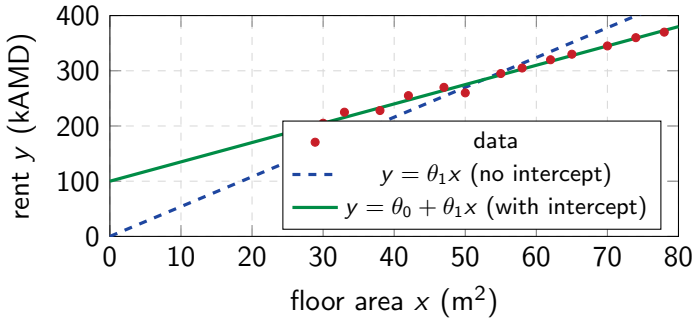
Outline

The intercept problem - can a line through the origin do it?

Suppose Yerevan studio rent vs. floor area. Even the smallest viable 25 m^2 studio doesn't cost (25 $\times$ per-m^2 price): there's a baseline (registration, condition, neighbourhood floor). A line forced through the origin can't absorb that baseline.



What we learn from the picture

- The dashed line (no intercept) is forced through (0, 0). To get near the data cloud it has to be much steeper than the cloud actually slopes.
- Result: it under-shoots small apartments and over-shoots large ones.
- The solid line (with intercept) is free to start at $\theta_0 \approx 100$ kAMD and rise gently. Much smaller residuals.

Conclusion: we need an intercept term θ_0. The next three frames make θ_0 disappear into the same dot product as the other coefficients.

Two parameters, one notation?

Why we want this: we're about to vectorize all n predictions as a single matrix multiplication. A clean dot product makes that one line of NumPy code instead of a loop.

We *want* to write every prediction as:

$$f(\mathbf{x}) = \boldsymbol{\theta}^\top \mathbf{x}.$$

But $\boldsymbol{\theta} = (\theta_0, \theta_1, \ldots, \theta_p)^\top \in \mathbb{R}^{p+1}$ has **one more entry** than $\mathbf{x} = (x_1, \ldots, x_p)^\top \in \mathbb{R}^p$.

Naive dot product:

$$\boldsymbol{\theta}^\top \mathbf{x} = \theta_1 x_1 + \cdots + \theta_p x_p \quad \text{(missing } \theta_0\text{!)}$$

The padding trick: prepend a 1

Replace every feature vector by an **augmented** version:

$$\mathbf{x} = (x_1, \ldots, x_p)^\top \longmapsto \tilde{\mathbf{x}} = (1, x_1, \ldots, x_p)^\top \in \mathbb{R}^{p+1}.$$

Then:

$$\boldsymbol{\theta}^\top \tilde{\mathbf{x}} = \theta_0 \cdot 1 + \theta_1 x_1 + \cdots + \theta_p x_p = \theta_0 + \theta_1 x_1 + \cdots + \theta_p x_p.$$

Now the intercept lives inside $\boldsymbol{\theta}$. No special case in any formula.

From now on we drop the tilde and just write $\mathbf{x} \in \mathbb{R}^{p+1}$ with a leading 1.

What this buys us, concretely

Without the trick:

- Prediction: $f(\mathbf{x}) = \theta_0 + \sum_{j=1}^{p} \theta_j x_j$
- Two cases for the gradient (one for θ_0, one for θ_j)
- In code: carry θ_0 as its own variable

With the trick:

- Prediction: $f(\mathbf{x}) = \boldsymbol{\theta}^\top \mathbf{x}$
- One gradient formula handles every parameter
- In code: `X = np.hstack([np.ones((n,1)), X])` once at the top, then everything is `X @ theta`

Caveat: regularization (L03) usually does *not* penalize θ_0. The penalty term acts on $\theta_{1:p}$ only - common gotcha when implementing Ridge by hand.

One observation $\rightarrow$ matrix-vector product

For a single augmented input $\mathbf{x}^{(i)} \in \mathbb{R}^{p+1}$:

$$\hat{y}^{(i)} = \boldsymbol{\theta}^\top \mathbf{x}^{(i)}.$$

Predictions for *all n* observations:

$$\begin{pmatrix} \hat{y}^{(1)} \\ \hat{y}^{(2)} \\ \vdots \\ \hat{y}^{(n)} \end{pmatrix} = \begin{pmatrix} \boldsymbol{\theta}^\top \mathbf{x}^{(1)} \\ \boldsymbol{\theta}^\top \mathbf{x}^{(2)} \\ \vdots \\ \boldsymbol{\theta}^\top \mathbf{x}^{(n)} \end{pmatrix}.$$

Each entry of the right-hand vector is the dot product of $\boldsymbol{\theta}$ with one input. We can collect all of them into a single matrix-vector product.

The design matrix $\mathbf{X}$

Stack the augmented inputs as the **rows** of $\mathbf{X}$:

$$\mathbf{X} = \begin{pmatrix} 1 & x_1^{(1)} & x_2^{(1)} & \cdots & x_p^{(1)} \\ 1 & x_1^{(2)} & x_2^{(2)} & \cdots & x_p^{(2)} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_1^{(n)} & x_2^{(n)} & \cdots & x_p^{(n)} \end{pmatrix} \in \mathbb{R}^{n \times (p+1)}.$$

Shape mnemonic: **rows are observations, columns are features.** First column is always 1 (intercept).

In NumPy: `X.shape == (n, p + 1)`.

The full prediction in one expression

All n predictions become a single matrix-vector product:

$$\boxed{\hat{\mathbf{y}} = \mathbf{X}\boldsymbol{\theta}} \quad \text{where} \quad \hat{\mathbf{y}} \in \mathbb{R}^n, \;\; \mathbf{X} \in \mathbb{R}^{n \times (p+1)}, \;\; \boldsymbol{\theta} \in \mathbb{R}^{p+1}.$$

Shape check (do this every time you write a new matrix expression):

$$\underbrace{(n \times (p+1))}_{\mathbf{X}} \cdot \underbrace{((p+1) \times 1)}_{\boldsymbol{\theta}} = \underbrace{(n \times 1)}_{\hat{\mathbf{y}}}.$$

Residuals and SSE also vectorize:

$$\mathbf{r} = \mathbf{y} - \hat{\mathbf{y}} = \mathbf{y} - \mathbf{X}\boldsymbol{\theta}, \qquad \mathcal{R}_{\text{emp}} = \sum_{i=1}^{n} r_i^2 = \mathbf{r}^\top \mathbf{r} = \|\mathbf{y} - \mathbf{X}\boldsymbol{\theta}\|_2^2.$$

Vectorized vs. loop: code

Slow (Python loop) - teaching example only, DO NOT use in real code:

```
yhat = np.zeros(n)
for i in range(n):                    # row by row
    s = 0.0
    for j in range(p + 1):            # element by element
        s += theta[j] * X[i, j]
    yhat[i] = s
```

Fast (vectorized NumPy) - the actual implementation:

```
yhat = X @ theta              # one matrix-vector product
residuals = y - yhat
sse = residuals @ residuals
```

The `@` operator is matrix multiplication (covered in `python_libs/02_numpy`).

Why vectorization wins

Two reasons the second version is dramatically faster:

1. **No per-element Python overhead.** Every iteration of the loop pays the cost of a Python bytecode dispatch. The vectorized version hands the whole job to a single call into compiled linear-algebra code (the BLAS library, written in C / Fortran).
2. **The CPU can process many numbers in parallel.** BLAS routines stream contiguous chunks of memory through SIMD instructions, where one CPU instruction operates on 4-16 floats at once. The Python loop processes one number at a time.

Rule of thumb on this laptop (Intel Iris Xe, 16 GB): for $n = 10^5$, $p = 50$, the loop takes seconds; `X @ theta` takes milliseconds.

Habit to build: when you catch yourself writing a Python `for` loop over rows of an array, stop and ask "what matrix op does this?".

The setup

We want the $\boldsymbol{\theta}$ that minimizes empirical risk:

$$\hat{\boldsymbol{\theta}} \in \arg\min_{\boldsymbol{\theta}} \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \left(y^{(i)} - \boldsymbol{\theta}^\top \mathbf{x}^{(i)} \right)^2 = \arg\min_{\boldsymbol{\theta}} \|\mathbf{y} - \mathbf{X}\boldsymbol{\theta}\|_2^2.$$

The function $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$ is a smooth (differentiable everywhere) function with no constraints on $\boldsymbol{\theta}$. So the strategy from calculus:

1. Expand the squared norm so we can differentiate.
2. Take the gradient w.r.t. $\boldsymbol{\theta}$.
3. Set the gradient to zero $\rightarrow$ this gives the *normal equations*.
4. Solve the resulting linear system for $\hat{\boldsymbol{\theta}}$.

Speedrun: the derivation in 4 lines

Before the careful version, here is the whole thing in 4 lines. Read these once, then we'll justify each step.

$$\mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) = \|\mathbf{y} - \mathbf{X}\boldsymbol{\theta}\|_2^2 = \mathbf{y}^\top \mathbf{y} - 2\,\boldsymbol{\theta}^\top \mathbf{X}^\top \mathbf{y} + \boldsymbol{\theta}^\top \mathbf{X}^\top \mathbf{X}\,\boldsymbol{\theta}$$

$$\nabla_{\boldsymbol{\theta}} \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) = -2\,\mathbf{X}^\top \mathbf{y} + 2\,\mathbf{X}^\top \mathbf{X}\,\boldsymbol{\theta}$$

$$\text{set to 0:} \quad \mathbf{X}^\top \mathbf{X}\,\hat{\boldsymbol{\theta}} = \mathbf{X}^\top \mathbf{y} \quad (\textit{normal equations})$$

$$\boxed{\hat{\boldsymbol{\theta}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}} \quad (\textit{OLS estimator})$$

Two facts make this work:

- $\nabla_{\boldsymbol{\theta}}\, \mathbf{a}^\top \boldsymbol{\theta} = \mathbf{a}$ and $\nabla_{\boldsymbol{\theta}}\, \boldsymbol{\theta}^\top A\, \boldsymbol{\theta} = 2A\,\boldsymbol{\theta}$ for symmetric A.
- $\mathbf{X}^\top \mathbf{X}$ is symmetric: $(\mathbf{X}^\top \mathbf{X})^\top = \mathbf{X}^\top (\mathbf{X}^\top)^\top = \mathbf{X}^\top \mathbf{X}$. ✓

Step 1: expand the squared norm

Recall: $\|\mathbf{v}\|_2^2 = \mathbf{v}^\top \mathbf{v}$ for any vector $\mathbf{v}$ (the squared norm is the dot product with itself). Apply with $\mathbf{v} = \mathbf{y} - \mathbf{X}\boldsymbol{\theta}$:

$$\begin{aligned}\mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) &= (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^\top (\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) \\ &= \mathbf{y}^\top \mathbf{y} \;-\; \mathbf{y}^\top \mathbf{X}\boldsymbol{\theta} \;-\; (\mathbf{X}\boldsymbol{\theta})^\top \mathbf{y} \;+\; (\mathbf{X}\boldsymbol{\theta})^\top (\mathbf{X}\boldsymbol{\theta}).\end{aligned}$$

Why the middle two terms are equal. Each one is a scalar:

$$\underbrace{\mathbf{y}^\top}_{1\times n}\ \underbrace{\mathbf{X}}_{n\times(p+1)}\ \underbrace{\boldsymbol{\theta}}_{(p+1)\times 1} \quad \to \quad 1 \times 1 \quad \to \quad \text{a number.}$$

A scalar equals its own transpose, so $\mathbf{y}^\top \mathbf{X}\boldsymbol{\theta} = (\mathbf{y}^\top \mathbf{X}\boldsymbol{\theta})^\top = \boldsymbol{\theta}^\top \mathbf{X}^\top \mathbf{y}$. Combine:

$$\mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) = \mathbf{y}^\top \mathbf{y} \;-\; 2\,\boldsymbol{\theta}^\top \mathbf{X}^\top \mathbf{y} \;+\; \boldsymbol{\theta}^\top \mathbf{X}^\top \mathbf{X}\,\boldsymbol{\theta}.$$

Step 2: vector-calculus rules we need

Two rules. For constants $\mathbf{a} \in \mathbb{R}^d$ and symmetric $A \in \mathbb{R}^{d \times d}$:

$$\boxed{\nabla_{\boldsymbol{\theta}}\, \mathbf{a}^\top \boldsymbol{\theta} = \mathbf{a}} \qquad \boxed{\nabla_{\boldsymbol{\theta}}\, \boldsymbol{\theta}^\top A\, \boldsymbol{\theta} = 2\, A\, \boldsymbol{\theta}}$$

Where rule 1 comes from (one-line derivation):

$$\mathbf{a}^\top \boldsymbol{\theta} = \sum_j a_j \theta_j \;\Rightarrow\; \frac{\partial}{\partial \theta_j}(\mathbf{a}^\top \boldsymbol{\theta}) = a_j \;\Rightarrow\; \nabla_{\boldsymbol{\theta}}(\mathbf{a}^\top \boldsymbol{\theta}) = \mathbf{a}.$$

Rule 2 follows similarly (see math module 07 - multivariate calculus).

1D sanity check. If $d = 1$ and a, A are scalars,

$$\tfrac{d}{d\theta}(a\theta) = a, \qquad \tfrac{d}{d\theta}(A\theta^2) = 2A\theta. \;\checkmark$$

And $A = \mathbf{X}^\top \mathbf{X}$ is symmetric because $(\mathbf{X}^\top \mathbf{X})^\top = \mathbf{X}^\top \mathbf{X}$, so rule 2 applies.

Step 3: take the gradient

Differentiate $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) = \mathbf{y}^\top\mathbf{y} - 2\,\boldsymbol{\theta}^\top\mathbf{X}^\top\mathbf{y} + \boldsymbol{\theta}^\top(\mathbf{X}^\top\mathbf{X})\boldsymbol{\theta}$ term-by-term:

- $\nabla_{\boldsymbol{\theta}}\,\mathbf{y}^\top\mathbf{y} = 0$ (no $\boldsymbol{\theta}$)
- $\nabla_{\boldsymbol{\theta}}\,\left(-2\,\boldsymbol{\theta}^\top\mathbf{X}^\top\mathbf{y}\right) = -2\,\mathbf{X}^\top\mathbf{y}$ (rule 1 with $\mathbf{a} = \mathbf{X}^\top\mathbf{y}$)
- $\nabla_{\boldsymbol{\theta}}\,\boldsymbol{\theta}^\top(\mathbf{X}^\top\mathbf{X})\,\boldsymbol{\theta} = 2\,(\mathbf{X}^\top\mathbf{X})\,\boldsymbol{\theta}$ (rule 2)

Sum:

$$\nabla_{\boldsymbol{\theta}}\,\mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) = -2\,\mathbf{X}^\top\mathbf{y} + 2\,\mathbf{X}^\top\mathbf{X}\,\boldsymbol{\theta}.$$

Step 4: set the gradient to zero

At a stationary point of $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$:

$$-2\,\mathbf{X}^\top \mathbf{y} + 2\,\mathbf{X}^\top \mathbf{X}\,\boldsymbol{\theta} = 0 \quad \Longrightarrow \quad \boxed{\mathbf{X}^\top \mathbf{X}\,\hat{\boldsymbol{\theta}} = \mathbf{X}^\top \mathbf{y}}$$

These are the **normal equations** - a linear system in $\boldsymbol{\theta}$.

Why "normal"? The residual $\mathbf{r} = \mathbf{y} - \mathbf{X}\hat{\boldsymbol{\theta}}$ ends up *orthogonal* (normal) to every column of $\mathbf{X}$. The system above says exactly

$$\mathbf{X}^\top \mathbf{r} = 0.$$

Geometrically: each column of $\mathbf{X}$ is a "feature direction". The optimal residual has no remaining correlation with any feature - if it did, we could reduce the loss by moving $\boldsymbol{\theta}$ along that direction.

Step 5: solve for $\hat{\boldsymbol{\theta}}$

If $\mathbf{X}^\top \mathbf{X}$ is invertible, left-multiply both sides of $\mathbf{X}^\top \mathbf{X}\,\hat{\boldsymbol{\theta}} = \mathbf{X}^\top \mathbf{y}$ by $(\mathbf{X}^\top \mathbf{X})^{-1}$:

$$\boxed{\hat{\boldsymbol{\theta}} = (\mathbf{X}^\top \mathbf{X})^{-1}\,\mathbf{X}^\top \mathbf{y}}$$

This is the **ordinary least squares (OLS) estimator**.

Why this is the global minimum (not just a stationary point). The Hessian of $\mathcal{R}_{\text{emp}}(\boldsymbol{\theta})$ is

$$\nabla^2_{\boldsymbol{\theta}}\, \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) = 2\,\mathbf{X}^\top \mathbf{X}.$$

$\mathbf{X}^\top \mathbf{X}$ is positive semi-definite, meaning the loss surface is a *bowl* (never curves down). A stationary point of a bowl is the bottom. So $\hat{\boldsymbol{\theta}}$ is the global minimum.

Bonus: closed-form $\rightarrow$ no iteration, no learning rate, no convergence questions. The price: $\mathbf{X}^\top \mathbf{X}$ has to be invertible (next section).

Worked numerical example

Let $\mathbf{X} = \begin{pmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{pmatrix}$, $\mathbf{y} = \begin{pmatrix} 2 \\ 3 \\ 5 \end{pmatrix}$. Compute $\hat{\boldsymbol{\theta}}$ by hand.

$$\mathbf{X}^\top \mathbf{X} = \begin{pmatrix} 3 & 6 \\ 6 & 14 \end{pmatrix}, \qquad \mathbf{X}^\top \mathbf{y} = \begin{pmatrix} 10 \\ 23 \end{pmatrix}$$

$$\det(\mathbf{X}^\top \mathbf{X}) = 3 \cdot 14 - 6 \cdot 6 = 6$$

$$(\mathbf{X}^\top \mathbf{X})^{-1} = \tfrac{1}{6} \begin{pmatrix} 14 & -6 \\ -6 & 3 \end{pmatrix}$$

$$\hat{\boldsymbol{\theta}} = \tfrac{1}{6} \begin{pmatrix} 14 & -6 \\ -6 & 3 \end{pmatrix} \begin{pmatrix} 10 \\ 23 \end{pmatrix} = \tfrac{1}{6} \begin{pmatrix} 2 \\ 9 \end{pmatrix} = \begin{pmatrix} 1/3 \\ 3/2 \end{pmatrix}.$$

Fitted line: $\hat{y} = \frac{1}{3} + \frac{3}{2} x$.

Residuals. $\hat{\mathbf{y}} = \mathbf{X}\hat{\boldsymbol{\theta}} = (\frac{11}{6}, \frac{10}{3}, \frac{29}{6})$, so

$$\mathbf{r} = \mathbf{y} - \hat{\mathbf{y}} = (\tfrac{1}{6}, -\tfrac{2}{6}, \tfrac{1}{6}).$$

Orthogonality check: $\mathbf{X}^\top \mathbf{r}$ should be 0.

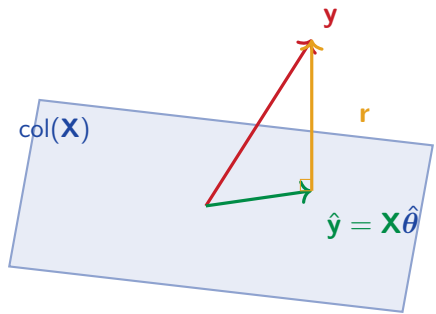
$$\tfrac{1}{6} - \tfrac{2}{6} + \tfrac{1}{6} = 0 \checkmark$$

$$1 \cdot \tfrac{1}{6} + 2 \cdot (-\tfrac{2}{6}) + 3 \cdot \tfrac{1}{6} = 0 \checkmark$$

Both columns of $\mathbf{X}$ are orthogonal to $\mathbf{r}$, exactly as the normal equations require.

Geometric picture

$\hat{\mathbf{y}} = \mathbf{X}\hat{\boldsymbol{\theta}}$ is the **orthogonal projection** of $\mathbf{y}$ onto the **column space** of $\mathbf{X}$ (the set of all vectors $\mathbf{X}\boldsymbol{\theta}$ as $\boldsymbol{\theta}$ ranges over $\mathbb{R}^{p+1}$ - the subspace reachable from our features).



OLS in one sentence: pick $\boldsymbol{\theta}$ so that the residual is perpendicular to every feature direction.

When does $\mathbf{X}^\top\mathbf{X}$ fail to be invertible?

Fact (from linear algebra): $\mathbf{X}^\top\mathbf{X}$ is invertible exactly when the $p+1$ columns of $\mathbf{X}$ are linearly independent.

Three common ways the columns become *dependent*:

- **Multicollinearity.** Two features are essentially the same. Example: weight in kg and weight in pounds (one is a constant multiple of the other).
- **Redundant encoding (the dummy trap).** Including *all* dummy columns for a categorical variable AND an intercept. The dummies always sum to the all-ones column.
- $p \geq n$**.** More features than observations. Columns live in $\mathbb{R}^n$ - you can't fit $p+1 > n$ linearly independent vectors in $\mathbb{R}^n$.

What to do when it fails

Options, in order of practicality:

1. **Drop the redundant column.** Cheap fix for the dummy trap and for obvious unit-of-measure duplicates.
2. **Use the pseudo-inverse:** `theta = np.linalg.pinv(X) @ y`. Works via SVD; returns the minimum-norm solution when the system is under-determined.
3. **Regularize.** Replace $\mathbf{X}^\top\mathbf{X}$ with $\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I}$. Always invertible for $\lambda > 0$. This is **Ridge regression** - L03.
4. **Gradient descent.** Works even when the closed form doesn't, and scales to large n, p - L02.

Computational cost

Forming and solving the normal equations costs:

- Building $\mathbf{X}^\top \mathbf{X}$: $\mathcal{O}(np^2)$ multiplications.
- Solving the $(p+1) \times (p+1)$ system (LU / Cholesky): $\mathcal{O}(p^3)$.
- Total: $\mathcal{O}(np^2 + p^3)$.

Big-$\mathcal{O}$ implications:

- Fine for $p \lesssim 10^3$. A laptop solves it instantly.
- Bad for $p \gtrsim 10^4$. The p^3 term dominates. Use gradient descent (L02) or stochastic methods.
- Numerically: prefer `np.linalg.lstsq(X, y)` or `np.linalg.solve(X.T @ X, X.T @ y)` over an explicit `np.linalg.inv(...)` call. Same answer, much better conditioning.

Same model, different features

Linear regression is linear **in the parameters $\boldsymbol{\theta}$**, not in the inputs $\mathbf{x}$. Nothing stops us from feeding it nonlinear functions of x.

For a single feature $x \in \mathbb{R}$, the degree-d polynomial model is

$$f(\mathbf{x}) = \theta_0 + \theta_1 x + \theta_2 x^2 + \cdots + \theta_d x^d.$$

"But x^2 is nonlinear!" Yes - the *fitted function* is nonlinear in x. But the *optimization problem* is still linear regression: we treat x^2 as just another column of the design matrix. Define the basis expansion

$$\phi(x) = (1, x, x^2, \ldots, x^d)^\top \in \mathbb{R}^{d+1},$$

then $f(\mathbf{x}) = \boldsymbol{\theta}^\top \phi(x)$ - linear in $\boldsymbol{\theta}$.

Polynomial design matrix

Stack the basis-expanded inputs into a new design matrix:

$$\mathbf{X}_\phi = \begin{pmatrix} 1 & x^{(1)} & (x^{(1)})^2 & \cdots & (x^{(1)})^d \\ 1 & x^{(2)} & (x^{(2)})^2 & \cdots & (x^{(2)})^d \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x^{(n)} & (x^{(n)})^2 & \cdots & (x^{(n)})^d \end{pmatrix} \in \mathbb{R}^{n \times (d+1)}.$$

Key observation: from OLS's perspective $\mathbf{X}_\phi$ is just another design matrix. The normal equation is unchanged:

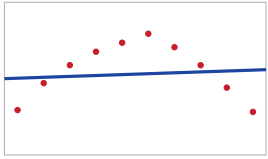
$$\hat{\boldsymbol{\theta}} = (\mathbf{X}_\phi^\top \mathbf{X}_\phi)^{-1} \mathbf{X}_\phi^\top \mathbf{y}.$$

In code: `from sklearn.preprocessing import PolynomialFeatures`. For multiple features, the same idea also generates *interaction* terms like $x_1 x_2$, $x_1^2 x_2$.

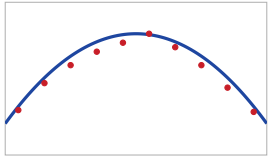
Predict-first: which curve generalizes?

Three fits on the same 10 noisy samples from $y = \sin(\pi x) + \varepsilon$, $x \in [0, 1]$.

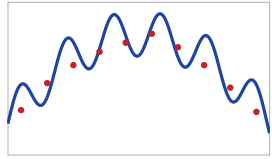
curve A



curve B



curve C



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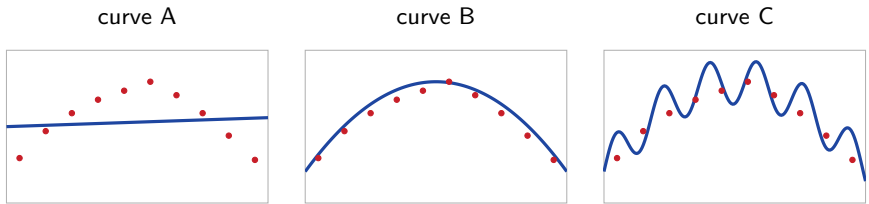

Predict, then read on: (1) Which has the smallest training error? (2) Which has the smallest test error? (3) Which would you deploy?

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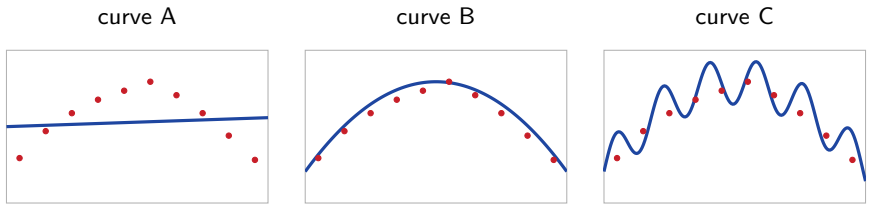
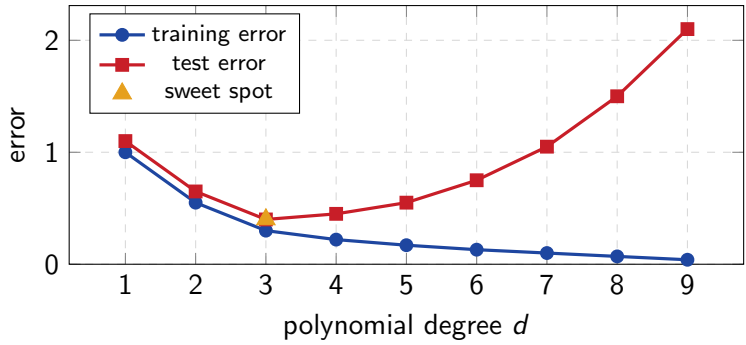


Predict, then read on: (1) Which has the smallest training error? (2) Which has the smallest test error? (3) Which would you deploy?

Answers: A is degree 1 (*underfit*, biggest train AND test error). C is degree 9 (*overfit*, tiny train error, biggest test error). **B** is degree 3 - small train error AND small test error. Deploy B.

The U-shape of test error



Training error keeps falling. Test error has a **U-shape**. Minimum at the sweet spot.
Numbers illustrative; exact values depend on noise level and sample size.

What polynomial regression teaches us

1. **Linearity is in θ, not in x.** Almost every model in classical ML (kernel methods, basis splines, fixed-feature neural networks) is "linear regression on engineered features".
2. **More features = more flexibility = more overfitting risk.** The U-shape is the bias-variance tradeoff (formalized in L04).
3. **We need a way to penalize complexity.** If we can't drop features by hand, can we penalize their size? $\rightarrow$ **regularization** (L03).
4. **We need a way to evaluate honestly.** Training error is not enough. $\rightarrow$ **hold-out + cross-validation** (L04, L05).

Wrap-up

- Pad inputs with a 1 so the intercept lives inside $\boldsymbol{\theta}$. One formula everywhere.
- Design matrix $\mathbf{X}$: rows are observations, columns are features. Predictions vectorize as $\hat{\mathbf{y}} = \mathbf{X}\boldsymbol{\theta}$.
- Normal equation $(\mathbf{X}^\top \mathbf{X})\,\hat{\boldsymbol{\theta}} = \mathbf{X}^\top \mathbf{y}$ comes from $\nabla \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) = 0$. Geometrically: residual perpendicular to every feature column.
- OLS fails when $\mathbf{X}^\top \mathbf{X}$ is singular. Fixes: drop a column, pseudo-inverse, ridge, or gradient descent.
- Polynomial regression is OLS with $\phi(x) = (1, x, x^2, \ldots, x^d)$. Same algebra, more flexibility - and more overfitting risk.

HW01b - implement and verify.

1. Implement OLS from scratch using only `np.linalg.solve(X.T @ X, X.T @ y)`.
2. Verify against `sklearn.linear_model.LinearRegression`: `np.allclose(theta_mine, sk.coef_, atol=1e-10)`.
3. Extend to polynomial degree 3 by hand-constructing $\mathbf{X}_\phi$. Compare to `PolynomialFeatures`.
4. Bonus: time the loop version vs. the vectorized version for $n = 10^5$, $p = 50$ and report the ratio.