The curse of dimensionality

Data Mining - CdL CLAMSES

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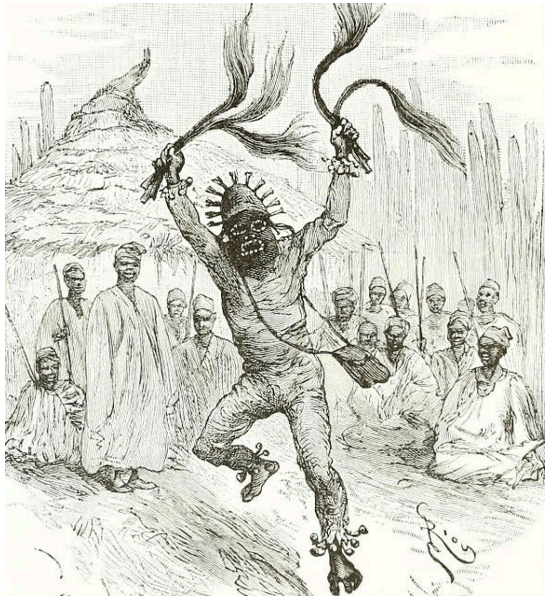

*"In view of all that we have said in the foregoing sections, the many obstacles we appear to have surmounted, what casts the pall over our victory celebration? It is the **curse of dimensionality**, a malediction that has plagued the scientist from the earliest days."*

Richard Bellman

- In Unit C we explored **linear** predictive models for **high-dimensional** data (i.e. p is large).
- In Unit D we explored **nonparametric** predictive models for **univariate** data, placing almost no assumptions on $f(x)$.
- Thus, the expectations are that this unit should cover models with the following features:
  - **High-dimensional**, with large p;
  - **Nonparametric**, placing no assumptions on $f(\boldsymbol{x})$.
- The title of this unit, however, is not "*fully flexible high-dimensional models*."
- Instead, it sounds like **bad news** is coming. Let us see why, unfortunately, this will be indeed the case.

Multidimensional local regression

- At least **conceptually**, kernel methods could be applied with **two** or **more covariates**.
- To estimate f on a specific point $\boldsymbol{x} = (x_1, \dots, x_p)^T$, a **natural extension** of the Nadaraya-Watson takes the form

$$\hat{f}(x) = \frac{1}{\sum_{i'=1}^{n} w_{i'}(\boldsymbol{x})} \sum_{i=1}^{n} w_i(\boldsymbol{x}) y_i = \sum_{i=1}^{n} s_i(\boldsymbol{x}) y_i,$$

  where the **weights** $w_i(\boldsymbol{x})$ are defined as

$$w_i(\boldsymbol{x}) = \prod_{j=1}^{p} \frac{1}{h_j} w\left(\frac{x_{ij} - x_j}{h_j}\right).$$

- This estimator is well-defined and it considers "**local**" points in p dimensions.
- If the theoretical definition of multidimensional nonparametric tools is not a problem, why are they **not used** in practice?

The curse of dimensionality I

- When the function $f(x)$ is entirely unspecified and a **local nonparametric** method is used, a **dense** dataset is needed to get a reasonably accurate estimate $\hat{f}(x)$.

- However, when p grows, the data points becomes **sparse**, even when n is "big" in absolute terms.
- In other words, a neighborhood of a generic point x contains a small fraction of observations.
- Thus, a **neighborhood** with a fixed percentage of data points is **no longer local**.

- To put it another way, to get a local neighborhood with 10 data points along each axis we need about 10^p data points.

- As a consequence, **much larger** datasets are needed even for moderate p, because the sample size n needs to grows **exponentially** with p.

The curse of dimensionality II

- The following illustration may help clarify this notion of **sparsity**. Let us consider data points that are uniformaly distributed on $(0,1)^p$, that is $\boldsymbol{x}_i \overset{\text{iid}}{\sim} \mathrm{U}^p(0,1)$.
- Then, the **median distance** from the origin $(0,\dots,0)^T$ to the **closest point** is:

$$\text{dist}(p,n) = \left\{1 - \left(\frac{1}{2}\right)^{1/n}\right\}^{1/p}.$$

- In the **univariate** case, such a median distance for $n = 100$ is quite small:

$$\text{dist}(1,100) = 0.007.$$

- Conversely, when the **dimension p increases**, the **median distance** becomes:

$$\text{dist}(2,100) = 0.083, \quad \text{dist}(10,100) = 0.608, \quad \text{dist}(50,100) = 0.905.$$

  Note that we get $\text{dist}(10,1000) = 0.483$ even with a much larger sample size.
- Most points are **close to the boundary**, making predictions very hard.

The curse of dimensionality III

- The following argument gives another **intuition** of the curse of dimensionality. Let us consider again **uniform** covariates $\boldsymbol{x}_i \overset{\text{iid}}{\sim} \mathrm{U}^p(0,1)$.
- Let us consider a subcube which contains a fraction $r \in (0,1)$ of the total number of observations n. In the univariate case $(p = 1)$, the side of this cube is r.
- In the more general case, it can be shown that on **average**, the **side** of the cube is

$$\text{side}(r, p) = r^{1/p},$$

  which is again exponentially increasing in p.
- Hence, when $p = 1$, the expected amount of points in the **local sub-interval** $(0, 1/10)$ is again $1/10$.
- Instead, when $p = 10$ the amount of point is the **local subcube** $(0,1)^{10}$ is

$$n\left(\frac{1}{10}\right)^{10} = \frac{n}{1.000.000.000}.$$

The curse of dimensionality (HTF, 2011)

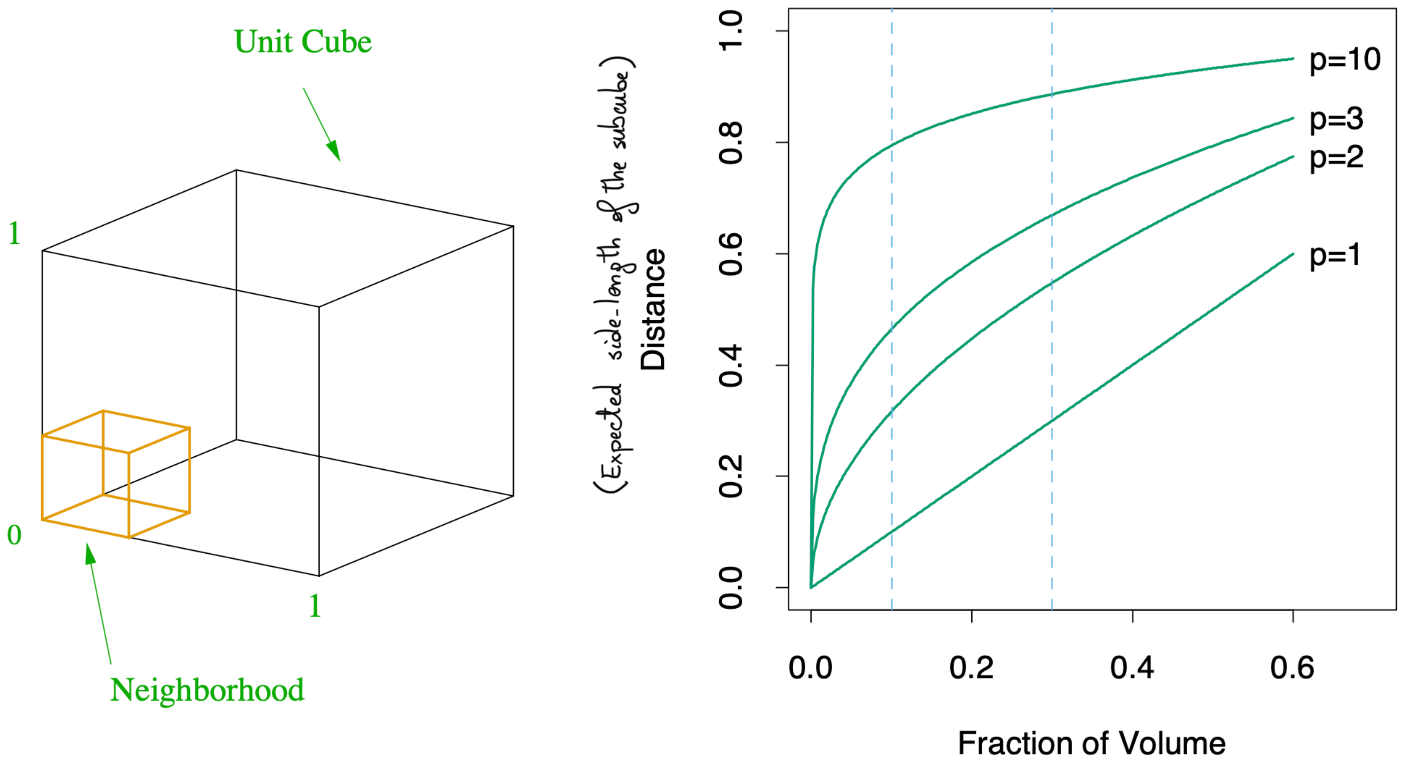

FIGURE 2.6. *The curse of dimensionality is well illustrated by a subcubical neighborhood for uniform data in a unit cube. The figure on the right shows the side-length of the subcube needed to capture a fraction r of the volume of the data, for different dimensions p. In ten dimensions we need to cover 80% of the range of each coordinate to capture 10% of the data.*

Implications of the curse of dimensionality

- In the local **kernel smoothing** approach, we can precisely quantify the impact of the **curse of dimensionality** on the **mean squared error**.
- Under some regularity conditions, the Nadaraya-Watson and the local linear regression estimator has **asymptotic mean squared error**

$$\mathbb{E}\left[\{f(x) - \hat{f}(x)\}^2\right] \sim n^{-4/5},$$

which is **slower** than the **parametric rate** n^{-1}, but still reasonably fast for predictions.
- Conversely, it can be shown that in **high-dimension** the **asymptotic rate** becomes

$$\mathbb{E}\left[\{f(\boldsymbol{x}) - \hat{f}(\boldsymbol{x})\}^2\right] \sim n^{-4/(4+p)}.$$

- Thus, the sample size for a p-dimensional problem to have the same accuracy as a sample size n in one dimension is $m \propto n^{cp}$, with $c = (4+p)/(5p) > 0$.
- To maintain a given degree of accuracy of a **local nonparametric** estimator, the sample size must increase **exponentially** with the dimension p.

Escaping the curse

- Is there a "**solution**" to the **curse of dimensionality**? Well, yes... and no.
- If $f(x)$ is assumed to be **arbitrarily complex** and our estimator $\hat{f}(x)$ is **nonparametric**, we are destined to face the curse.
- However, in **linear models** you never encountered the curse of dimensionality. Indeed:

$$\frac{1}{n}\sum_{i=1}^{n}\mathbb{E}\left\{(\boldsymbol{x}_i^T\beta - \boldsymbol{x}_i^T\hat{\beta})^2\right\} = \sigma^2\frac{p}{n},$$

  which is increasing **linearly** in p, but **not exponentially**.
- Linear models make **assumptions** and impose a **structure**. If the assumptions are correct, the estimates exploit **global features** and are less affected by the local sparsity.
- Nature is not necessarily a linear model, so we explored the nonparametric case.
- Nonetheless, making (correct) **assumptions** and therefore imposing (appropriate) restrictions is **beneficial**, to the extent that it is **unavoidable** in high dimensions.

Escaping the curse

- The **multidimensional** methods you will study (GAM, trees, random forest, boosting, neural networks, etc.) deal with the curse of dimensionality by making (implicit) assumptions.
- These **assumptions** differentiate because of:
  - The particular **nature** of the knowledge they impose (e.g., no interactions, piecewise constant functions, etc.);
  - The **strength** of this assumption;
  - The **sensibility** of the methods to a potential violation of the assumptions.
- Thus, several alternative ideas and methods are needed; no single "best" algorithm exists.
- This is why having a well-trained statistician on the team is important because they can identify the method that best suits the specific applied example.
- ...or at least, they will be aware of the **limitations** of the methods.

References

- **Main references**

  - **Section 4.3** of Azzalini, A. and Scarpa, B. (2011), *Data Analysis and Data Mining*, Oxford University Press.
  - **Section 2.5** of Hastie, T., Tibshirani, R., and Friedman, J. (2009), *The Elements of Statistical Learning*, Second Edition, Springer.
  - **Sections 4.5 and 5.12** of Wasserman, L. (2006), *All of Nonparametric statistics*, Springer.