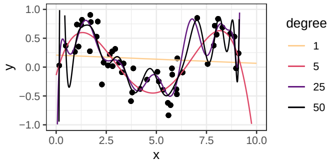
Introduction to Machine Learning

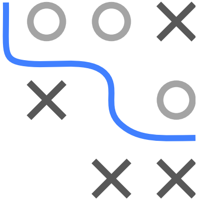
Supervised Regression: Polynomial Regression Models



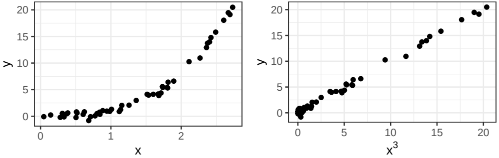
Learning goals

- Learn about general form of linear model
- See how to add flexibility by using polynomials
- Understand that more flexibility is not necessarily better

INCREASING FLEXIBILITY



- Recall our definition of LM: model y as linear combo of features
- But: isn't that pretty **inflexible**?
- E.g., here, y does not seem to be a linear function of x...



... but relation to x^3 looks pretty linear!

- Many other trafos conceivable, e.g., $\sin(x_1)$, $\max(0, x_2)$, $\sqrt{x_3}, \dots$
- Turns out we can use LM much more **flexibly** (and: it's still linear)
  $\rightsquigarrow$ interpretation might get less straightforward, though

THE LINEAR MODEL

- Recall what we previously defined as LM:

$$f(x) = \theta_0 + \sum_{j=1}^{p} \theta_j x_j = \theta_0 + \theta_1 x_1 + \cdots + \theta_p x_p \tag{1}$$

- Actually, just special case of "true" LM
- **The linear model** with **basis functions** ϕ_j:

$$f(\mathbf{x}) = \theta_0 + \sum_{j=1}^{p} \theta_j \phi_j(x_j) = \theta_0 + \theta_1 \phi_1(x_1) + \cdots + \theta_p \phi_p(x_p)$$

- In Eq. 1, we implicitly use identity trafo: $\phi_j = \mathrm{id}_x : x \mapsto x \quad \forall j$
  $\rightsquigarrow$ we often say LM and imply $\phi_j = \mathrm{id}_x$

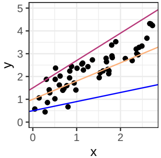
THE LINEAR MODEL

- Are models like $f(\mathbf{x}) = \theta_0 + \theta_1 x^2$ **really linear**?
  - Certainly not in covariates:

$$\begin{aligned} a \cdot f(x, \boldsymbol{\theta}) + b \cdot f(x_*, \boldsymbol{\theta}) &= \theta_0(a+b) + \theta_1(ax^2 + bx_*^2) \\ &\neq \theta_0 + \theta_1(ax + bx_*)^2 \\ &= f(ax + bx_*, \boldsymbol{\theta}) \end{aligned}$$

  - Crucially, however, **linear in params**:

$$\begin{aligned} a \cdot f(x, \boldsymbol{\theta}) + b \cdot f(x, \boldsymbol{\theta}^*) &= a\theta_0 + b\theta_0^* + (a\theta_1 + b\theta_1^*)x^2 \\ &= f(x, a\boldsymbol{\theta} + b\boldsymbol{\theta}^*) \end{aligned}$$



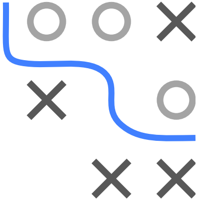
$\boldsymbol{\theta} = (0.5, 0.4)^\top$
$\boldsymbol{\theta} = (1.0, 0.8)^\top$
$\boldsymbol{\theta} = (1.5, 1.2)^\top$

- NB: we still call design matrix $\mathbf{X}$, incorporating possible trafos:

$$\mathbf{X} = \begin{pmatrix} 1 & \phi_1(x_1^{(1)}) & \dots & \phi_p(x_p^{(1)}) \\ \vdots & \vdots & & \vdots \\ 1 & \phi_1(x_1^{(n)}) & \dots & \phi_p(x_p^{(n)}) \end{pmatrix}$$

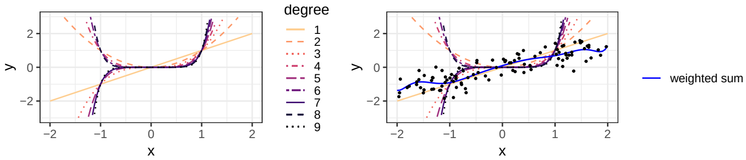
$\rightsquigarrow$ solution via normal equations as usual

POLYNOMIAL REGRESSION



- Simple & flexible choice for basis funs: ***d*-polynomials**
- Idea: map x_j to (weighted) sum of its monomials up to order $d \in \mathbb{N}$

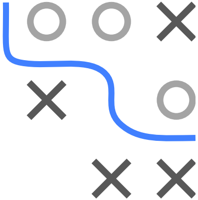
$$\phi^{(d)} : \mathbb{R} \to \mathbb{R}, \quad x_j \mapsto \sum_{k=1}^{d} \beta_k x_j^k$$



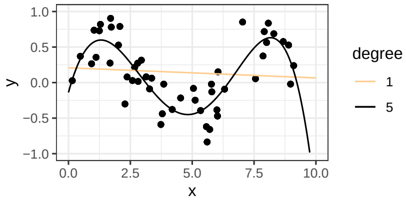
- How to estimate coefficients β_k?
  - Both LM & polynomials **linear** in their params $\rightsquigarrow$ merge
  - E.g., $f(\mathbf{x}) = \theta_0 + \theta_1 \phi^{(d)}(x) = \theta_0 + \sum_{k=1}^{d} \theta_{1,k} x^k$

$$\rightsquigarrow \mathbf{X} = \begin{pmatrix} 1 & x^{(1)} & (x^{(1)})^2 & \dots & (x^{(1)})^d \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x^{(n)} & (x^{(n)})^2 & \dots & (x^{(n)})^d \end{pmatrix}, \quad \boldsymbol{\theta} \in \mathbb{R}^{d+1}$$

POLYNOMIAL REGRESSION – EXAMPLES



Univariate regression, $d \in \{1, 5\}$



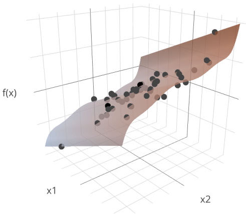
- Data-generating process:

$$y = 0.5\sin(x) + \epsilon,$$
$$\epsilon \sim \mathcal{N}(0, 0.3^2)$$

- Model:

$$f(x) = \theta_0 + \sum_{k=1}^{d} \theta_{1,k} x^k$$

Bivariate regression, $d = 7$



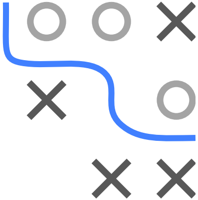
- Data-generating process:

$$y = 1 + 2x_1 + x_2^3 + \epsilon,$$
$$\epsilon \sim \mathcal{N}(0, 0.5^2)$$

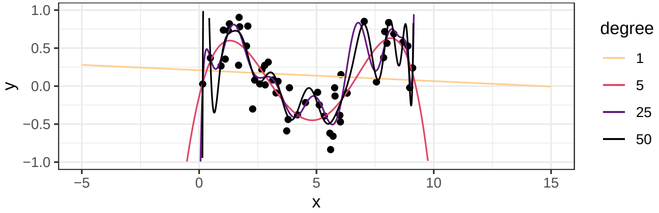
- Model:

$$f(x) = \theta_0 + \theta_1 x_1 + \sum_{k=1}^{7} \theta_{2,k} x_2^k$$

COMPLEXITY OF POLYNOMIALS



- Higher d allows to learn more complex functions
  $\rightsquigarrow$ richer hyp space / higher **capacity**



- Should we then simply let $d \to \infty$?
  - **No**: data contains random **noise** – not part of true DGP
  - Model with overly high capacity learns all those spurious patterns $\rightsquigarrow$ poor generalization to new data
  - Also, higher d can lead to oscillation esp. at bounds (Runge's phenomenon[1])

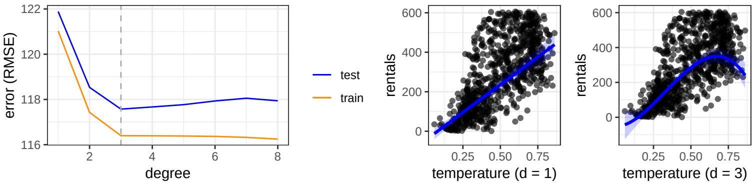
[1] Interpolation of m equidistant points with d-polynomial only well-conditioned for $d < 2\sqrt{m}$.
Plot: 50 points, models with $d \geq 14$ instable (under equidistance assumption).

BIKE RENTAL EXAMPLE

- OpenML task `dailybike`: predict `rentals` from weather conditions
- Hunch: non-linear effect of `temperature` $\rightsquigarrow$ include with polynomial:

$$f(\mathbf{x}) = \sum_{k=1}^{d} \theta_{\text{temperature},k} x_{\text{temperature}}^{k} + \theta_{\text{season}} x_{\text{season}} + \theta_{\text{humidity}} x_{\text{humidity}}$$

- Test error[2] confirms suspicion $\rightsquigarrow$ minimal for $d = 3$



d	θ_0	$\theta_{\text{temp},1}$	$\theta_{\text{temp},2}$	$\theta_{\text{temp},3}$	θ_{sSPRING}	θ_{sSUMMER}	θ_{sFALL}	θ_{hum}	**test error**
1	377.3	2778.2			101.0	57.0	80.1	-230.0	**121.9**
3	419.3	2645.8	-963.1	-430.9	71.9	75.8	56.6	-283.8	**117.6**

- Conclusion: flexible effects can improve fit/performance

[2] Reliable insights about model performance only via separate test dataset not used during training (here computed via 10-fold *cross validation*). Much more on this in Evaluation chapter.