 \sum_i x_i {x_i}^\top w - 2 \sum_i x_i y_i + 2\lambda w$$

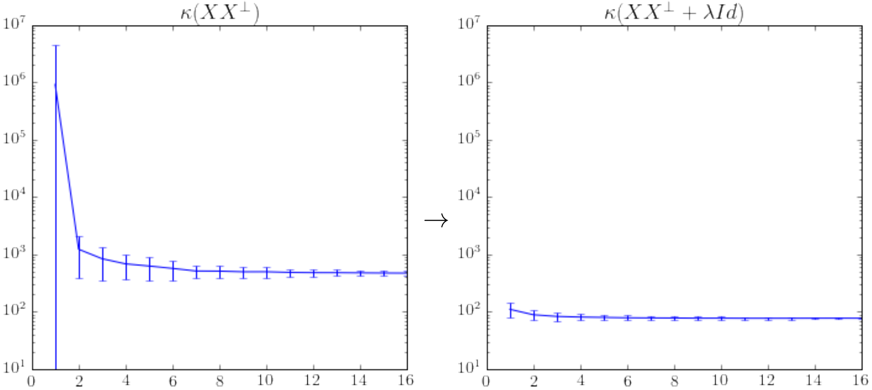
Set gradient to zero:

$$\underbrace{\sum_i x_i {x_i}^\top w + \lambda w}_{= (\sum_i x_i {x_i}^\top \ + \ \lambda \, \mathrm{Id}_{n \times n}) w} \quad = \sum_i x_i y_i$$

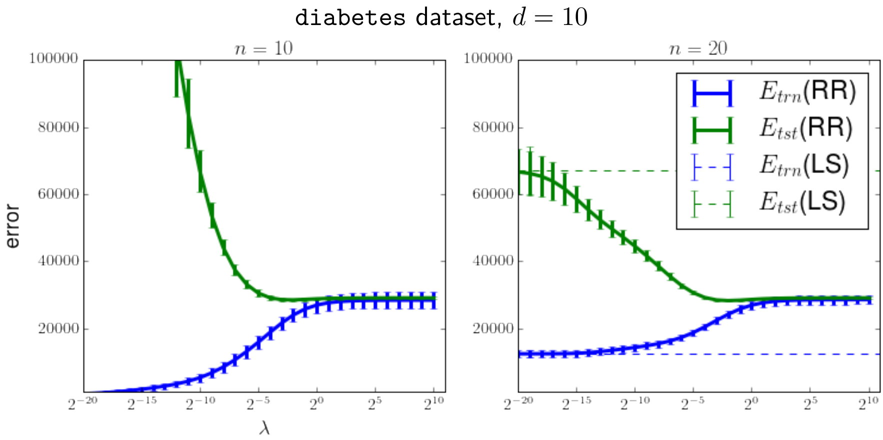
For $\lambda > 0$, we can *always* solve for $w$ (regardless if $n \geq d$),

$$w = \big( \sum_i x_i {x_i}^\top + \lambda \, \mathrm{Id} \big)^{-1} \sum_i x_i y_i$$

Already small regularization strongly increases robustness (here: $\lambda = 0.0001n$)



Training and test error for different regularization constants:



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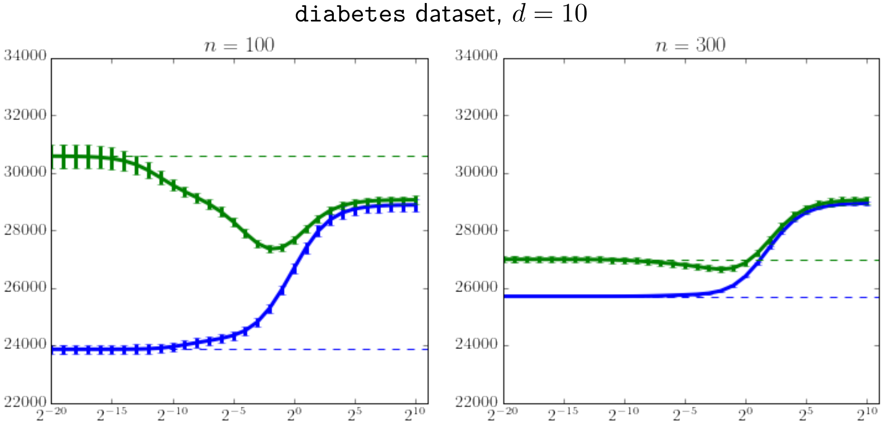

Question:

- How to select one model from many possible ones.
- How to set free parameters of a model (e.g. regularization)?

**Training and Choosing between Multiple Models (suboptimal, don't use)**

**input** data $\mathcal{D}$, set of method $\mathcal{A} = \{A_1, \dots, A_K\}$
  randomly split $\mathcal{D} = \mathcal{D}_{trn} \dot\cup \mathcal{D}_{tst}$ disjointly
  **for all** possible procedures $A_i \in \mathcal{A}$ **do**
    $f_i \hookleftarrow A_i[\mathcal{D}_{trn}]$
    $E(f_i) \hookleftarrow$ performance of $f_i$ on $\mathcal{D}_{tst}$
  **end for**
**output** $f \hookleftarrow f_i$ for $i = \mathbf{argmin}_i\, E(f_i)$    // pick best performing $f_i$

Question:

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Problem: How good is the selected model? We don't know!
$\mathcal{D}_{tst}$ was used to select $f$, so it became part of the *training* stage.

## Model Selection

**Proper model selection:** We simulate the model evaluation step during the training procedure. This requires one additional data split:

### Training and Selecting between Multiple Models

**input** data $\mathcal{D}$
**input** set of method $\mathcal{A} = \{A_1, \dots, A_K\}$
randomly split $\mathcal{D} = \mathcal{D}_{trnval} \dot\cup \mathcal{D}_{tst}$ disjointly
set aside $\mathcal{D}_{tst}$ to a safe place (and do not look at it)

randomly split $\mathcal{D}_{trnval} = \mathcal{D}_{trn} \dot\cup \mathcal{D}_{val}$ disjointly
**for all** possible procedures $A_i \in \mathcal{A}$ **do**
$f_i \leftarrow A_i[\mathcal{D}_{trn}]$
$E_{val}(f_i) \leftarrow$ performance of $f_i$ on $\mathcal{D}_{val}$
**end for**
$f \leftarrow f_i$ for $i = \mathbf{argmin}_i\, E_{val}(f_i)$ // pick best performing $f_i$

(optional) $f \leftarrow A_i[\mathcal{D}_{trnval}]$ // retrain best method on full data

$E_{tst}(f) \leftarrow$ performance of $f$ on $\mathcal{D}_{tst}$
**output** trained model $f$, performance estimate $E_{tst}(f)$

**Discussion.**

- Each model is trained on $\mathcal{D}_{trn}$ and evaluated on disjoint $\mathcal{D}_{val}$ ✓
- Which model is selected depends on $\mathcal{D}_{trn}$ and $\mathcal{D}_{val}$ ✓
- Only then the "new" $\mathcal{D}_{tst}$ is used to evaluate the single final model ✓

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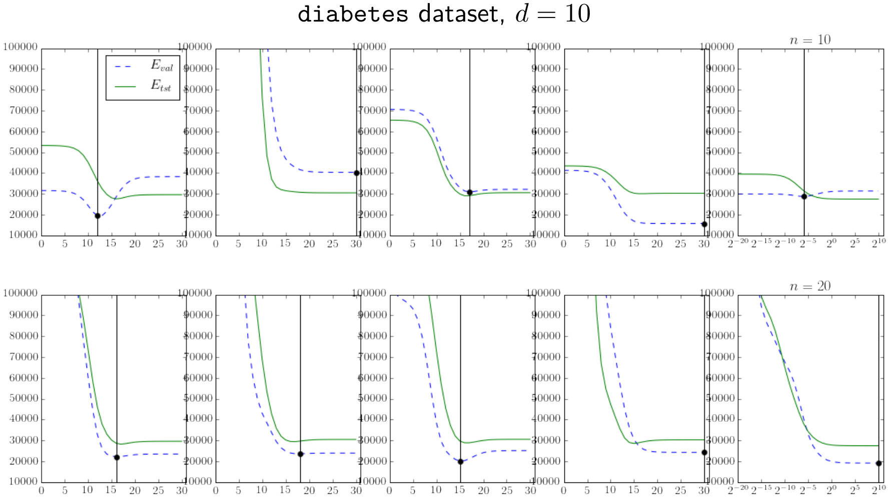
**Problems.**

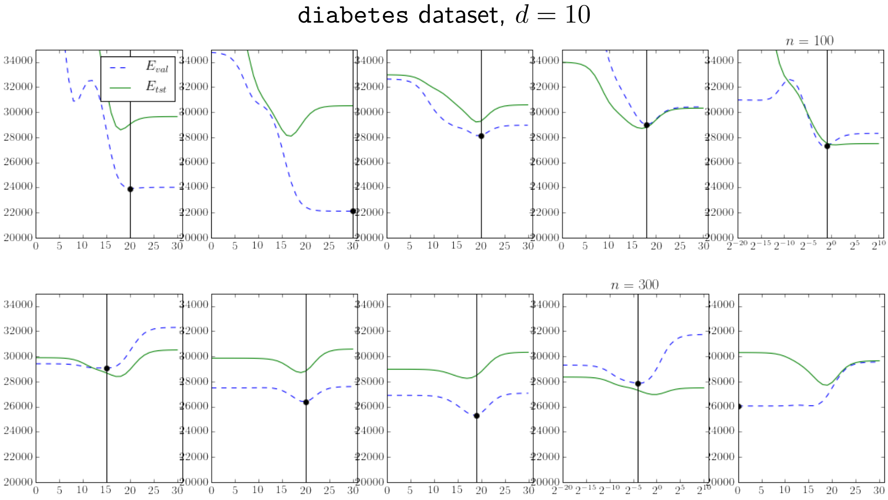
- small $\mathcal{D}_{val}$ is bad: $E_{val}$ could be bad estimate of $f_i$'s true performance, and we might pick a suboptimal method.
- large $\mathcal{D}_{val}$ is bad: $\mathcal{D}_{trn}$ is much smaller than $\mathcal{D}_{trnval}$, so the classifier learned on $\mathcal{D}_{trn}$ might be much worse than necessary.
- retraining the best model on $\mathcal{D}_{trnval}$ might overcome that, but that comes at a risk: just because a model/parameter was the best for $\mathcal{D}_{trn}$, does not mean it is also the best for the larger $\mathcal{D}_{trnval}$.

Validation error and test error for different regularization constants:



# Model Selection

Validation error and test error for different regularization constants:




Parameters from model selection are rarely optimal, but usually reasonable.

Can we use *all data* for training as well as model selection?

### Leave-One-Out Evaluation (for a single model/algorithm)

**input** algorithm $A$
**input** data $\mathcal{D}$ (*trnval* part only: *tst* part was set aside earlier)
  **for all** $(x_i, y_i) \in \mathcal{D}$ **do**
    $f_{\neg i} \leftarrow A[\ \mathcal{D} \setminus \{(x_i, y_i)\}\ ]$ // $\mathcal{D}_{trn}$ is $\mathcal{D}$ with $i$-th example removed
    $r_i \leftarrow$ performance of $f_i$ on $(x_i, y_i)$ // i.e. $\mathcal{D}_{val}$ is $\{(x_i, y_i)\}$
  **end for**
**output** $E_{loo}(f) = \frac{1}{n} \sum_{i=1}^{n} r_i$ // average leave-one-out risk

**Properties.**

- Each $r_i$ is a unbiased (but high variance) estimate of the quality of $f_{\neg i}$
- $\mathcal{D} \setminus \{(x_i, y_i)\}$ is almost the same as $\mathcal{D}$, so we can hope that each $f_{\neg i}$ is almost the same as $f = A[\mathcal{D}]$.
- Therefore, $E_{loo}$ can be expected a good estimate of $E$ on new data

**Problem:** slow, trains $n$ times on $n-1$ examples instead of once on $n$
**Problem:** all training sets are almost the same, $r_i$ are correlated

Compromise: use fixed number of small $\mathcal{D}_{val}$

**$K$-fold Cross Validation (CV)**

**input** algorithm $A$, loss function $\ell$, data $\mathcal{D}$ (trnval part)

split $\mathcal{D} = \dot{\bigcup}_{k=1}^{K} \mathcal{D}_k$ into $K$ equal sized disjoint parts

**for** $k = 1, \ldots, K$ **do**

$f_{\neg k} \leftarrow A[\,\mathcal{D} \setminus \mathcal{D}_k\,]$

$r_k \leftarrow$ performance of $f_{\neg k}$ on $\mathcal{D}_k$

**end for**

**output** $R_{K\text{-CV}} = \frac{1}{K} \sum_{k=1}^{K} r_k$ ($K$-fold cross-validation risk)

**Observation.**

- for $K = |\mathcal{D}|$ same as leave-one-out error.
- approximately $k$ times increase in runtime.
- most common: $k = 10$ or $k = 5$.

**Remaining problem**: training sets overlap, so the error estimates are not independent, and it's hard to interpret error bars or design statistical tests