Linear Regression

SWC Neuroinformatics 2024

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Intro

Linear regression is ***everywhere***

The practicalities are endless

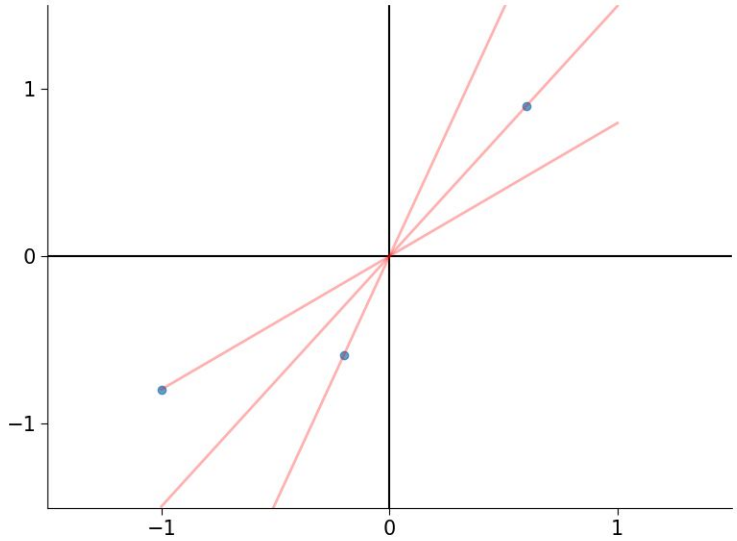
It is worthwhile taking time to go through the basics

Outline

- The Least Squares solution in 1 and multiple dimensions
- Model complexity, Bias-Variance tradeoff, and regularization
- Probabilistic / Bayesian interpretation of linear regression
- Some examples

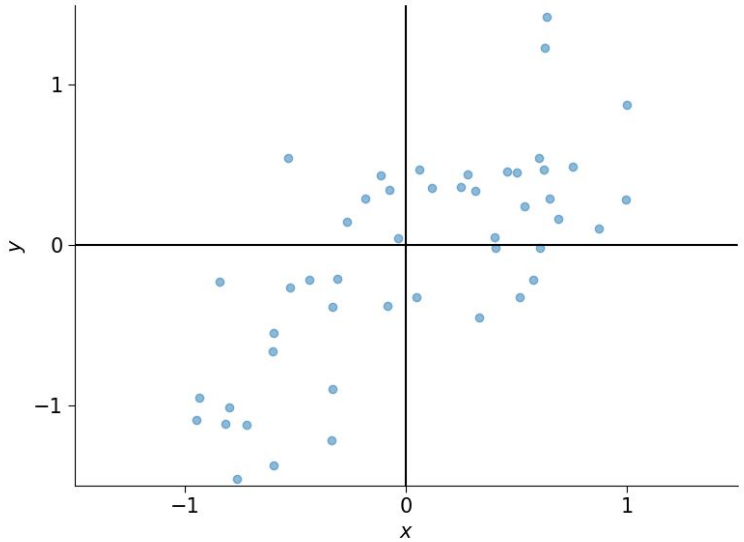
The problem

- Given a sample (x^i, y^i), find a good way to describe the dependence of *y* on *x*.
- Immediate questions:
  - What makes a fit “good”?
  - What type of dependences are we willing to consider?
- Keep in mind: we would like our model to be able to predict *unseen* future data
- Restrict to **linear** model: **y ~ bx**
  - If there was a single point, we could fit perfectly
  - What shall we do if there are multiple points?



Least Squares

- Instead of trying to perfectly fit each point, minimise the sum of squared errors
- The minimisation is over the parameter, ***b***
- Why squared error?
  - Mathematically convenient
  - The “right” thing under some assumptions (later)
- Deriving the solution



Multiple predictors

- Each **x** is now a vector $[x_1\ x_2\ \ldots\ x_p]^T$
- Linear mapping $x \mapsto y$ is parameterised by a vector of coefficients, $\mathbf{y \sim x^T b}$

Deriving the solution

Interpretation:

- The analogy to the 1D case
- The predictions for **y** are $\mathbf{Xb = X(X^TX)^{-1}X^Ty}$: the *orthogonal projection* of **y** onto the space spanned by the input vectors

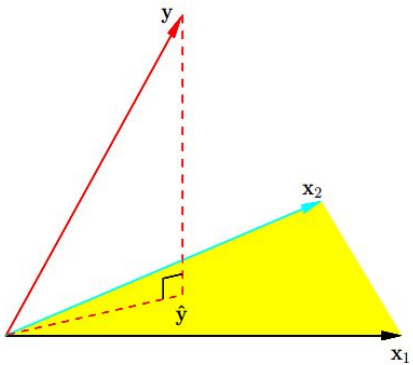


Fig source: The Elements of Statistical Learning

Adding an offset

- By positing **y ~ bx** we have constrained the regression line to pass through the origin
- We can instead assume **y ~ bx + c** to allow an offset (aka ‘bias’, ‘intercept’)

$$b^* = \mathrm{Cov}[x,y]/\mathrm{Var}[x] \qquad c^* = E[y] - bE[x]$$

- The optimal (minimising MSE) line goes through the sample average
- Therefore we can alternatively *center* the data, and consider the homogeneous model
  - Note that this recovers the “full” solution, as **Cov[x,y]=E[xy]** and **Var[x]=E[x^2]**

- Alternatively, we can view **y ~ bx + c** as a multiple predictors case
- For that, we redefine the examples, with mapping $x \mapsto [x, 1]$.
- **Exercise**: show the solutions match: $[b^* \; c^*]^T = (X^TX)^{-1}X^Ty$, after the remapping

The asymmetry in regression

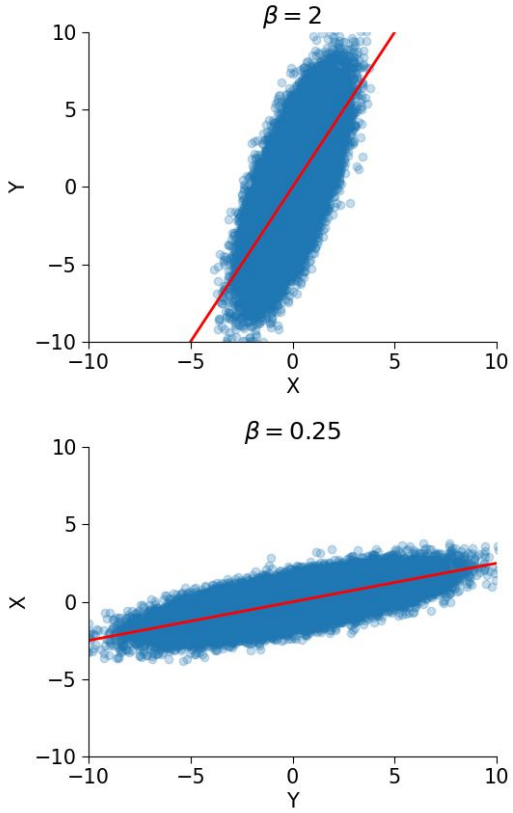
- Regressing **y ~ bx** and **x ~ ay** isn't the same – in general, a ≠ 1/b

- This is due to the division by Var[x]!

$$b_{y\sim x} = E[xy]/E[x^2]$$
$$b_{x\sim y} = E[xy]/E[y^2]$$

- Changes the role of the "noise"

In this example: x ~ N(0,1), y=2x+e, e~N(0,2²)



Inference and hypothesis testing

- So far we didn't commit too much to the true data distribution
- If we add some assumptions, we can say more about the result

In particular, we assume that:

- observations **y** were generated by an **unknown** linear model
- additive gaussian noise
- independent (and equal variance) noise between different observations

Mathematically, assume that $\mathbf{y=X\beta+\varepsilon}$, with $\boldsymbol{\varepsilon \sim N(0,\sigma^2 I)}$

Inference and hypothesis testing

We can now work out the distribution of the estimator $\boldsymbol{\beta}$ – this is a simple exercise in manipulating gaussian distributions:

$$\begin{aligned}\boldsymbol{\beta} &= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} \\ &= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T(\mathbf{X}\boldsymbol{\beta}+\boldsymbol{\varepsilon}) \\ &= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{X}\boldsymbol{\beta} + (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\boldsymbol{\varepsilon} \\ &= \boldsymbol{\beta} + (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\boldsymbol{\varepsilon}\end{aligned}$$

And therefore, we have $\boldsymbol{\beta} \sim \mathbf{N}(\boldsymbol{\beta}, (\mathbf{X}^T\mathbf{X})^{-1}\sigma^2)$

- Unbiased
- Lowest variance among all linear unbiased estimators (*Gauss Markov Theorem)*

Inference and hypothesis testing

- Now that we have the distribution of **β** we can perform hypothesis testing
- For example, we might want to test whether $\beta_i \neq 0$:
  - Write the distribution of β_i under the null, i.e., under $\beta_i = 0$, and compare the observed value
  - In our case, this would be a simple Z-test (since we assumed known variance)
  - If the variance is unknown, it can be estimated, resulting in a *t*-distribution for the standardised β_i

- The assumptions allow the usage of many standard statistical tools (t-test, F-test, etc)

- Can be slightly relaxed if we are willing to use nonparametric tests (e.g., bootstrap)

Rethinking the “linear” in linear regression

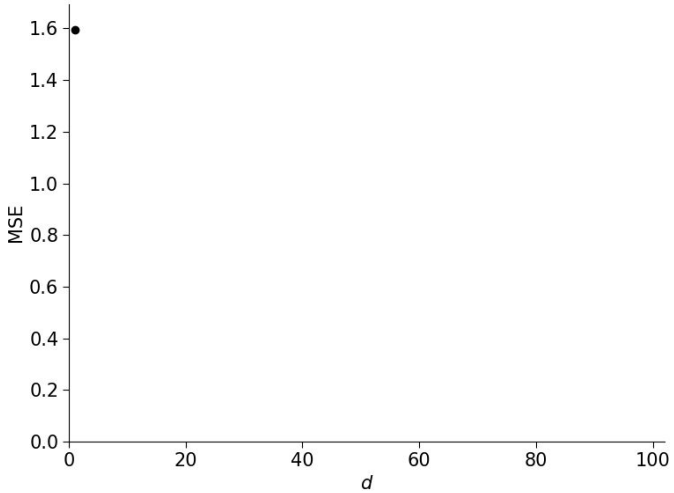
- The important thing was linearity **in the parameters**
- We can add more predictors, which are functions of the original variables, resulting in non-linear functions of those

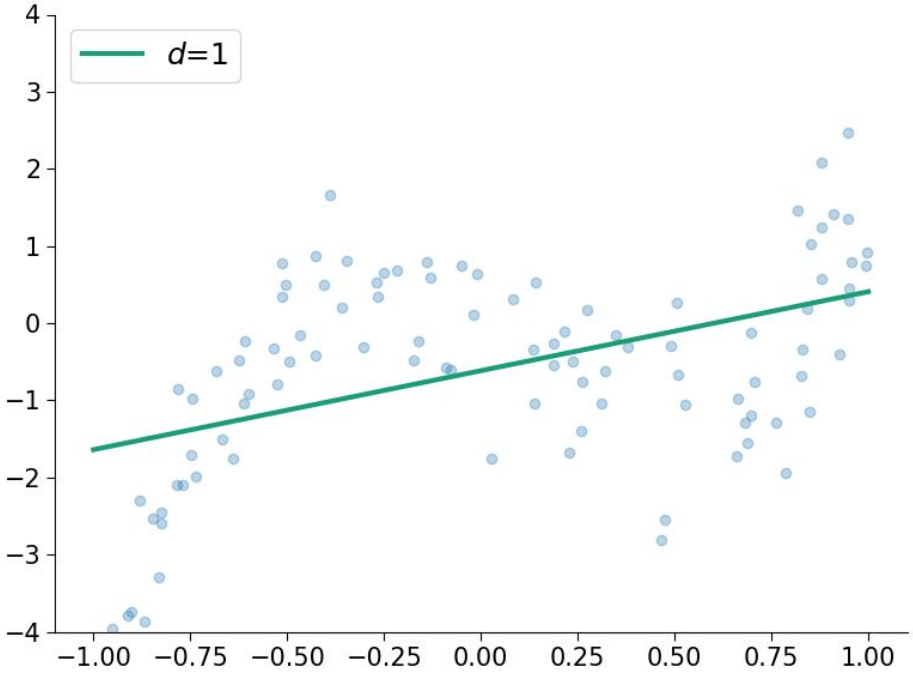
Example: polynomial regression

- Suppose we have 1D inputs x. We map $\mathbf{x} \mapsto [x \;\; x^2 \;\; x^3 \ldots x^d]^T$, and solve for **b**
- Then effectively we have a model $\mathbf{y \sim b_1 x + b_2 x^2 + \ldots + b_d x^d}$ – a *d* degree polynomial

- What happens as we increase **d**?
  - We are making the model less and less constrained
  - Since poly(d) $\subset$ poly(d+1), we can only decrease the error by taking larger and larger **d**
  - Is this the right thing to do?

Model complexity





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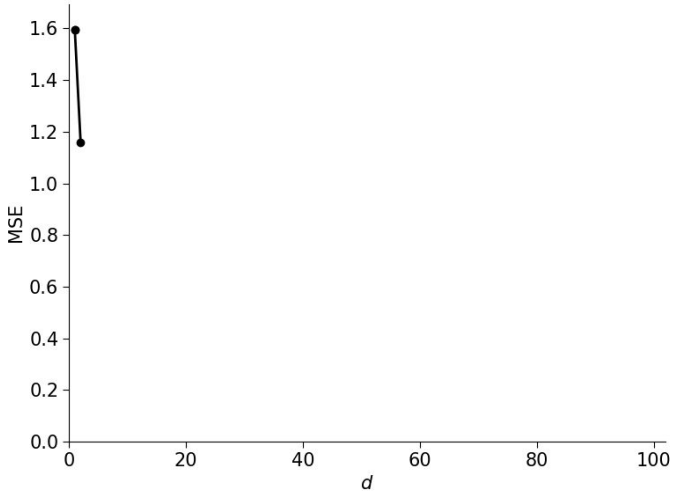

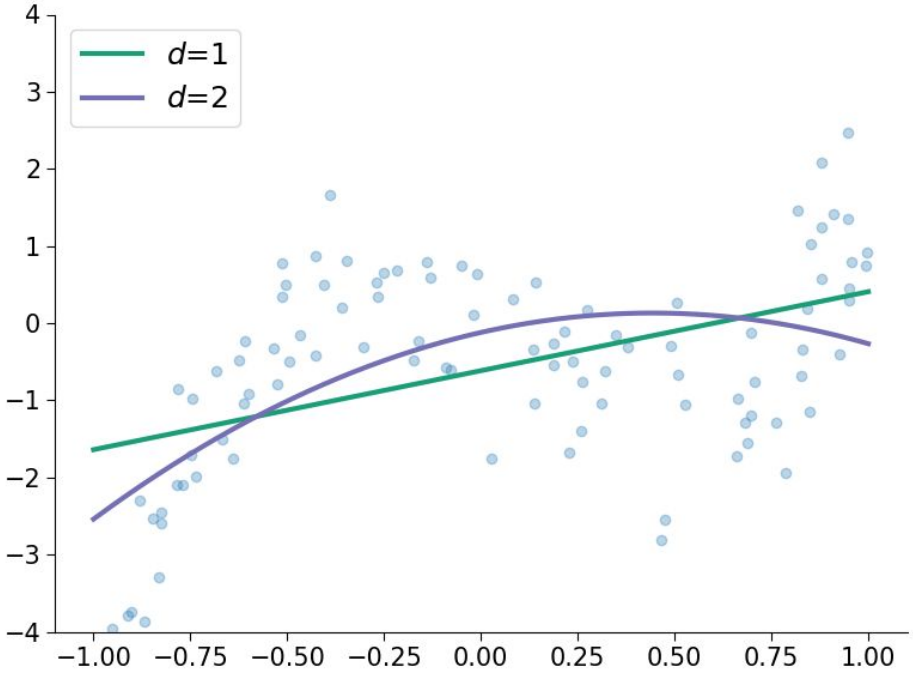

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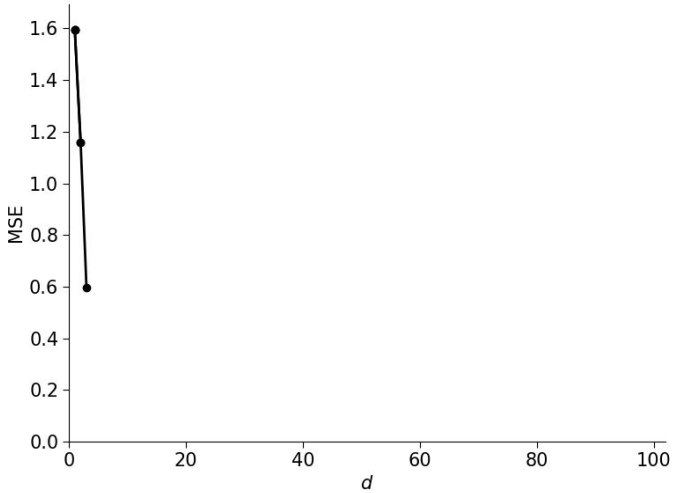

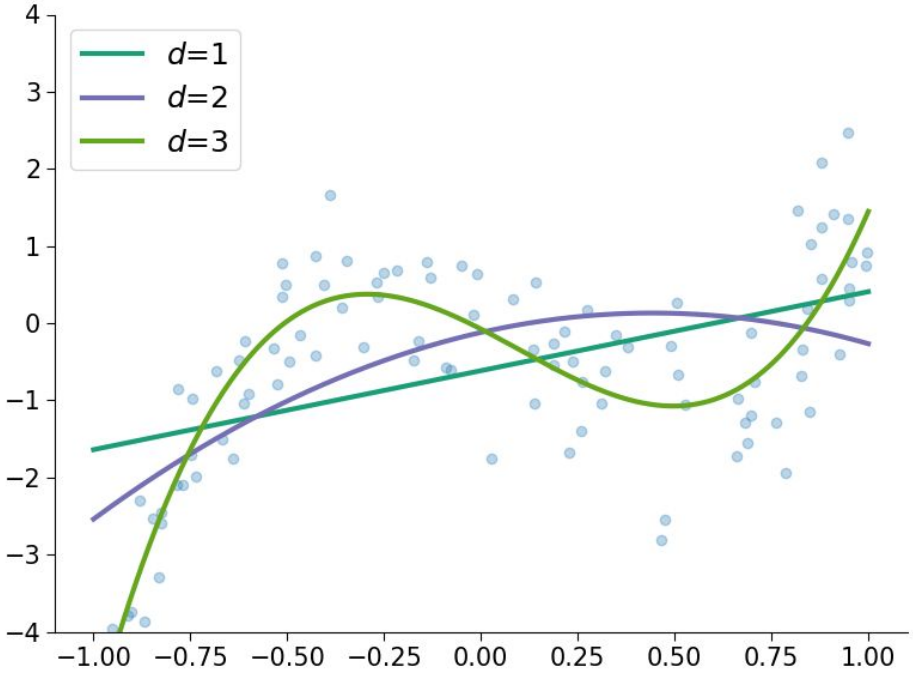

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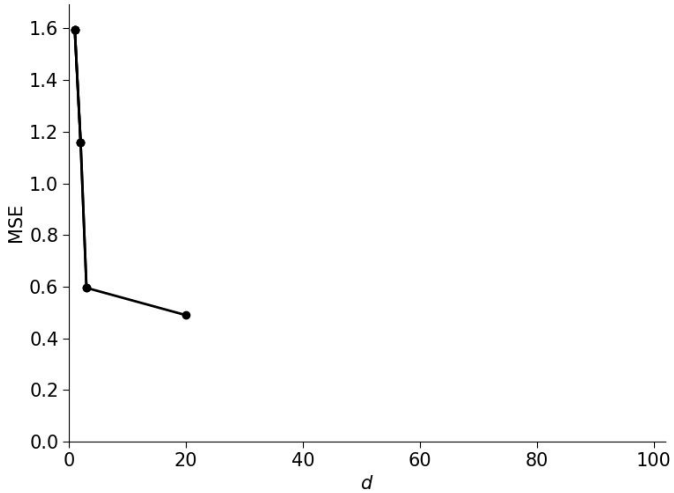

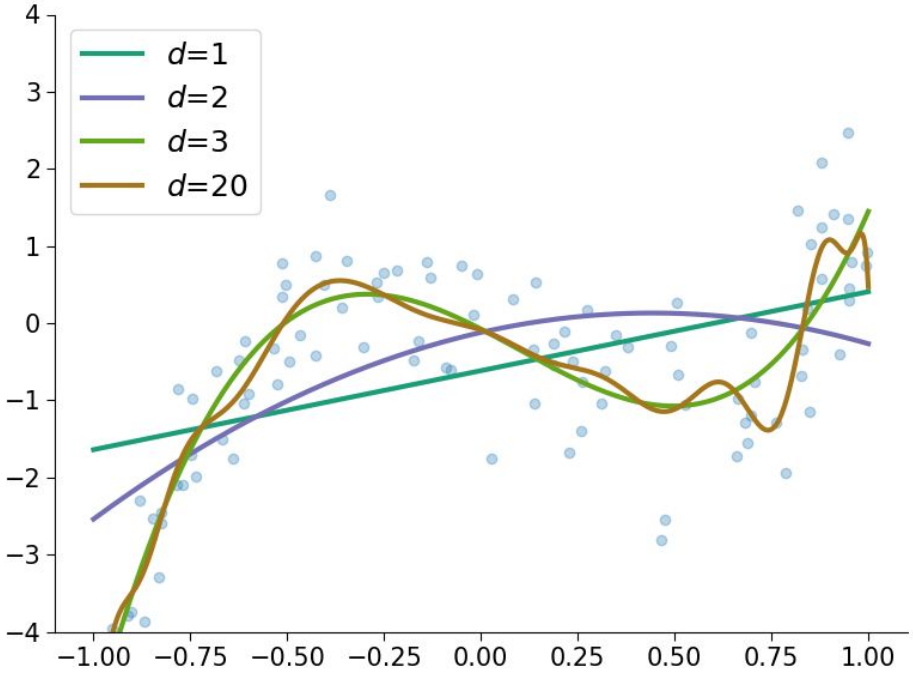

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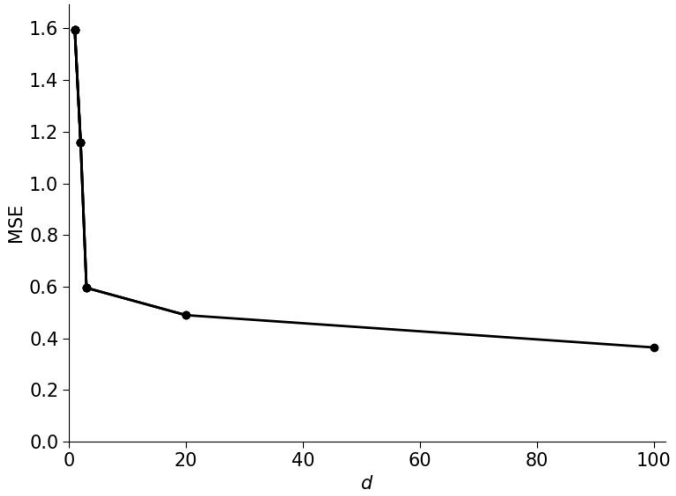

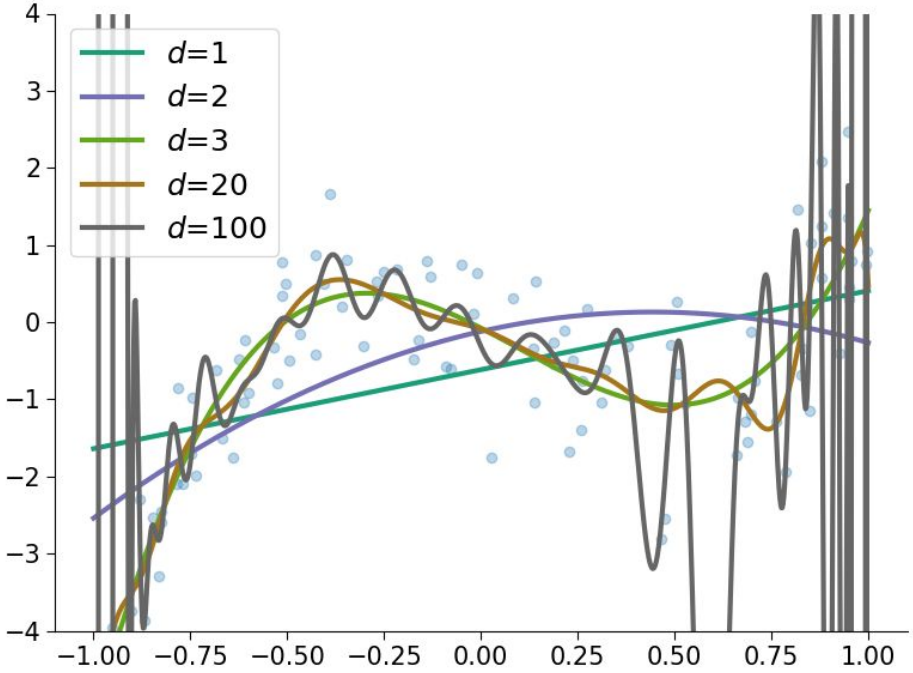

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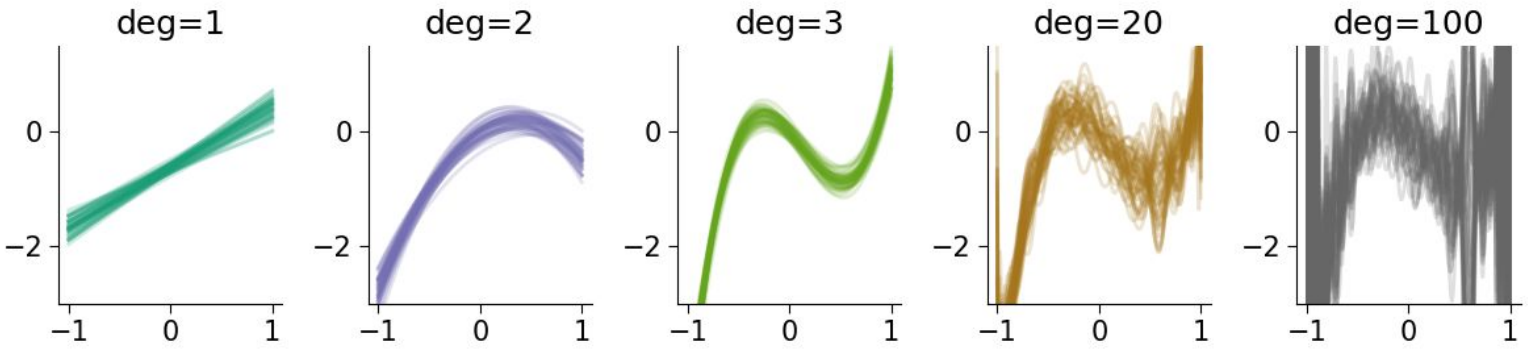


The bias-variance tradeoff

The complex models have:

- Low **bias** – they will fit whatever sample we give them
- High **variance** – different samples will result in very different predictions

The simple models have:

- High **bias** – they will systematically differ from the observations
- Low **Variance** – different samples result in similar predictions

The expected generalization error depends on both bias and variance

Bias-Variance decomposition of MSE

- Assume the true data is generated by $\mathbf{y = f(x) + \varepsilon}$
- We estimate $\hat{f}$ based on a sample $(x^1,y^1, \dots , x^N,y^N)$
- what is the expected error on a **new** datapoint **x**?

$$\mathbf{E[(y-\hat{f})^2] = E[(f + \varepsilon - \hat{f})^2]}$$

$$\mathbf{= E[\varepsilon^2 + f^2 - 2f\hat{f} + \hat{f}^2]} \qquad (\varepsilon \text{ uncorrelated with } \hat{f})$$

$$\mathbf{= \sigma^2 + f^2 - 2fE[\hat{f}] + Var[\hat{f}] + E^2[\hat{f}]} \qquad (E[X^2]=Var[X]+E^2[X])$$

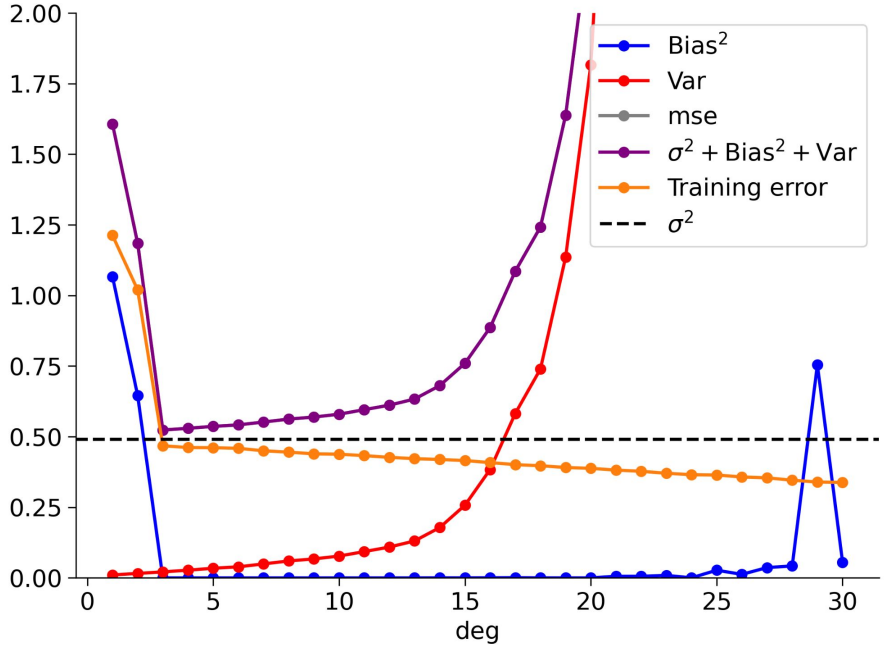
$$\mathbf{= \sigma^2 + (E[\hat{f}]-f)^2 + Var[\hat{f}]}$$

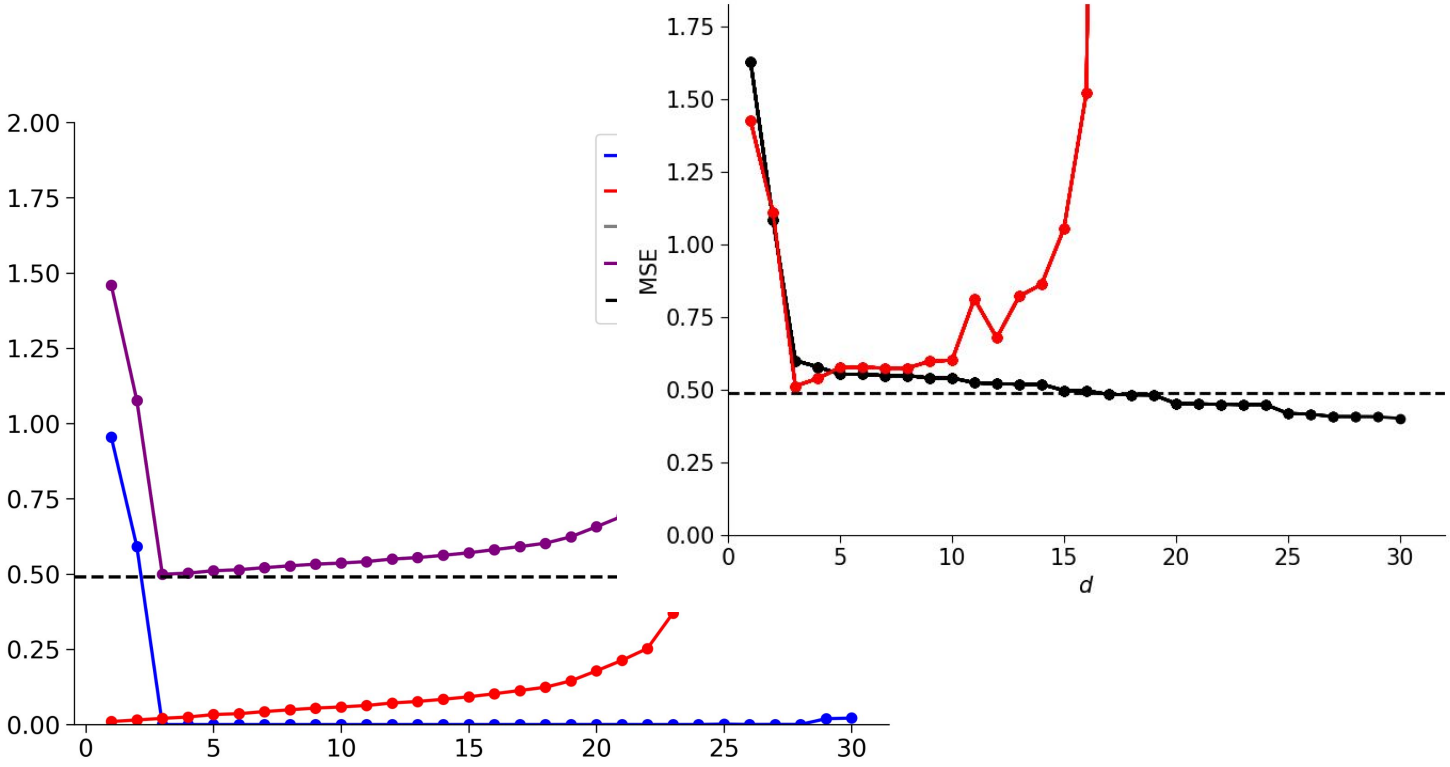
The total expected error: Irreducible error + Bias squared + Variance

The polynomial regression example, again

- Training error keep decreasing
- Generalization error diverges

Making the model more and more complex was **not** the right thing to do

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Regularization

- It is sometimes beneficial to explicitly constraint model complexity, even if we make it biased as a result. This is known as regularization

- The typical way: constraint the magnitude of $\boldsymbol{\beta}$, “shrinking” parameters towards 0
- Solve a different optimisation problem. For example:

$$\boldsymbol{\beta} = \min\{(\mathbf{y}-\mathbf{X}\boldsymbol{\beta})^T(\mathbf{y}-\mathbf{X}\boldsymbol{\beta}) + \lambda\boldsymbol{\beta}^T\boldsymbol{\beta}\} \qquad \text{(Ridge regression)}$$

$$\boldsymbol{\beta} = (\mathbf{X}^T\mathbf{X}+\lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y} \qquad \text{(Solution)}$$

- Alternatively, could use L_1 (rather than L_2) norm, resulting in the Lasso objective

Regularization – Ridge and Lasso

- Both methods shrink the parameters, but there are some differences
- Ridge will shrink magnitude of all parameters without setting them to 0
- Lasso will result in a sparse solution, setting small parameters to 0

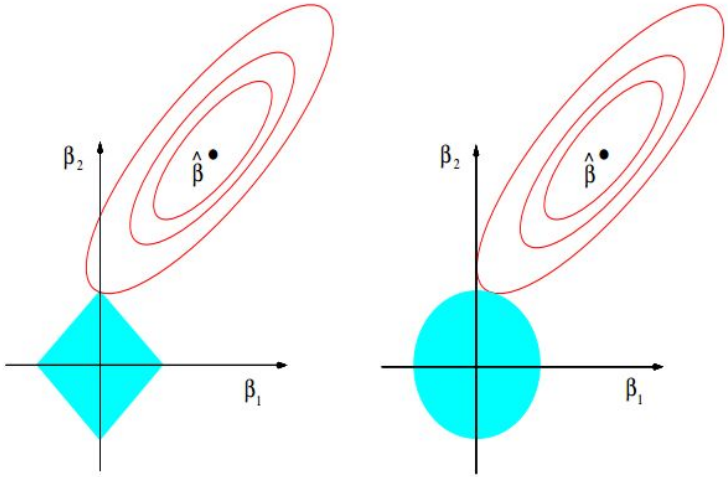


Fig source: The Elements of Statistical Learning

Ridge regression – geometric intuition

- Recall – the SVD decomposition $\mathbf{X=U\Sigma V^T}$
- Plugging into the (ordinary) solution:

$$\mathbf{Xb = X(X^TX)^{-1}X^Ty = UU^Ty}$$

- The orthogonal projection onto the column space of **X**, as we've seen before
- The ridge regression solution is

$$\mathbf{Xb = X(X^TX+\lambda I)^{-1}X^Ty = U\Sigma(\Sigma^2+\lambda I)^{-1}\Sigma U^Ty}$$

- Same projection, but each component is scaled down by $d_i^2/(d_i^2+\lambda)$

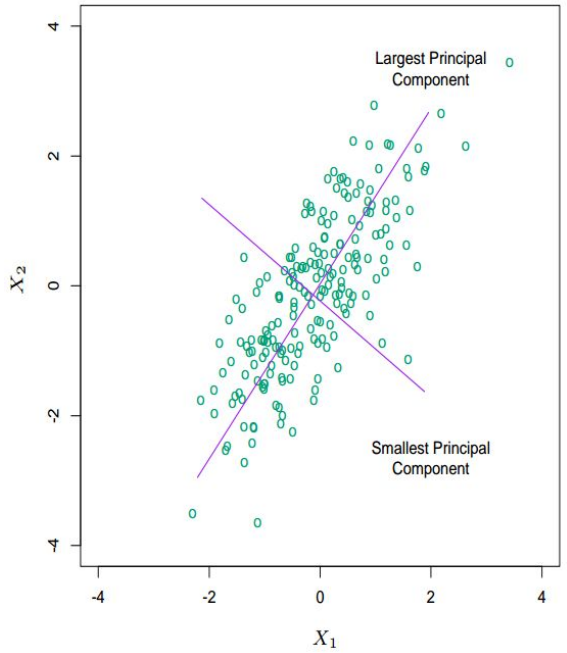


Fig source: The Elements of Statistical Learning

Probabilistic interpretation of linear regression

- Back to the basics: why minimise the **square error**?
- If we assume that the data was generated by an unknown linear model with additive gaussian noise, this is equivalent to **maximising the likelihood**:

$$\begin{aligned} \log P(y_1, \dots, y_N|b) &= \log P(y_1|b) + \dots + \log P(y_N|b) \\ &= -0.5*\sigma^{-2}(y_1 - x_1 b)^2 - \dots - 0.5*\sigma^{-2}(y_N - x_N b)^2 + C \end{aligned}$$

- Therefore, the **maximum-likelihood estimator** for β is the least square estimator

Adding a prior

- We use the data to update our belief about the true parameter.
- But what if we already have some prior belief? We use Bayes' theorem:

$$p(\beta \mid D) \propto p(\beta)\, p(D|\beta)$$

- For example, we might assume a-priori that $\boldsymbol{\beta \sim N(0, \tau I)}$. Then, the log posterior is:

$$\log p(\beta \mid D) = C \; -0.5\, \tau^{-1} \beta^T \beta - 0.5 \sigma^{-2} (y - X\beta)^T (y - X\beta)$$

- Maximizing this is the same as solving ridge regression, with $\boldsymbol{\lambda = \sigma^2/\tau}$
- Consider the extreme cases:

"Uniform"/flat prior: Large $\boldsymbol{\tau}$, resulting in $\boldsymbol{\lambda \to 0}$, reducing to OLS

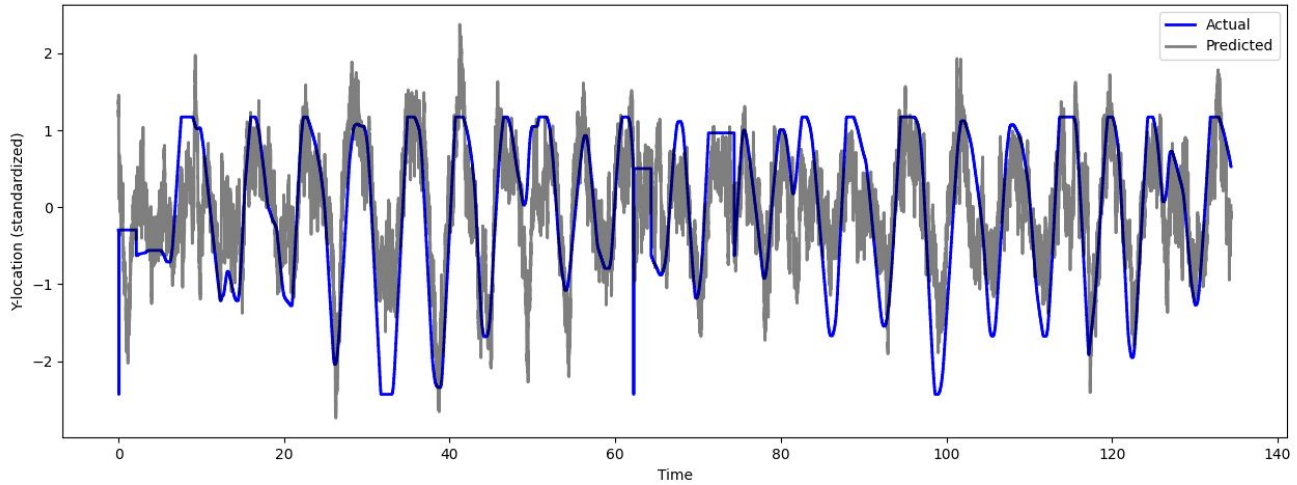
Strong prior: Small $\boldsymbol{\tau}$, resulting in $\boldsymbol{\lambda \to \infty}$, retaining $\beta = 0$

Towards Bayesian Linear Regression

- The Gaussian case is special because of conjugacy
  - posterior remains a gaussian with updated parameters
- In this case, the MAP is also the posterior mean
- The general case (non-zero prior mean, general prior covariance) is also tractable
- Serves as the basic intuition/building blocks for many more Bayesian models

Example 1: Decoding

- We try to predict stimulus/behavior from neural data
- Example: subjects using joystick to move a cursor, following target location
- Predict the cursor location from ECoG data



Data: https://compneuro.neuromatch.io/projects/ECoG/README.html ; paper: Shalck et al. 2007, https://iopscience.iop.org/article/10.1088/1741-2560/4/3/012

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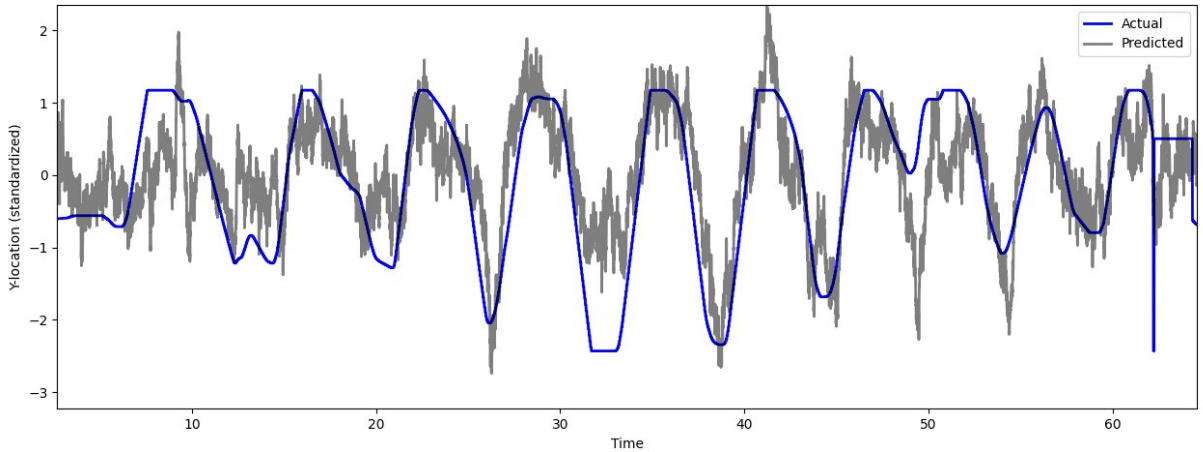

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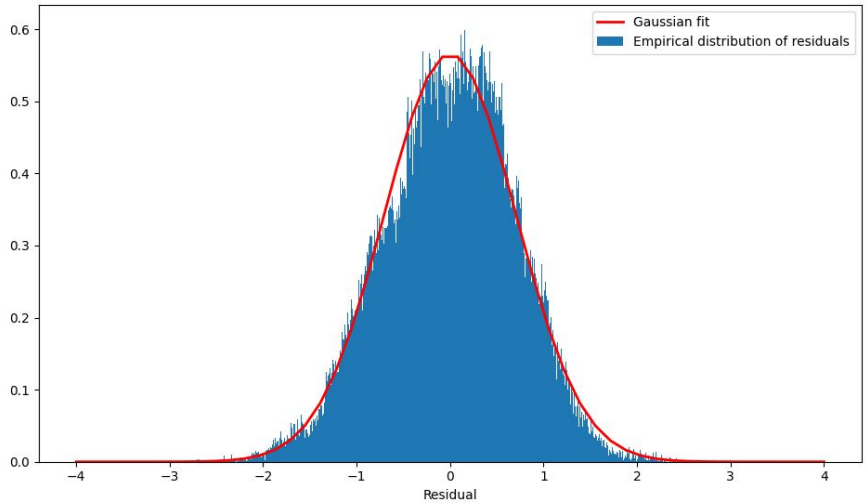

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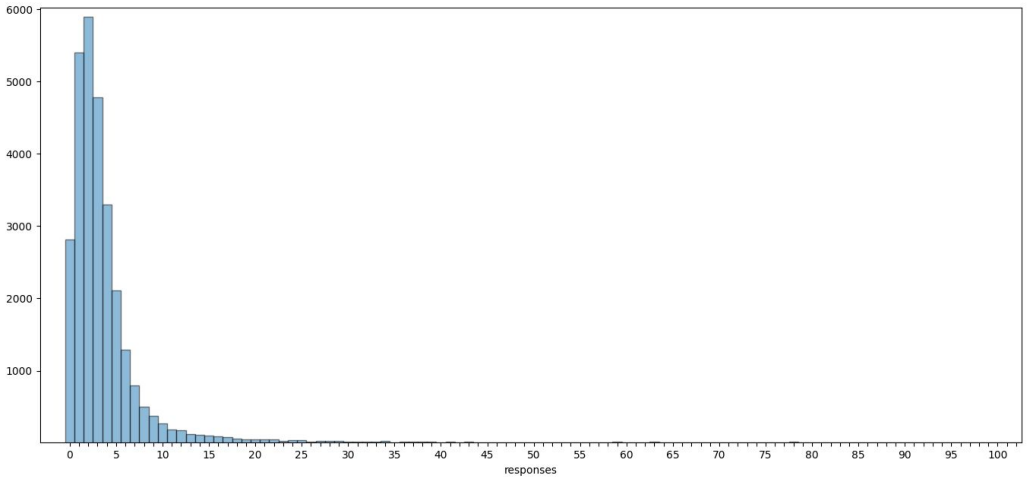
Example 2: Encoding (Receptive Fields)

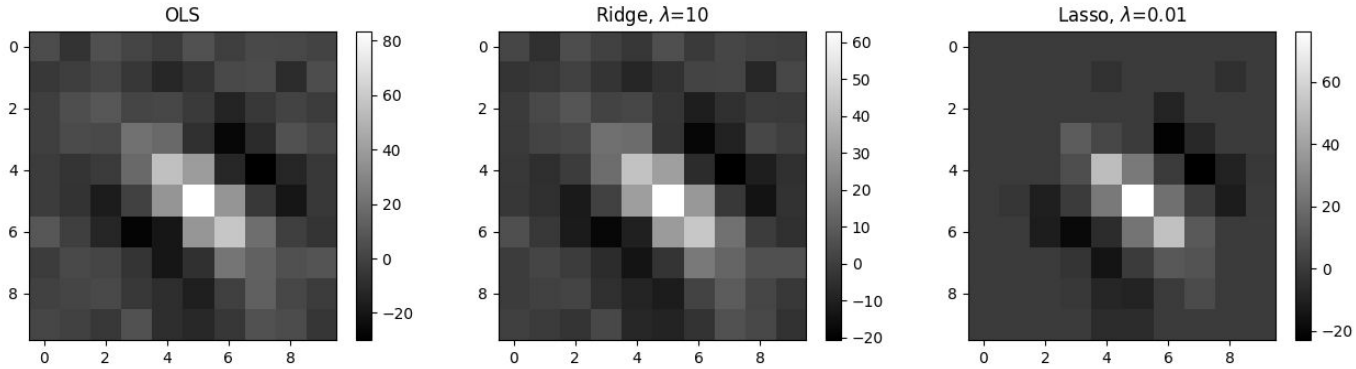
- Instead of neural→stimulus, we try to predict stimulus→neural
- Example: presented images, simple cell responses (spike counts)
- we really **shouldn't** treat this as ordinary linear regression, but we will anyway



Data: https://www.gatsby.ucl.ac.uk/~rapela/projects/vrst/ ; paper: Rapela et al. 2006 https://jov.arvojournals.org/article.aspx?articleid=2192869

Example 2: Encoding (Receptive Fields)

- Coefficients has the same dimensions as the input – in our case, it it's an image
- A way of describing the fitted (linear) receptive field of the cell!



Data: https://www.gatsby.ucl.ac.uk/~rapela/projects/vrst/ ; paper: Rapela et al. 2006 https://jov.arvojournals.org/article.aspx?articleid=2192869

Generalizations to different types of data

- The assumptions beyond the noise model:
  - Errors are symmetric around 0
  - Small errors are more likely than large errors

- Makes sense for continuous observations corrupted by measurement noise
- What if we have different type of observations?
  - Integers (e.g., number of spikes)
  - Binary outcomes (e.g., behavioral decision)
  - Categorical outcomes

- Different generalization exist (logistic regression, poisson regression, etc)
- Typically, cannot be solved in closed form (but can be optimised efficiently)

Conclusions and further directions

- The model is almost always wrong

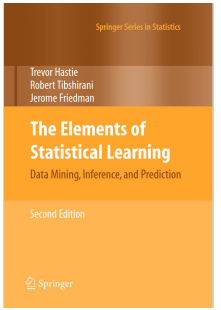
- Linear models are simple enough to analyze analytically. This makes them:
  - Extremely useful in their own right
  - Important for building intuition and understanding of more complicated models

- Ultimately, we built a model for **correlations** among predictors and outcomes
- Extra caution should be taken in interpreting the results as a “causal” story, particularly if fitted to observational data

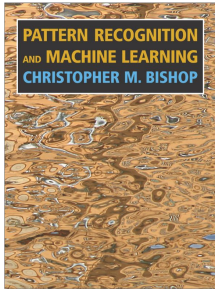
- Many topics we haven’t covered
  - Cross-validation, GLMs, (fully) Bayesian linear regression, subset selection, …

Sources and materials

The Elements of Statistical Learning, Hastie, Tibshirani, Friedman (available online)



Pattern recognition and machine learning, Bishop



Nueormatch academy tutorials
https://compneuro.neuromatch.io/tutorials/intro.html

LOTS of material online – but not everything is equally good