Quantifying Uncertainty

DS3 Göttingen 2019

August 7th 2019

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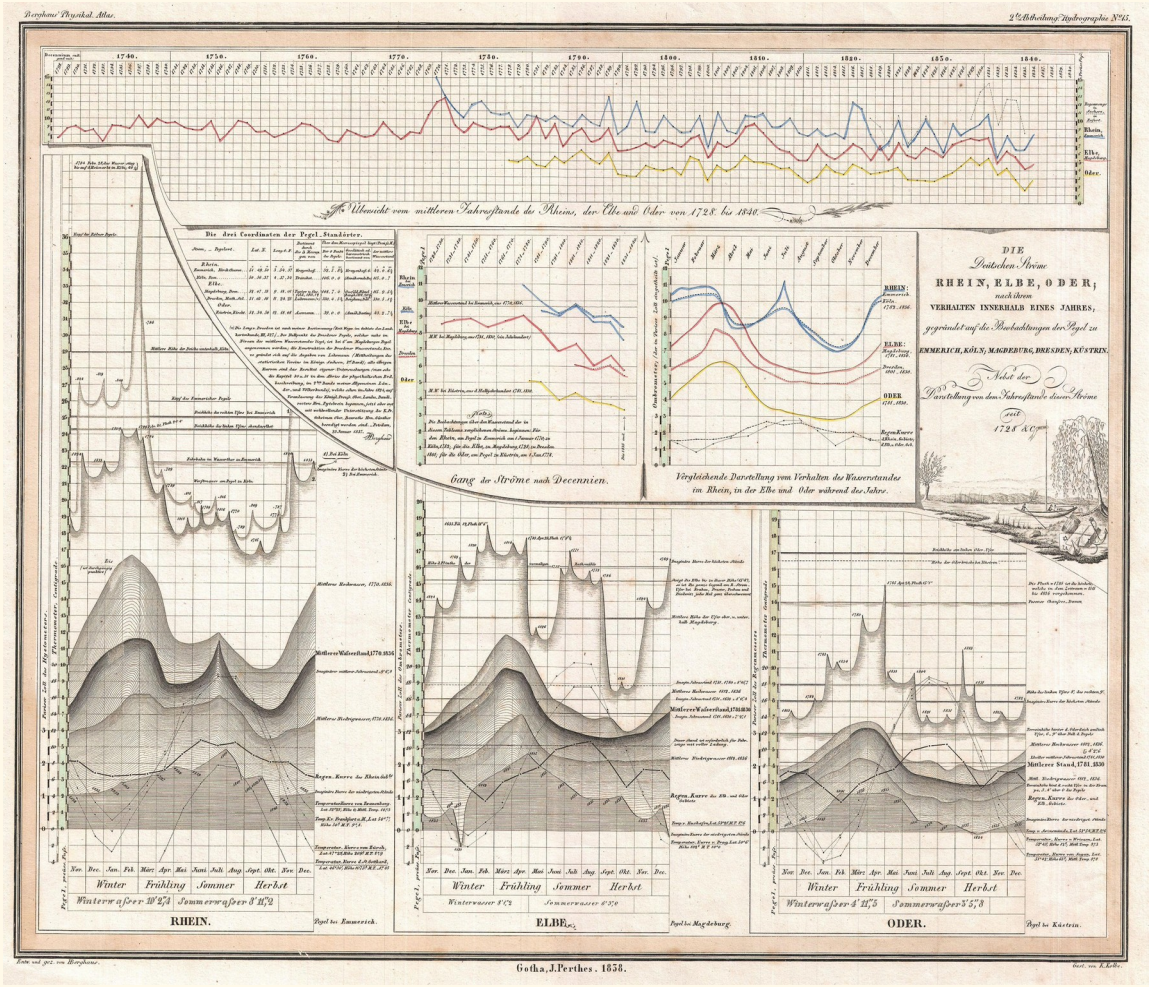
Data Science until 80 years ago



River charts by Dr. Heinrich Berghaus from 1838 (public domain)
https://commons.wikimedia.org/wiki/File:1838_Perthes_Chart_of_the_Rhine,_Elbe,_and_Order_Rivers_-_Geographicus_-_RheinElbeOder-perthes-1838.jpg

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Data Science Today (?)

Tianhe-2 super computer
(creator: user O01326; license: https://creativecommons.org/licenses/by-sa/4.0/deed.en;
source: https://commons.wikimedia.org/w/index.php?title=File:Tianhe-2.jpg&oldid=222583306)

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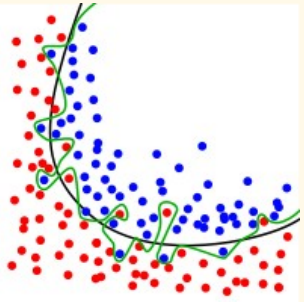
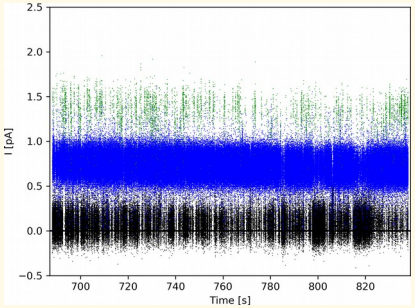
This is more like it…

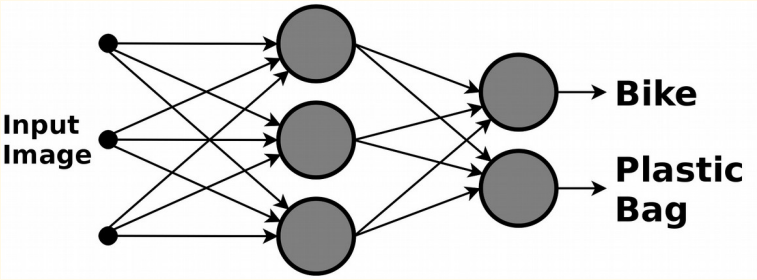
Data Science – How it‘s done.

(creator: user O01326; license: https://creativecommons.org/licenses/by/2.0/deed.en;
source: https://commons.wikimedia.org/w/index.php?title=File:TechCrunch_Disrupt_NY_2015_(17206523159).jpg&oldid=351399991)

A Tale of Two Cities







Statistics

- For small and large data sets
- For low and high dimension
- Classification, Modelling, Summary
- **Quantifies Uncertainty**
- Based on mathematical ingenuity

Neural Networks

- Needs large data sets
- Superior in high dimension
- Mostly classification
- Uncertainty empirically checked
- Based on technical ingenuity

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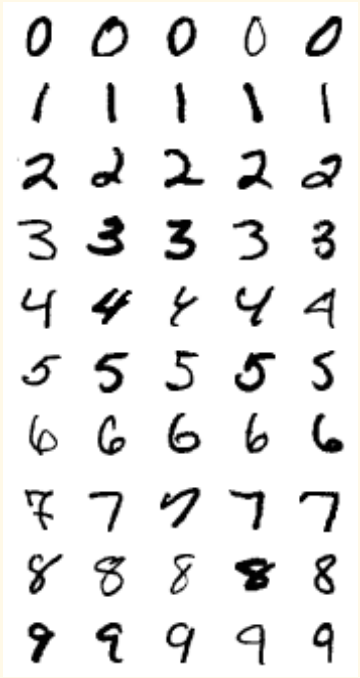
How superior are Neural Networks?

MNIST data set of handwritten digits. Task: identify digits correctly!
large training data set (60,000 images)**, high dimension** (28x28=784)



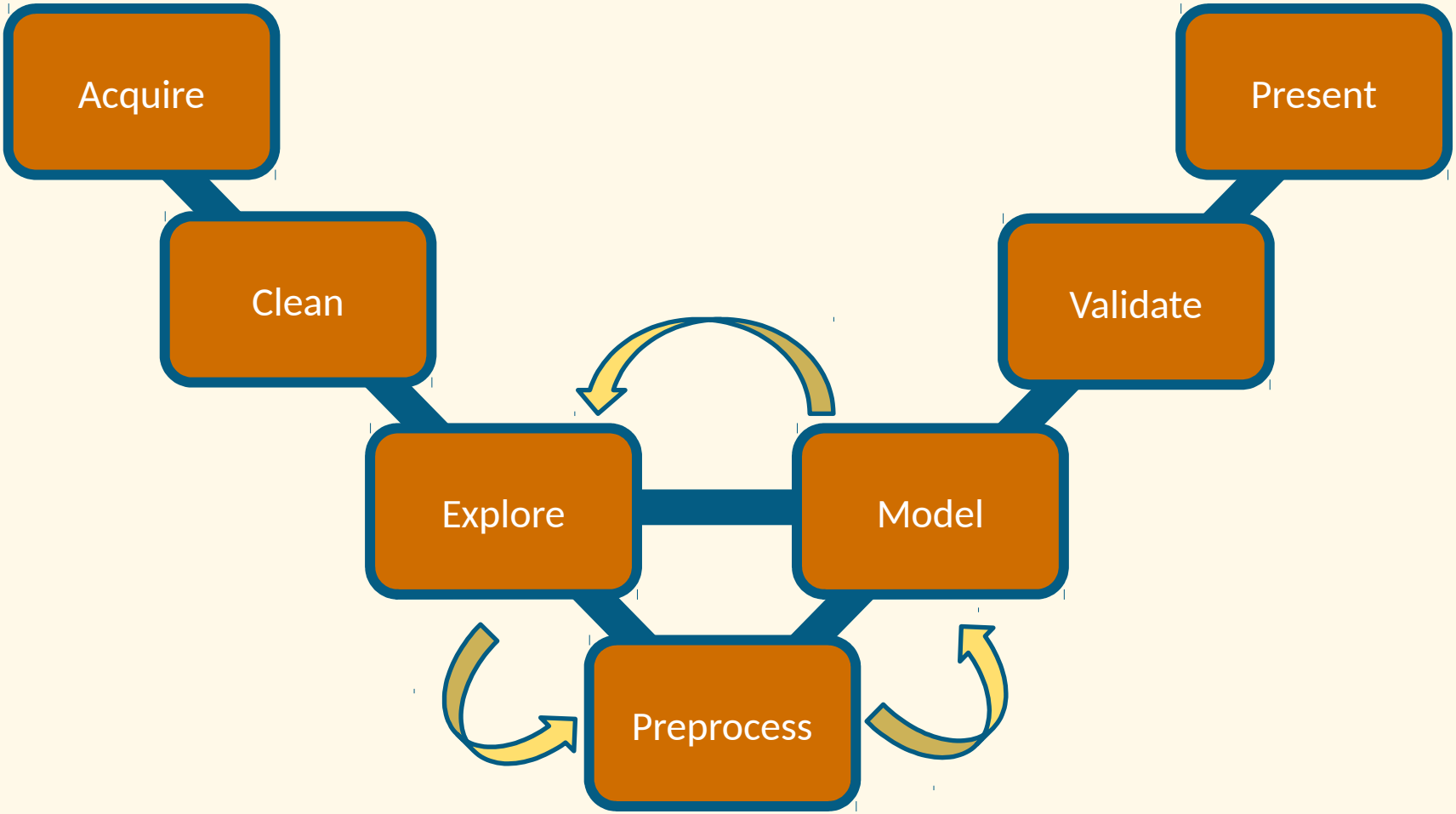
Some example digits[1]

Method	Error Rate	Publication
Gaussian kernel support vector machine	1.4%	
K-nearest-neighbors non-linear deformation (P2DHMDM)	0.52%	Keysers et al. IEEE PAMI 2007
committee of 35 convolutional neural networks	0.23%	Ciresan et al. CVPR 2012

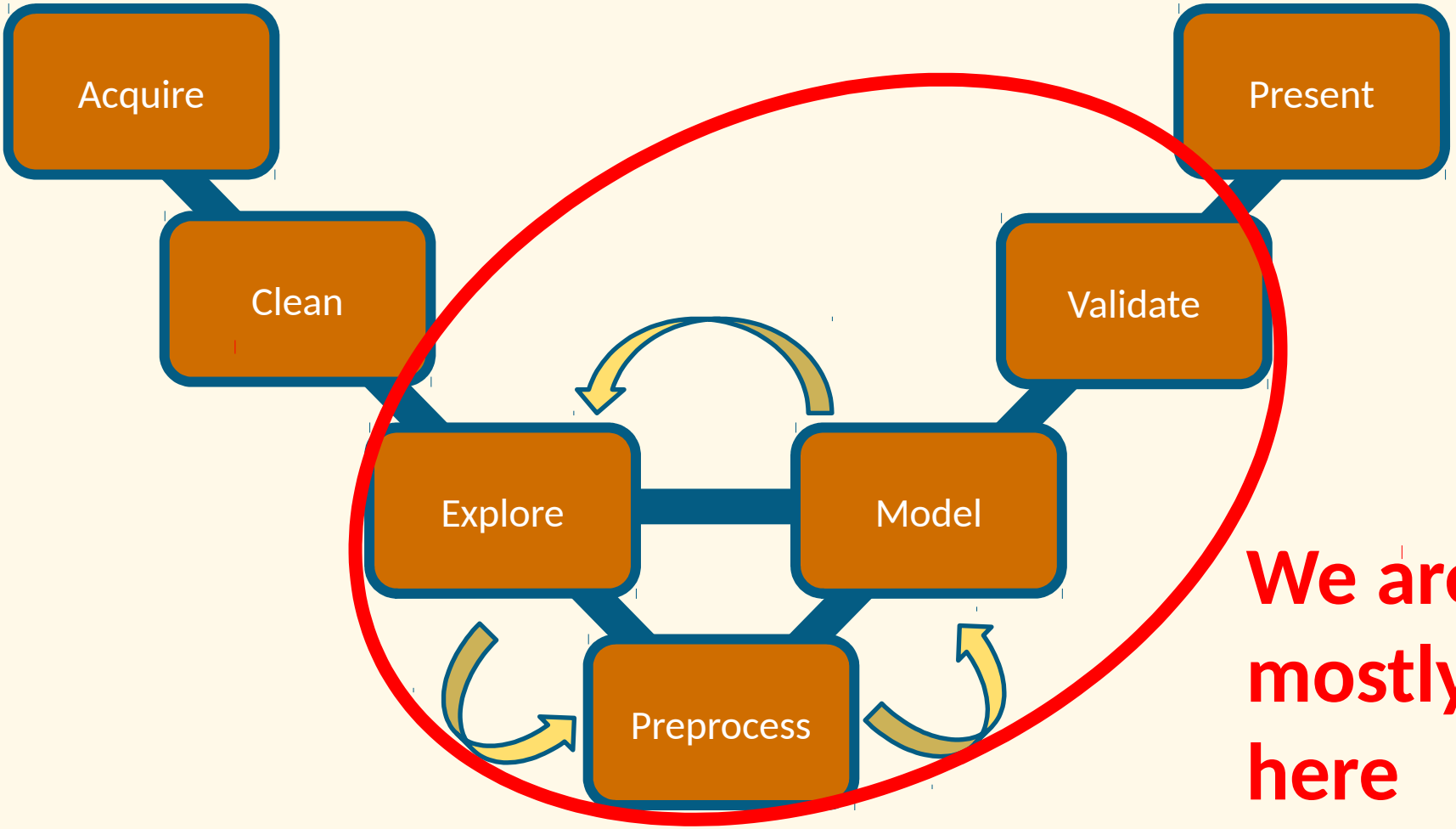
Information from http://yann.lecun.com/exdb/mnist/

[1](original creator: user Jost swd15; license: https://creativecommons.org/licenses/by-sa/4.0/deed.en; source: https://commons.wikimedia.org/w/index.php?title=File:MnistExamples.png&oldid=276154723)

Data Science Building Blocks



Data Science Building Blocks



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Intro: Statistical Experiment

- One system or exact copies, on which one can measure arbitrarily often.
- Measurement results “x” are random; one function f(x) determines the probabilities for all measurements.
- Every measurement result is independent of all other measurements.
- Example: rolling a die, f(x) = 1/6 for x = 1, …, 6.

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Regression

- Consider an Experiment, where $x_k = g(t_k) + \varepsilon(t_k)$,
- g(t) is a fixed function,
- values of ε(t) are random (with mean 0) and probabilities are determined by functions $f_t(\varepsilon(t))$.
- Trying to determine g(t) is called regression.

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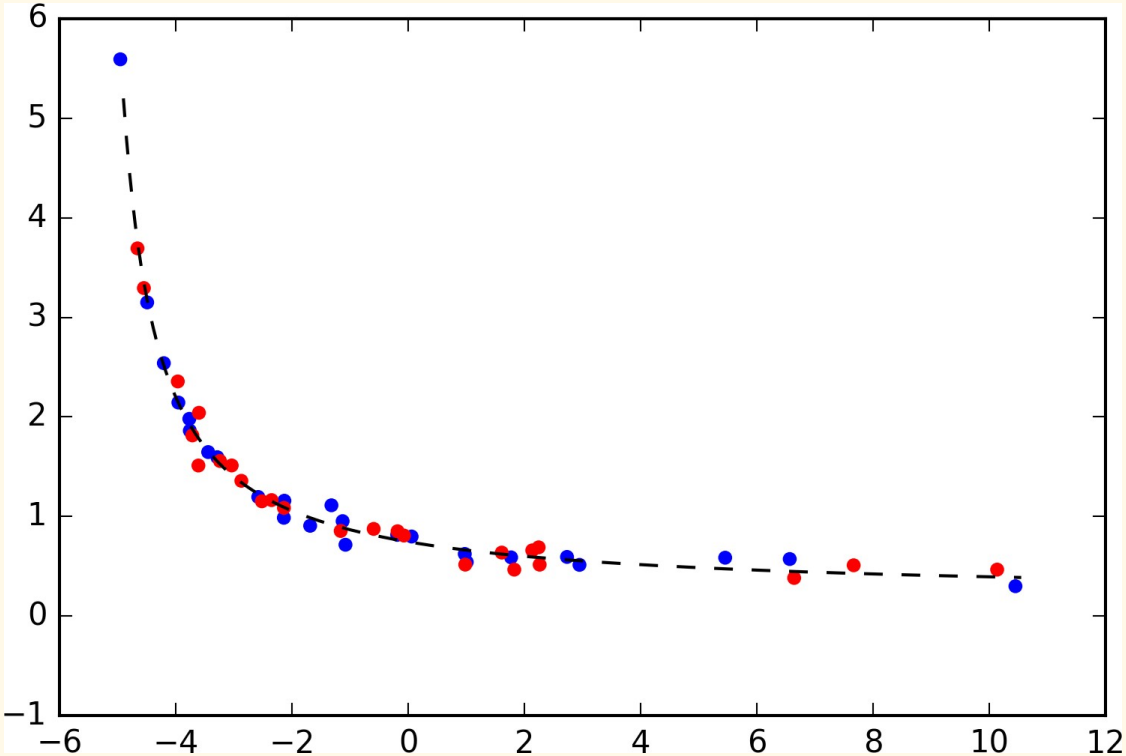
Overfitting: A Regression Example



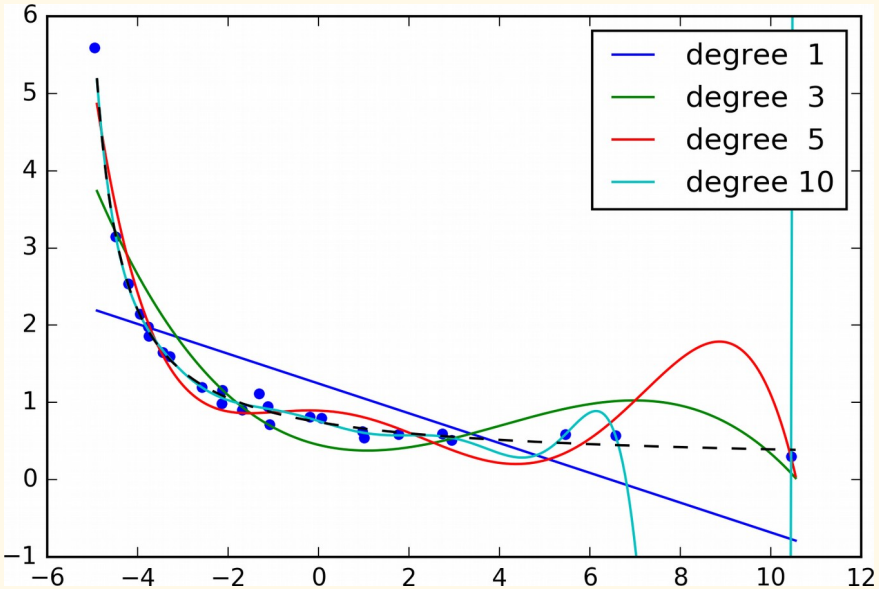
25 Training data

25 Test data

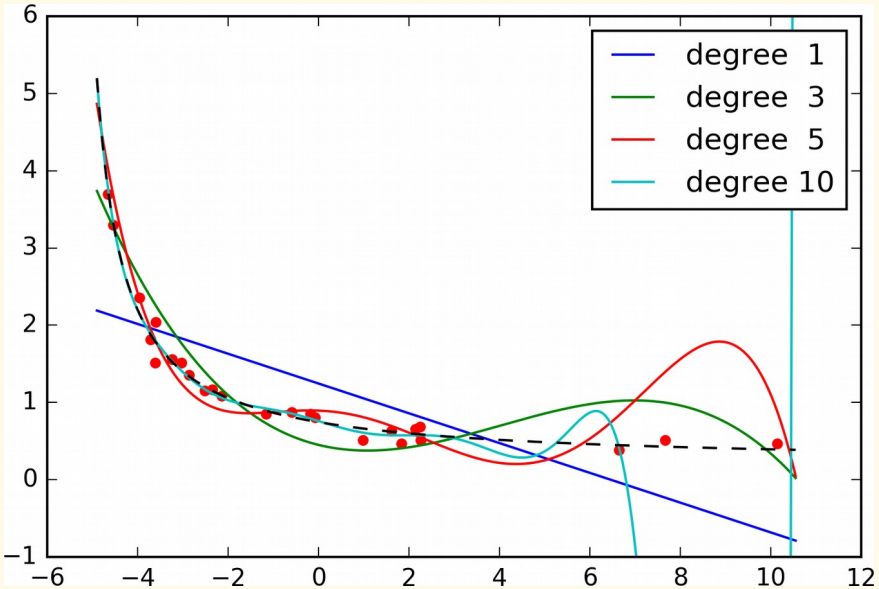
Dashed: g(t)

Polynomial Fits

$$g_d(t) = a_d\, t^d + \ldots + a_1\, t^1 + a_0$$



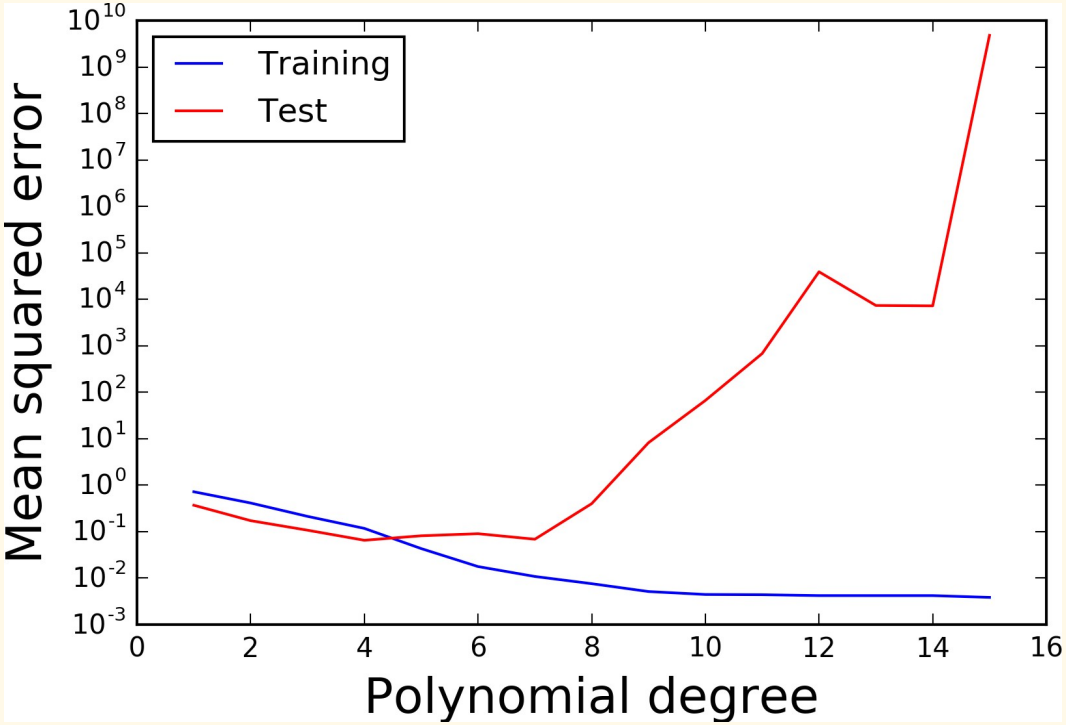
Training data: Good fits



Test data: Bad fits

How to Quantify the Error?

$$\mathrm{MSE} = \frac{1}{n}\left(\left(x_1 - g\left(t_1\right)\right)^2 + \ldots + \left(x_n - g\left(t_n\right)\right)^2\right)$$

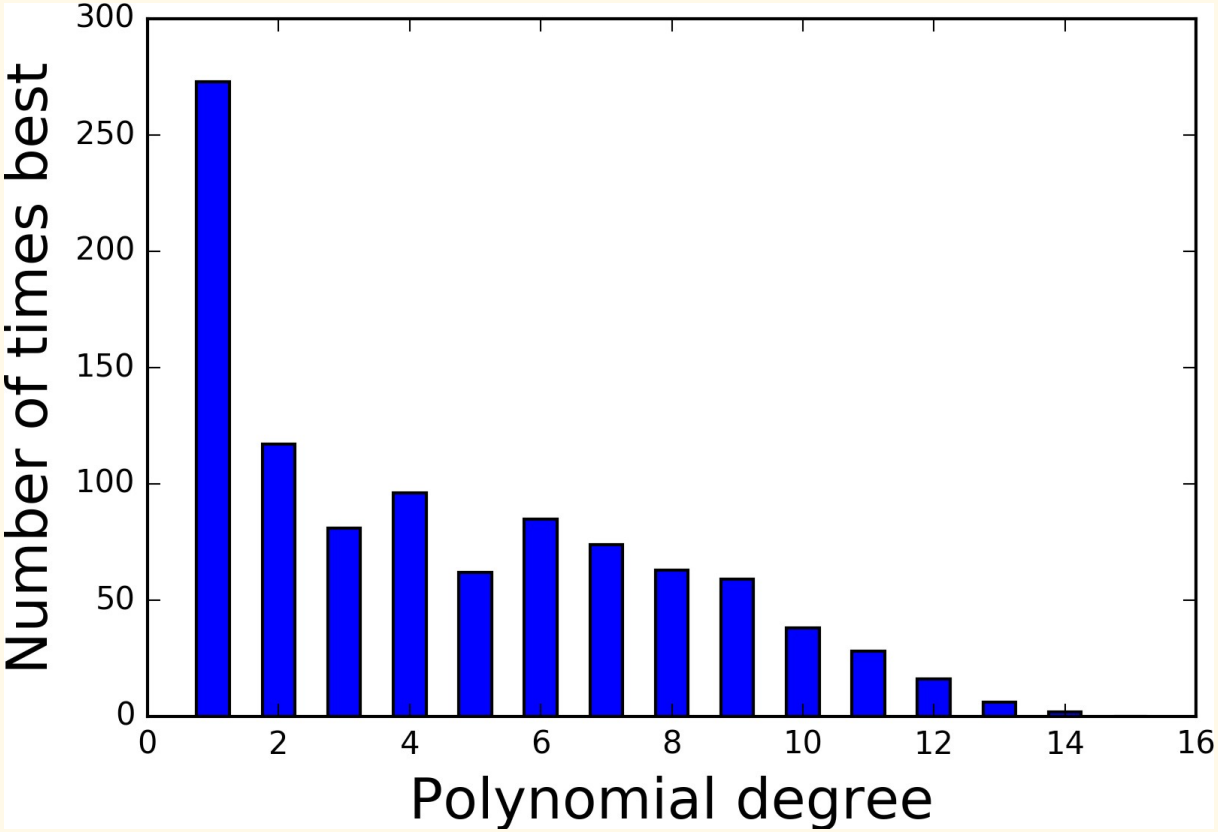


Higher polynomial degree:

better performance on **training** data,

worse performance on **test** data!

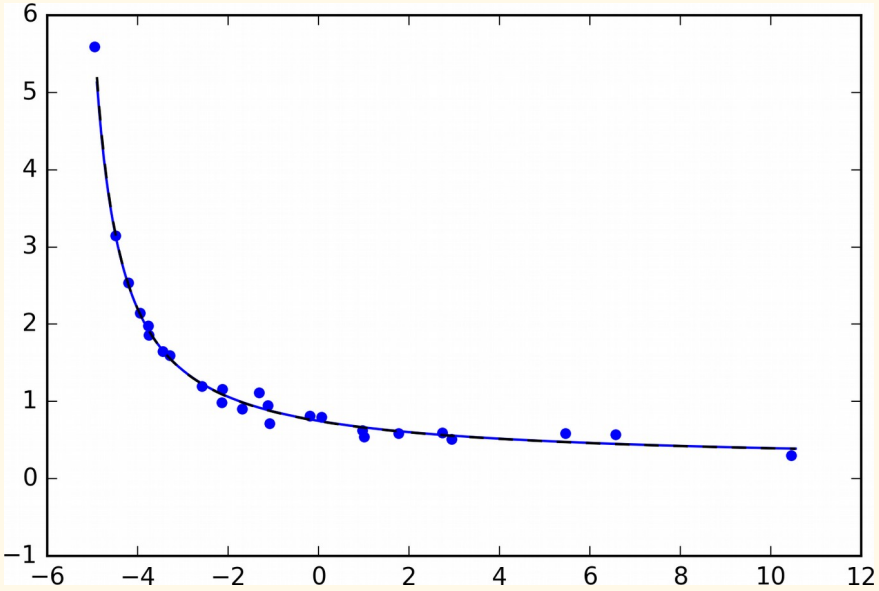
Which Degree is Best?



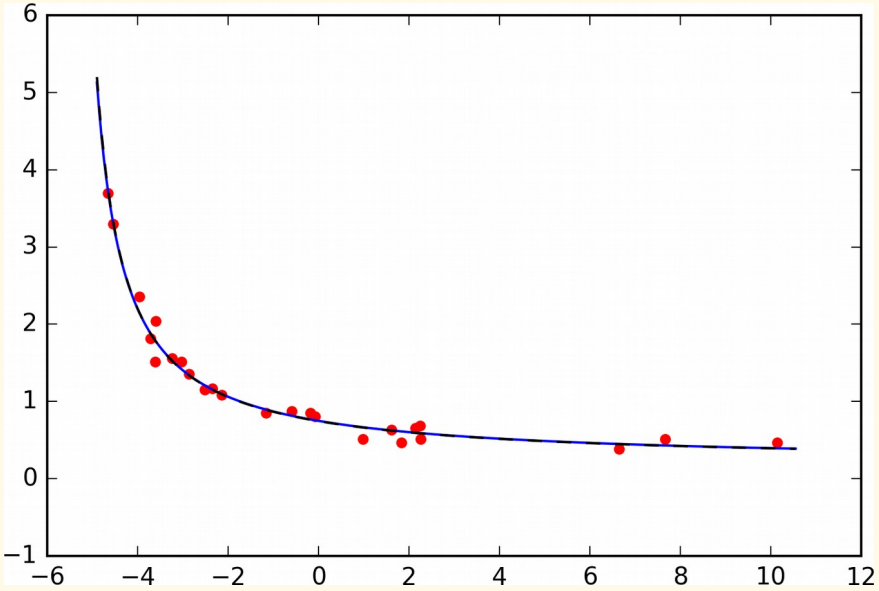
Which polynomial degree has the smallest MSE on test data, 1000 simulated data sets.

A Better Model

$$g(t) = \frac{a_1}{t + a_2} + a_3$$

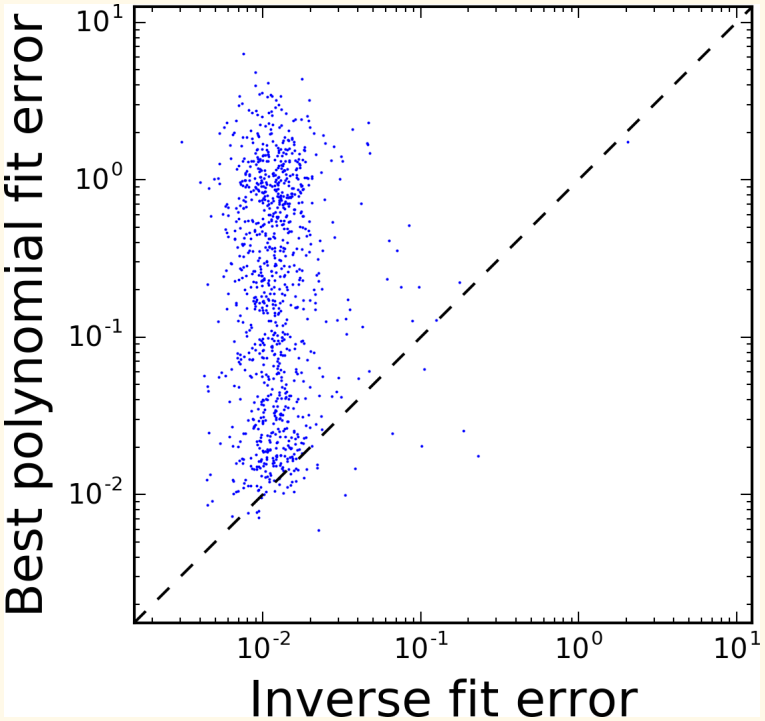


Training data: Good fits



Test data: Good fits

How Much Better is it?



Comparison of MSE on test data for 1000 simulated data sets: 1/x model does much better! (Log scale!)

Observations

- In general, more model parameters improve the fit for training data, but *too many parameters spoil the fit for test data*!
- Why does this happen? Can one *diagnose this for real data* before looking at test data?
- A *better model* (for the given data) is much more useful than more parameters.

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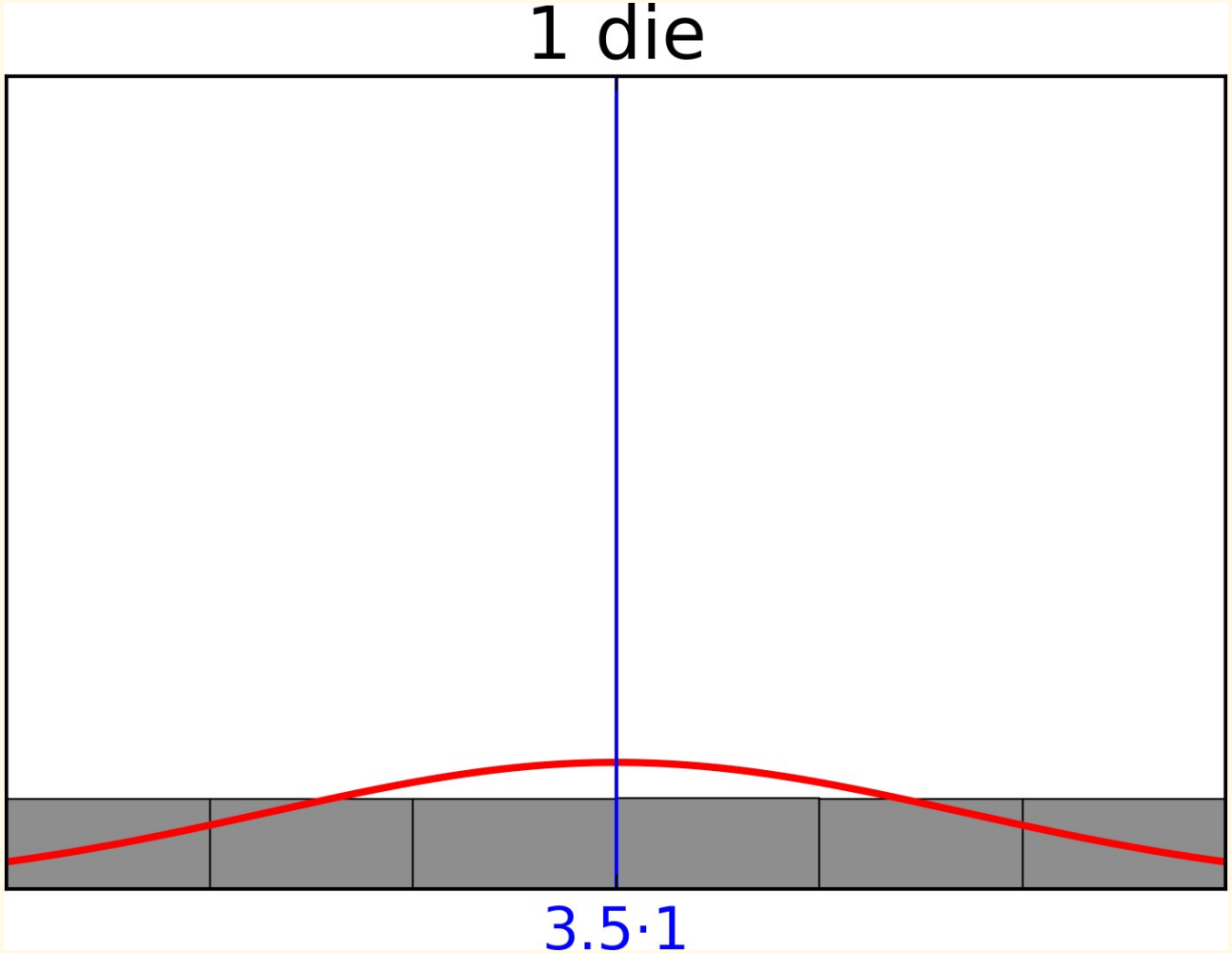
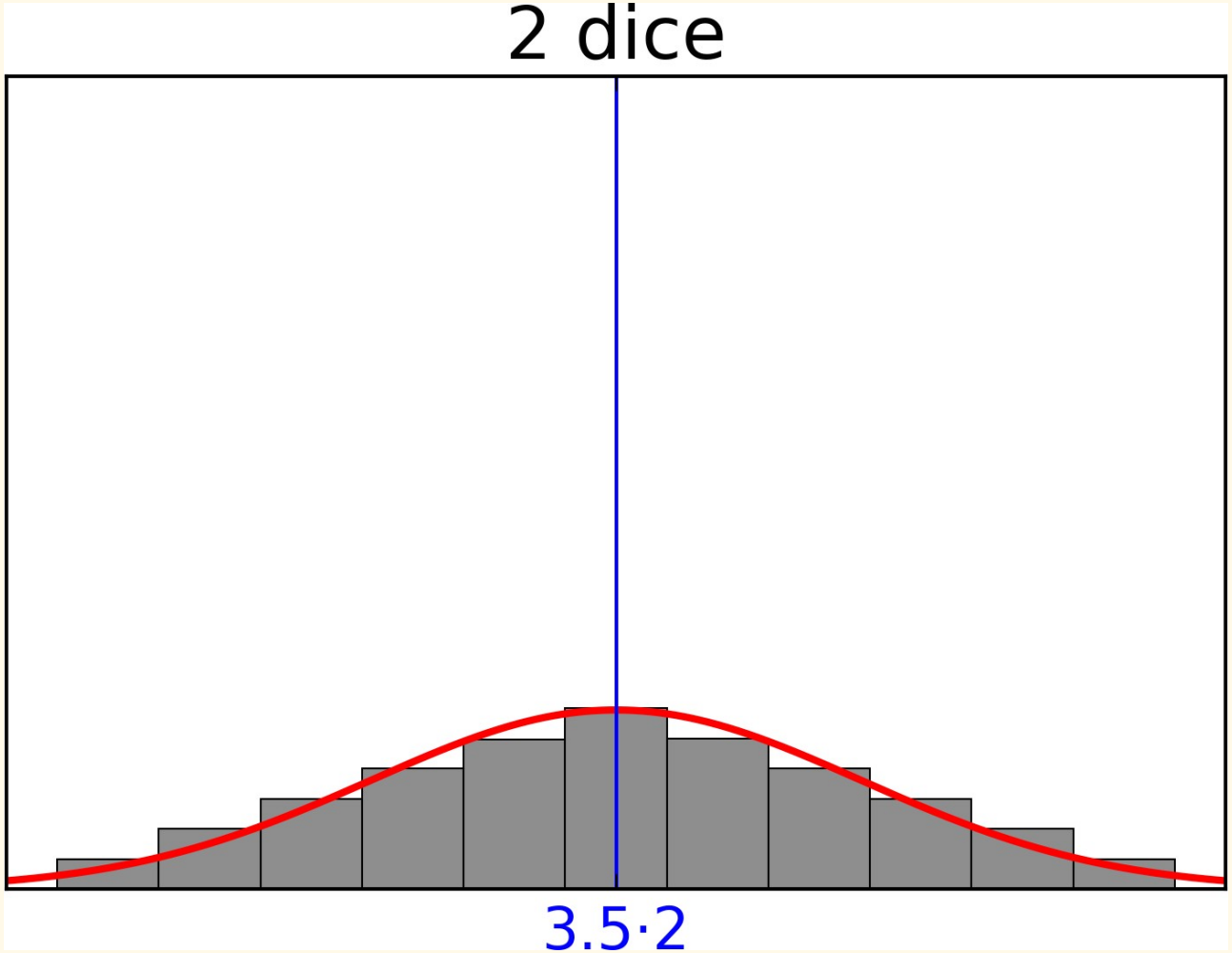
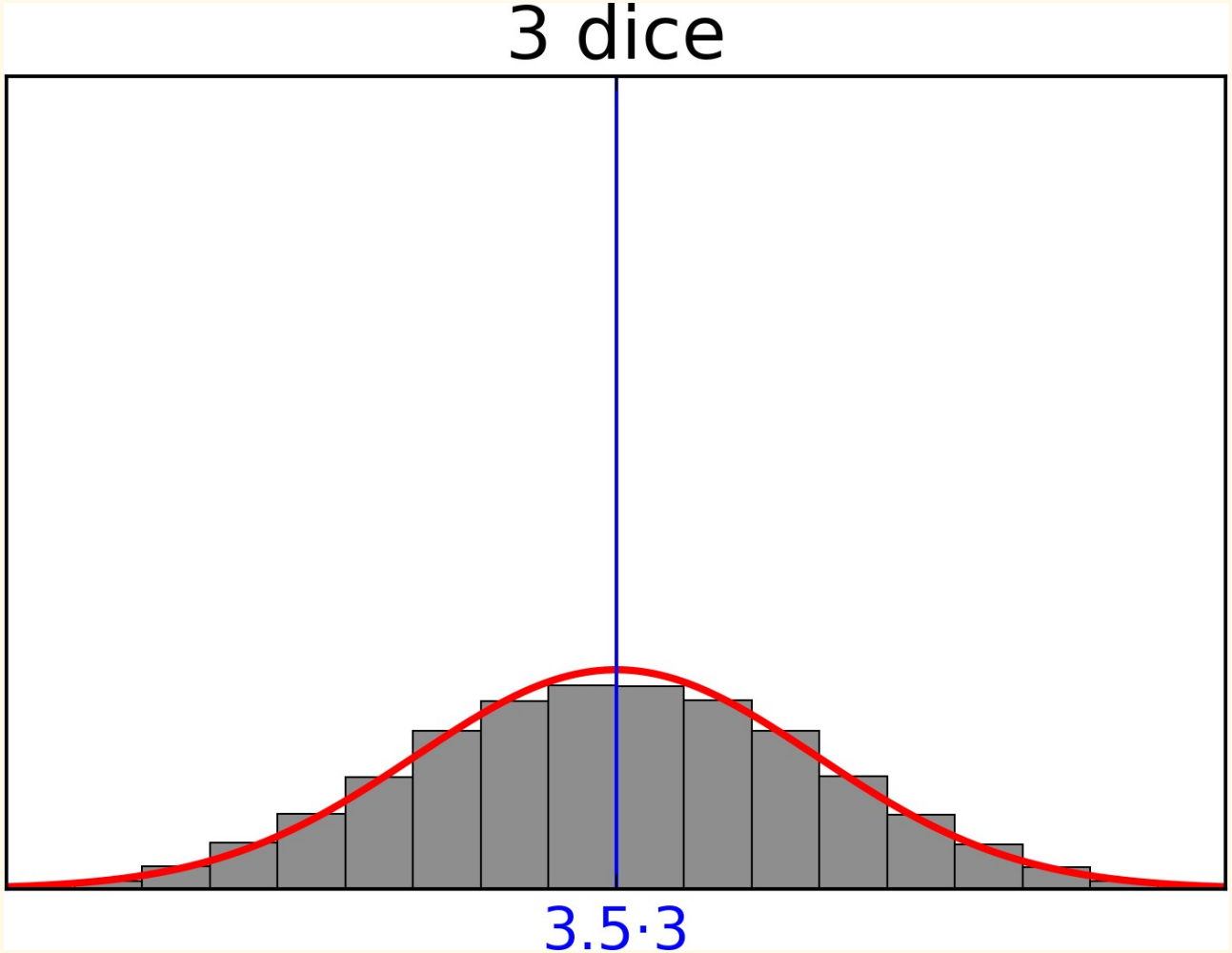
Throwing Dice



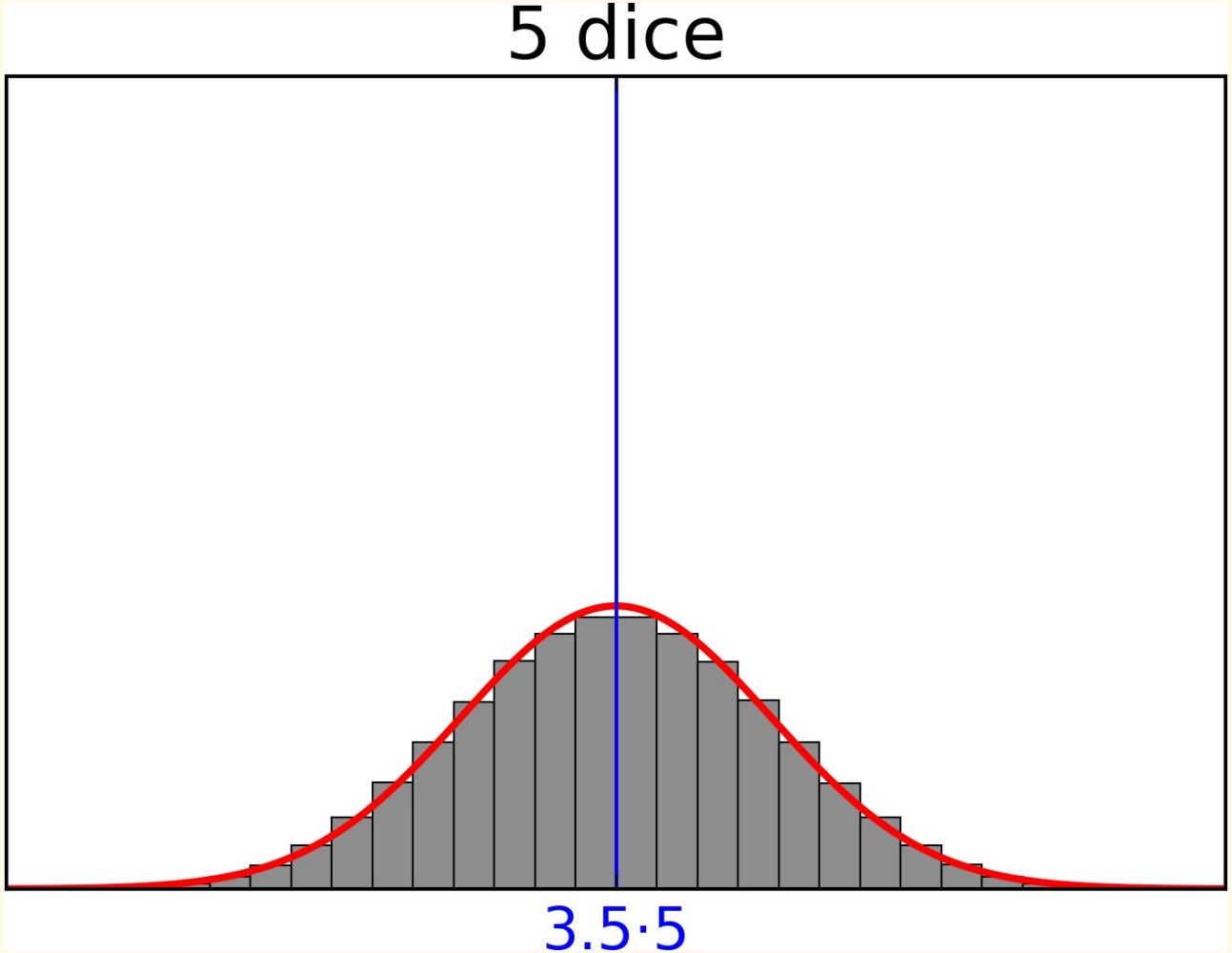
Throwing Dice



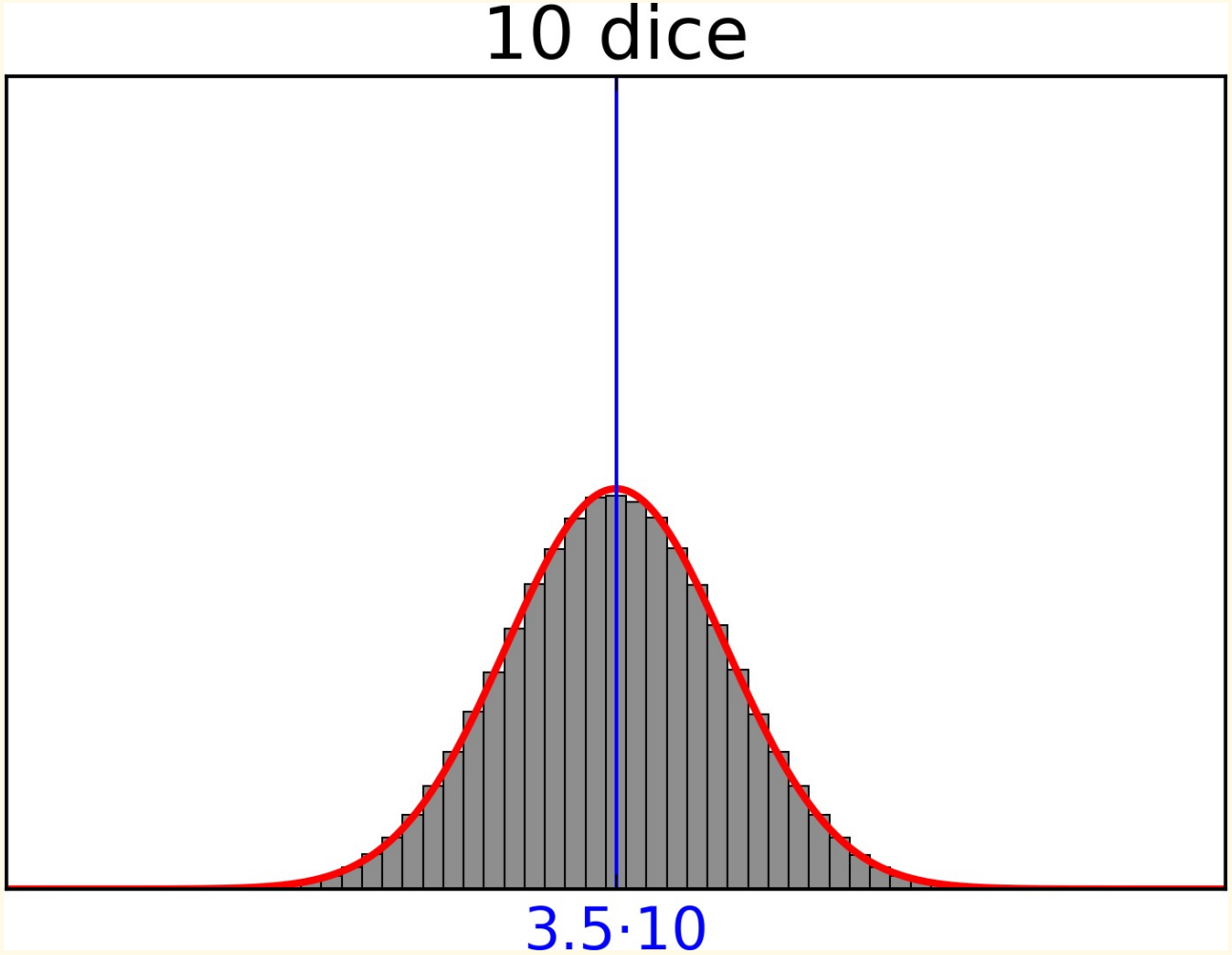
Throwing Dice



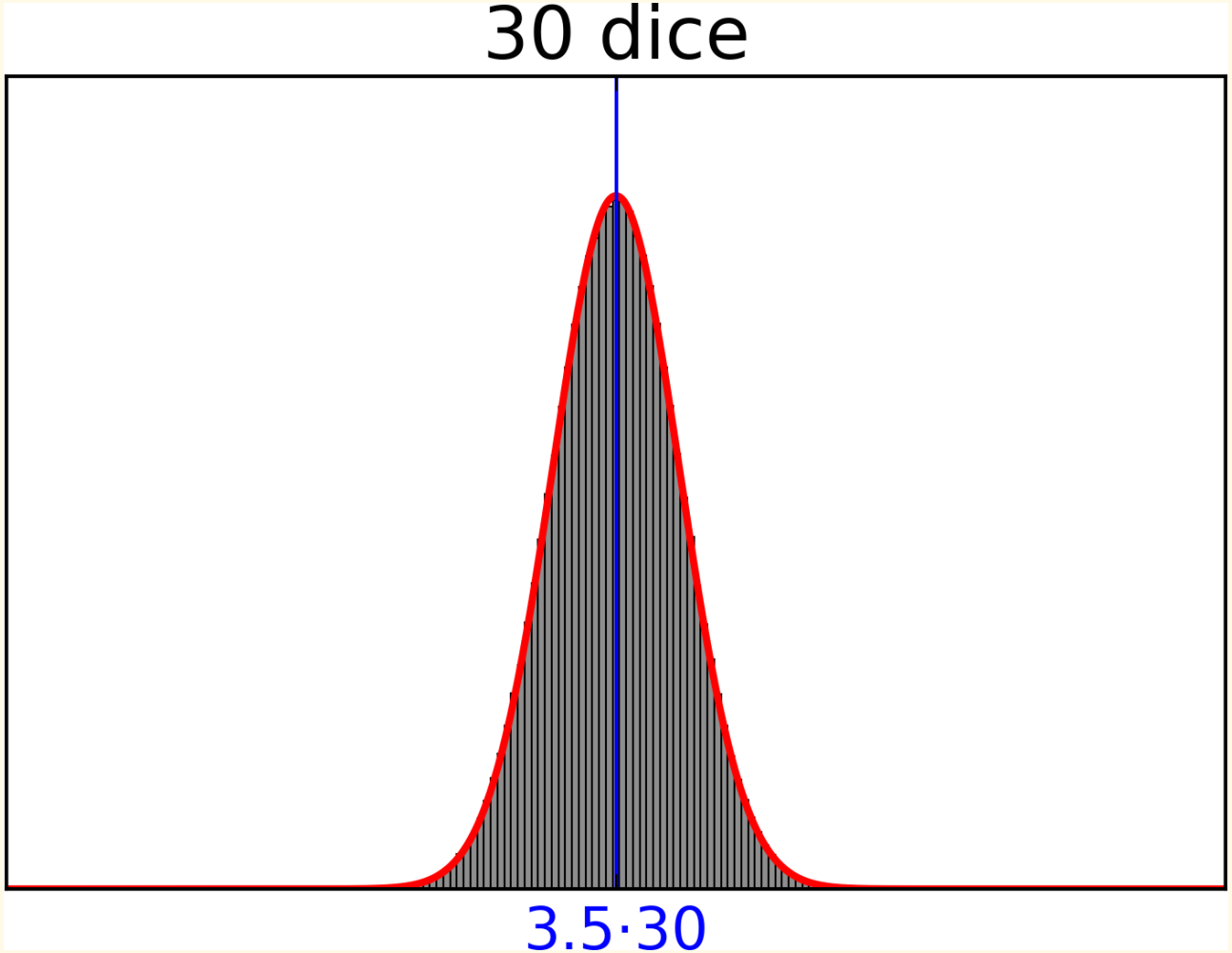
Throwing Dice



Throwing Dice



Throwing Dice



What Happened Here?

- The mean of n dice $\mu_n := (d_1+d_2+\ldots+d_n)/n$ is distributed symmetrically around $\mu_0=3.5$.
- The distribution of μ_n becomes *sharper with increasing n*.
- The distribution approaches a *Gaussian bell shape*.
- Is there some *general principle* at work here?

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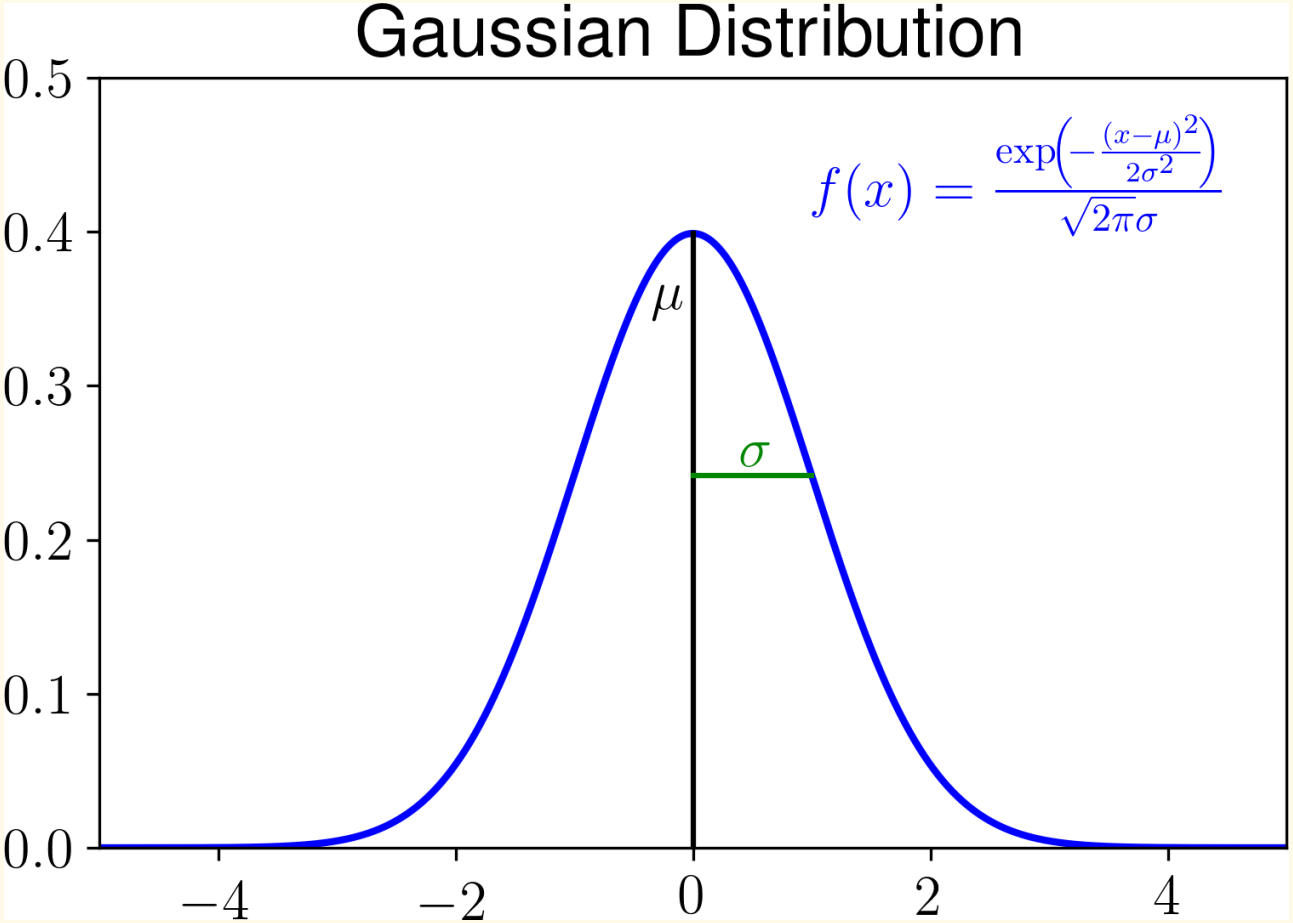
Mean μ and Standard Deviation σ



The Central Limit Theorem

Assume the following:

- $x_1, x_2, \ldots, x_n$ are measurements from a statistical experiment and call $\mu_n := (x_1 + x_2 + \ldots + x_n)/n$.
- For the density function f(x) of measurement results, $\mu_0 = \int_{-\infty}^{\infty} x f(x) dx$ and $\int_{-\infty}^{\infty} x^2 f(x) dx$ exist.

Then the distribution of $\sqrt{n}(\mu_n - \mu_0)$ approaches a Gaussian bell shape centered at 0 for $n \to \infty$.

Caveat: In reality, we do not know f(x), so we do not always know, if the Central Limit Theorem holds!

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What does this mean?

- $\sigma_n := \sqrt{\frac{1}{n}\left(\left(x_1-\mu_n\right)^2+\left(x_2-\mu_n\right)^2+\ldots+\left(x_n-\mu_n\right)^2\right)}$ is called the standard deviation and estimates the *spread of measured values*.

- The Central Limit Theorem yields the *standard error of the mean* $\epsilon_n := \frac{\sigma_n}{\sqrt{n}} = \frac{1}{n}\sqrt{\left(x_1-\mu_n\right)^2+\left(x_2-\mu_n\right)^2+\ldots+\left(x_n-\mu_n\right)^2}$ which estimates the spread of means of sets of n measured values.

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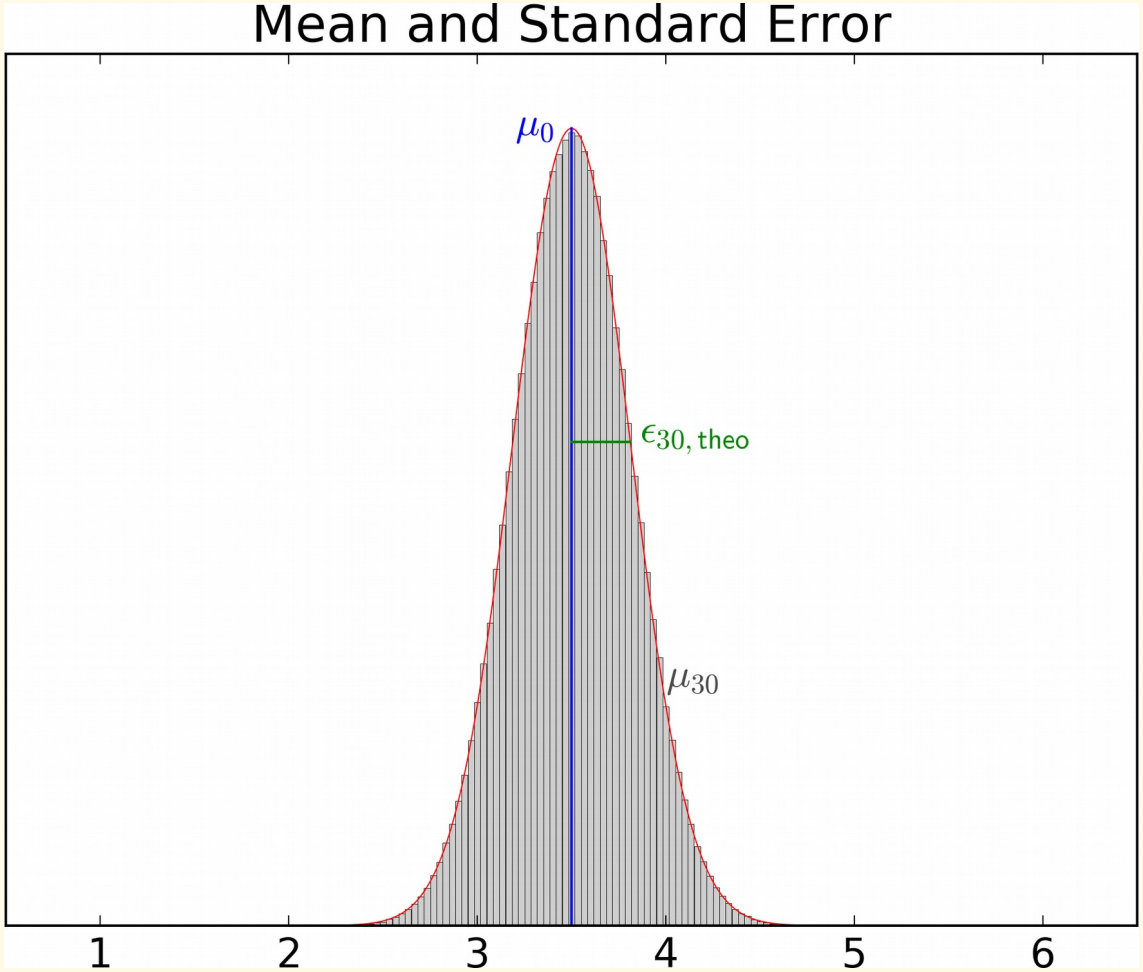
Behold the Standard Error



Quantifying Uncertainty

- The standard error ε_n is an estimator for the standard deviation of the distribution of μ_n.

- If the distribution of μ_n is the Gaussian distribution,
  the probability that $\mu_n - \mu_0 < \varepsilon_n$ is ~68%,
  the probability that $\mu_n - \mu_0 < 2\varepsilon_n$ is ~95%,
  the probability that $\mu_n - \mu_0 < 3\varepsilon_n$ is ~99,9%.

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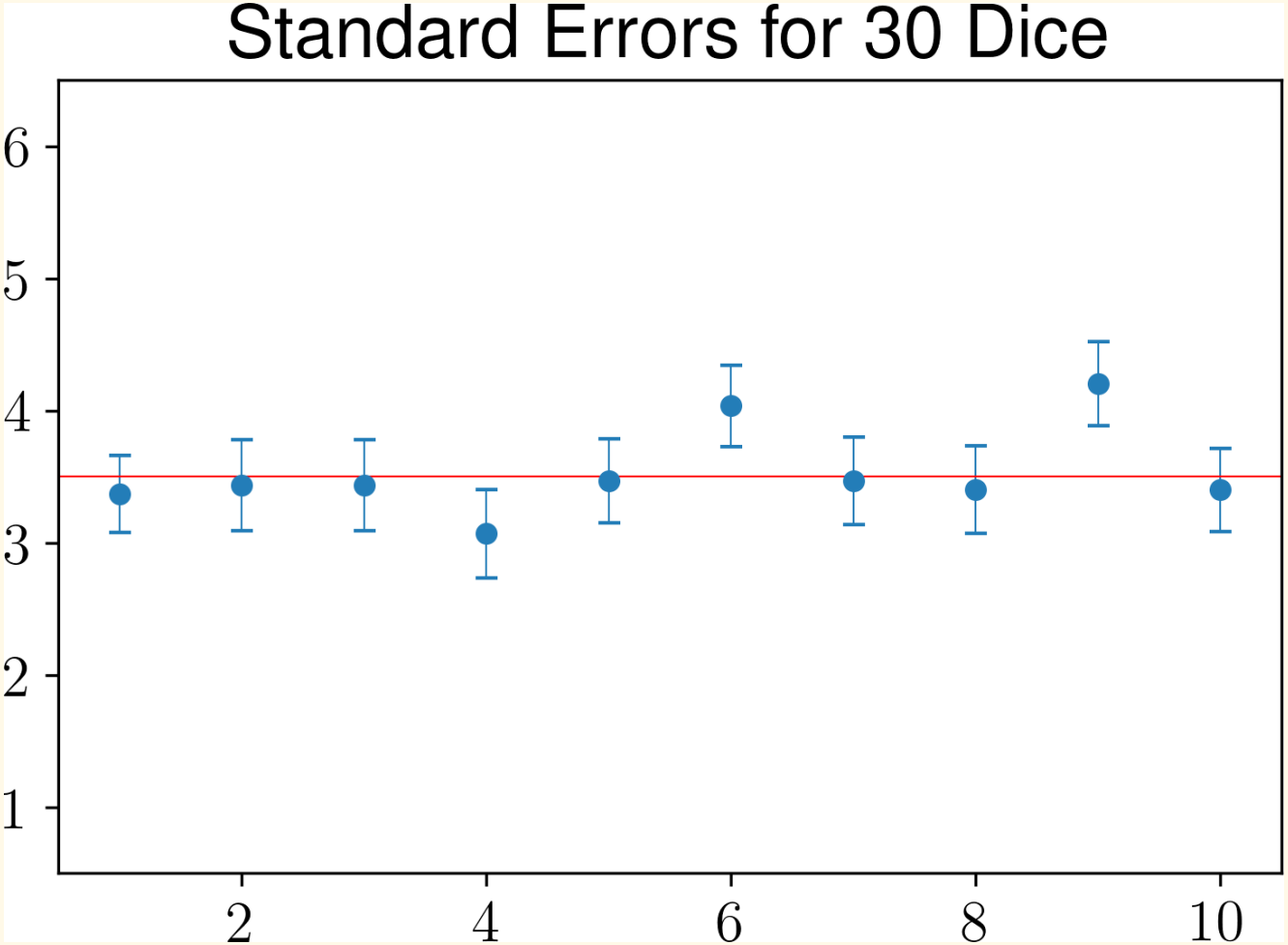
And this is how it looks...



The Root of Overfitting

- Central limit theorem for regression yields uncertainties of regression parameters.
- More model parameters *lead to higher parameter uncertainty*! For $g_d(t) = a_d\, t^d + \ldots + a_1\, t^1 + a_0$ the uncertainty of a_d is often larger than a_d itself!
- Therefore, the models are *not reliable for test data*.
- *Reliability can be quantified* in terms of parameter uncertainties!

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Artificial Neural Networks

- One layer is a map: $L_j : \mathbb{R}^{p_j} \times \mathbb{R}^{n_{j-1}} \to \mathbb{R}^{n_j}$
  p_j : number of parameters
  n_{j-1} : number of input values (nodes of previous layer)
  n_j : number of output values (nodes of this layer)

- A network of several layers is a map:
  $L_k \circ \ldots \circ L_2 \circ L_1 : \mathbb{R}^{p_k} \times \ldots \times \mathbb{R}^{p_2} \times \mathbb{R}^{p_1} \times \mathbb{R}^{n_0} \to \mathbb{R}^{n_k}$

- *Many fitted parameters*: one per network node!
  Neural networks are prone to overfitting!

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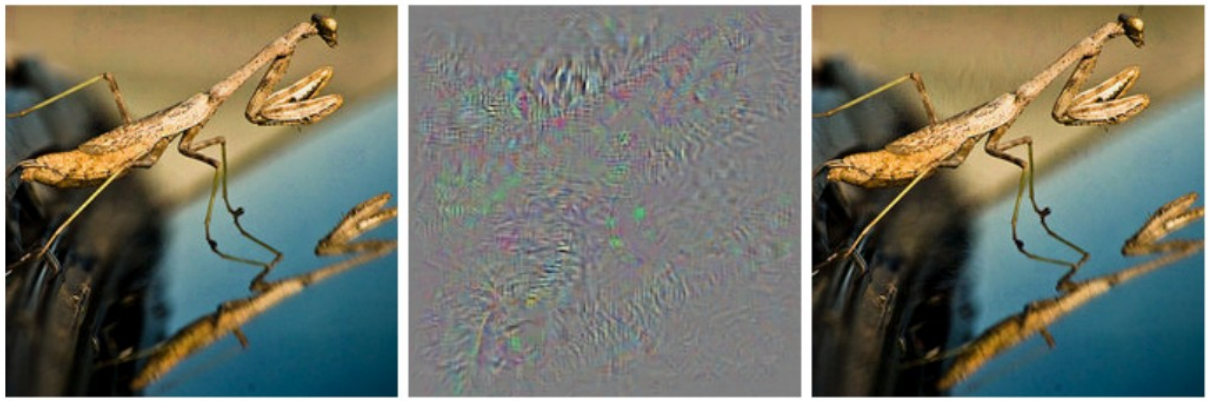
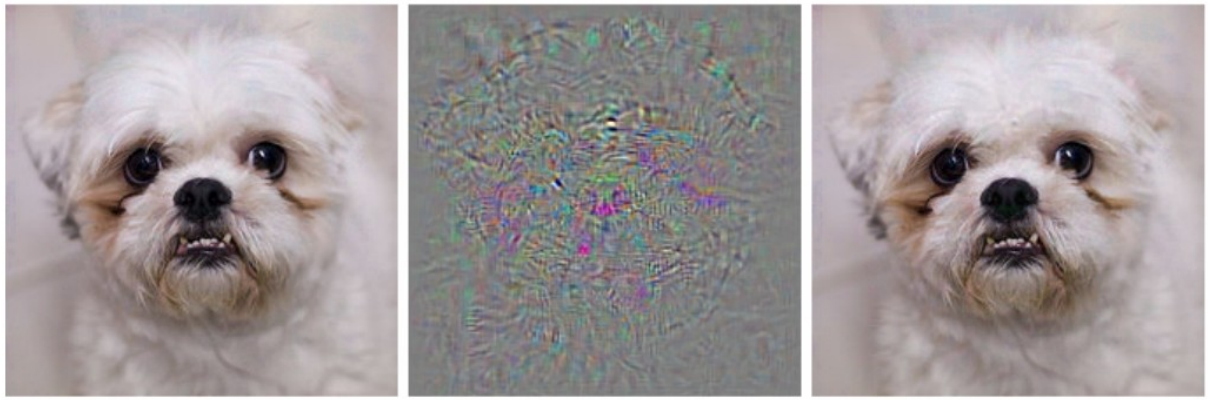
Adversarial Data

Mantis



Ostrich

Dog



Ostrich

- C. Szegedy, W. Zaremba, I. Sutskever, J. Bruna, D. Erhan, I. Goodfellow, and R. Fergus, “Intriguing properties of neural networks,” arXiv preprint arXiv:1312.6199, 2013. **Source of above image!**
- A. Nguyen, J. Yosinski, and J. Clune, “Deep neural networks are easily fooled: High confidence predictions for unrecognizable images,” arXiv preprint arXiv:1412.1897, 2014.

Adversarial Data – Definition

- Consider training data $x_1, x_2, \ldots, x_n$ in a high dimensional data space $\mathbb{R}^d$ and a neural network with p parameters which returns one of L labels: $NN : \mathbb{R}^p \times \mathbb{R}^d \to \{1, 2, \ldots, L\}$

- By training on $x_1, x_2, \ldots, x_n$ the parameter values P are determined.

- An *adversarial data point* for a given x_j of the training data is a point $y_j \in \mathbb{R}^d$ such that $NN(P, x_j) \neq NN(P, y_j)$ but the distance $|x_j - y_j|$ is very small.

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Mocking the Flawed Technology

Stephan Huckemann

FOLGEN

Professor for Non-Euclidean Statistics, University of Goettingen
Bestätigte E-Mail-Adresse bei math.uni-goettingen.de - Startseite

Statistical Shape Analysis Pattern Recognition Fingerprint Recognition Biomechanics Biomedical Imaging

TITEL	ZITIERT VON	JAHR
Intrinsic shape analysis: Geodesic PCA for Riemannian manifolds modulo isometric Lie group actions S Huckemann, T Hotz, A Munk Statistica Sinica, 1-58	~~161~~	2010
Intrinsic shape analysis: Geodesic PCA for Riemannian manifolds modulo isometric Lie group actions S Huckemann, T Hotz, A Munk Statistica Sinica, 1-58	161	2010
Adversarial spheres J Gilmer, L Metz, F Faghri, SS Schoenholz, M Raghu, M Wattenberg, ... arXiv preprint arXiv:1801.02774	88	2018
Global models for the orientation field of fingerprints: an approach based on quadratic differentials S Huckemann, T Hotz, A Munk IEEE Transactions on Pattern Analysis and Machine Intelligence 30 (9), 1507-1519	82	2008
Principal component analysis for Riemannian manifolds, with an application to triangular shape spaces S Huckemann, H Ziezold Advances in Applied Probability 38 (2), 299-319	82	2006

How does Adversarial Data work?

J. Gilmer, L. Metz, F. Faghri, S. S. Schoenholz, M. Raghu, M. Wattenberg, and I. Goodfellow. “Adversarial spheres,” arXiv preprint arXiv:1801.02774, 2018.

Consider two data sets of random vectors:

1) $x_j \in \mathbb{R}^{d+1}, \quad |x_j| = 1.0$ uniformly distributed

2) $y_j \in \mathbb{R}^{d+1}, \quad |y_j| = 1.3$ uniformly distributed

For d >> 100 and training data sets of 1,000,000 points, even though *99% of the sphere surfaces* are correctly classified, the *average distance* of a wrongly classified *adversarial point on either sphere* from any training data point can be smaller than 0.1.

The maximal average distance d depending on error surface μ can be bounded using the central limit theorem.

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The Curse of Dimensionality

Theorem

Consider a random vector **X** = $(X_1, X_2, \ldots, X_{d+1})$ of length one, uniformly distributed on the Sphere S^d. Then

$$\text{for any } \epsilon > 0 : \lim_{d \to \infty} P\left(|X_1| < \epsilon\right) = 1$$

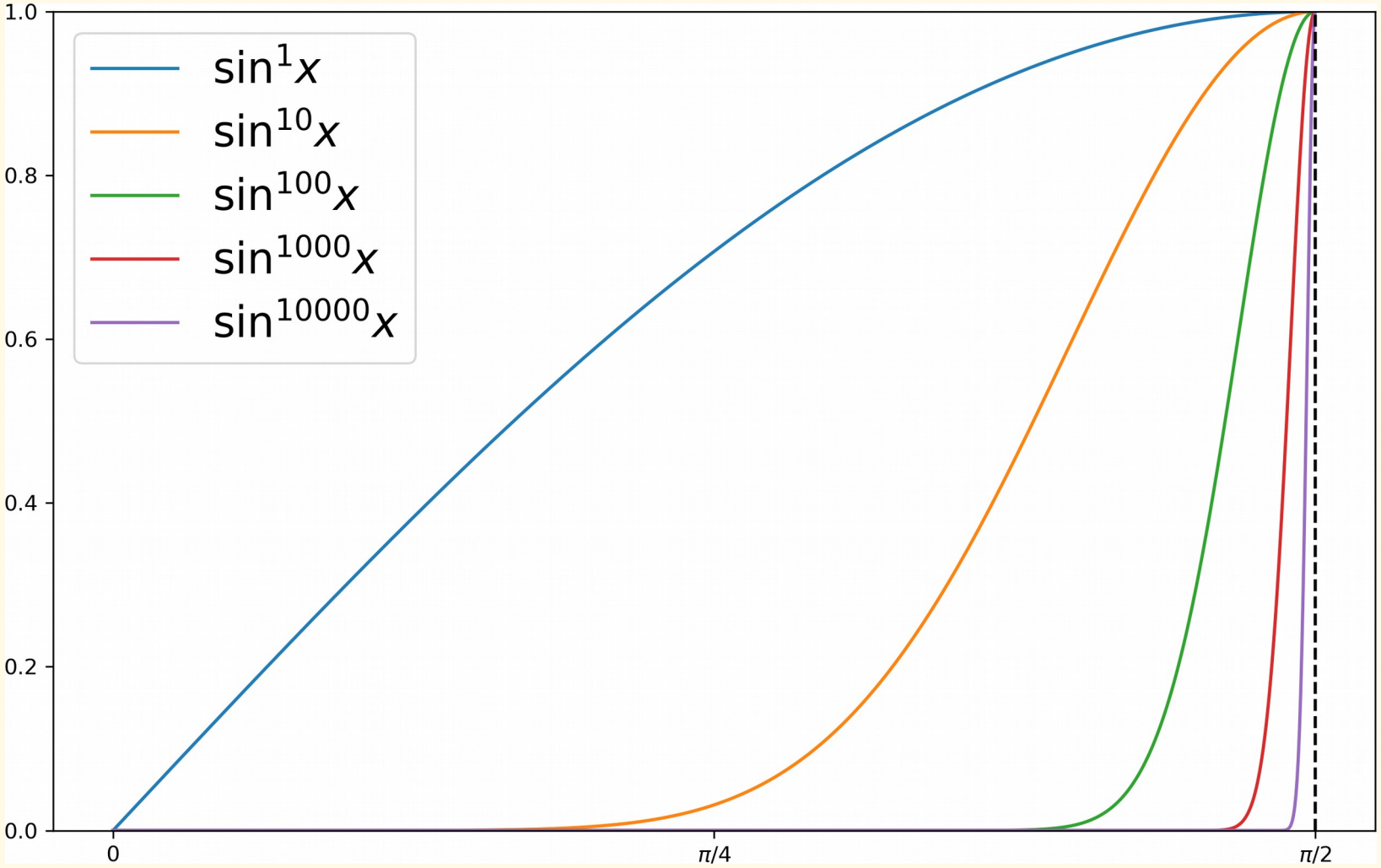
Proof

For $\alpha := \arccos(\epsilon)$ and $f_d(a,b) := \int_a^b \sin^{d-2} x \, dx$ one can write

$$P\left(|X_1| < \epsilon\right) = \frac{f_d(\alpha, \pi/2)}{f_d(0, \pi/2)} = 1 - \frac{f_d(0, \alpha)}{f_d(0, \pi/2)}$$

and note that $\lim_{d \to \infty} f_d(0, a) = 0$. This proves the theorem.

Illustration of the Curse



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Summary

- Neural Networks have two problems:

  1) Overfitting (many parameters)

  2) Curse of Dimensionality (high data dimension)

- Statistical analysis can help identify problems.

- Solution approach so far: **MOAR DATA!**

- "Neural Networks are terrible at *ignoring useless information*." *Sparsity* could help.

E. R. Balda, A. Behboodi, N. Koep and R. Mathar. "Adversarial Risk Bounds for Neural Networks through Sparsity based Compression," arXiv preprint arXiv:1906.00698, 2019.

And now to something completely different…

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Revisiting the Mean

The distribution and sample means

$$\mu_0 = \int_{-\infty}^{\infty} x f(x)\, dx \qquad \mu_n = \frac{1}{n}\sum_{k=1}^{n} x_k = \frac{1}{n}\left(x_1 + x_2 + \ldots + x_n\right)$$

cannot be generalized to other spaces. So consider

$$\mu_0 = \operatorname*{argmin}_{\mu \in \mathbb{R}} \int_{-\infty}^{\infty} (x-\mu)^2 f(x)\, dx$$

$$\mu_n = \operatorname*{argmin}_{\mu \in \mathbb{R}} \frac{1}{n}\sum_{k=1}^{n} (x_k - \mu)^2$$

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The Fréchet Mean

To see that the new definitions of the means are equivalent, calculate the minima. The new forms of the means are called population and sample *Fréchet mean*. For a metric space M with metric d:

$$\frac{d}{d\mu}\left(\frac{1}{n}\sum_{k=1}^{n}\left(x_k-\mu\right)^2\right)=0$$

$$\Leftrightarrow \frac{d}{d\mu}\left(\mu^2-2\mu\frac{1}{n}\sum_{k=1}^{n}x_k+\frac{1}{n}\sum_{k=1}^{n}x_k^2\right)=0$$

$$\Leftrightarrow \left(2\mu-\frac{2}{n}\sum_{k=1}^{n}x_k\right)=0$$

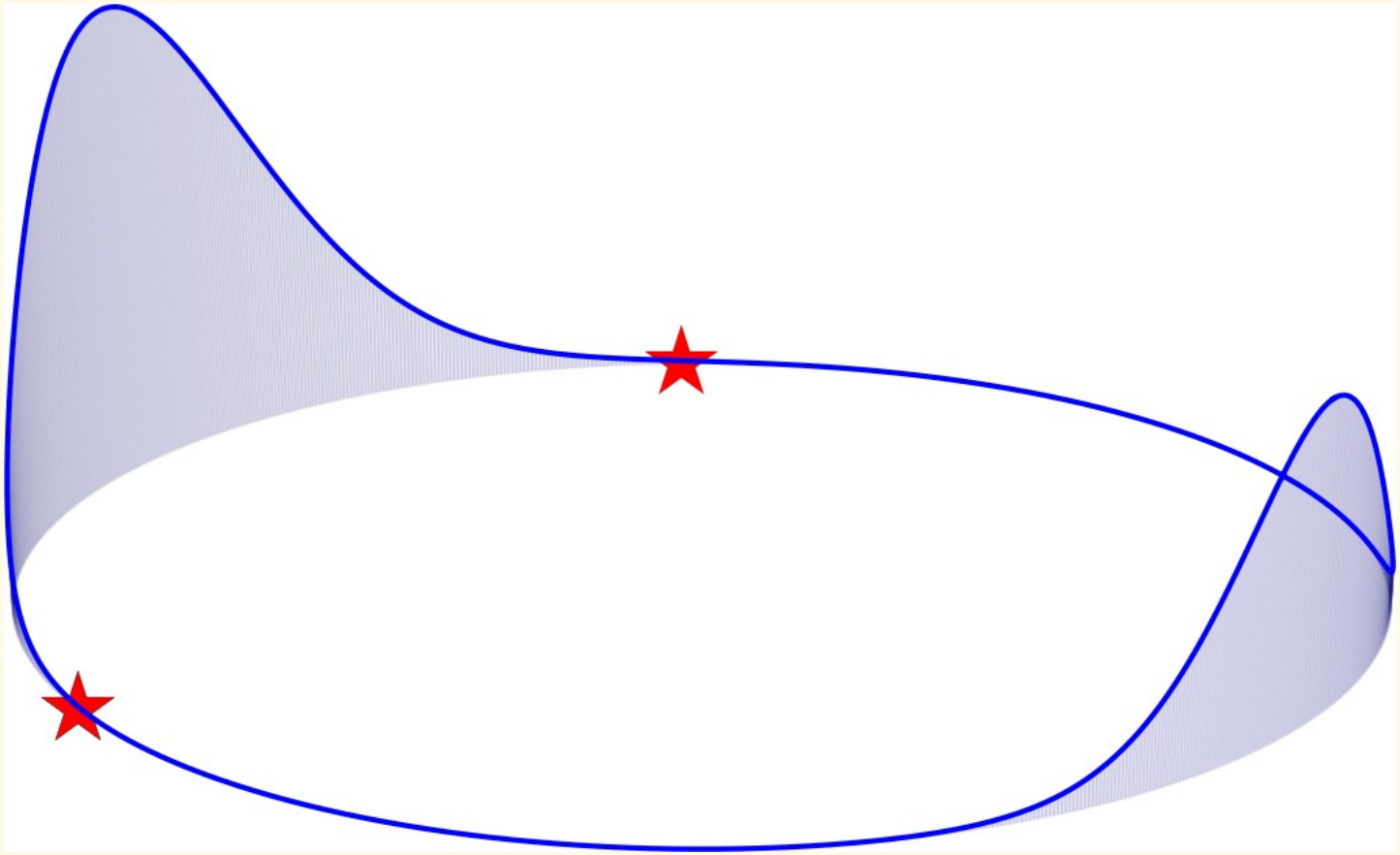
$$\Leftrightarrow \mu=\frac{1}{n}\sum_{k=1}^{n}x_k$$

$$\mu_0=\underset{\mu\in M}{\operatorname{argmin}}\int_M d\left(x,\mu\right)^2 f\left(x\right)dx$$

$$\mu_n=\underset{\mu\in M}{\operatorname{argmin}}\frac{1}{n}\sum_{k=1}^{n}d\left(x_k,\mu\right)^2$$

The Mean on Curved Spaces

On curved spaces, the mean can be ambiguous:



The Central Limit Theorem (CLT)

The Central Limit Theorem can be generalized to the Fréchet mean if

1) μ_0 is unique.

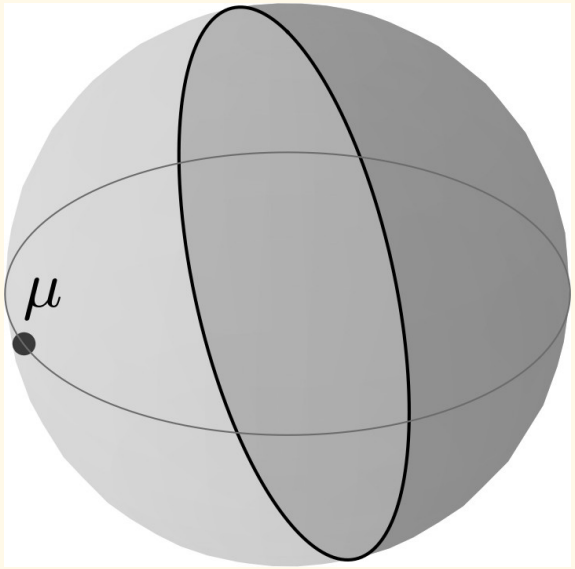
2) The population Fréchet function $F_0(\mu) := \int_M d(x,\mu)^2 f(x)\,dx$ has a second order Taylor expansion

$$F_0(\mu) = F_0(\mu_0) + \frac{d^2 F_0}{d\mu^2}(\mu_0)\,\mu^2 + O(\mu^3)$$

(This can be made precise if M is a *manifold*.)

What if…

- If the mean is not unique, the Central Limit Theorem can be adjusted.
- If the Taylor expansion does not work, things are more complicated…



A point mass on the north pole and a uniform distribution on the southern hemisphere: Quite troublesome…

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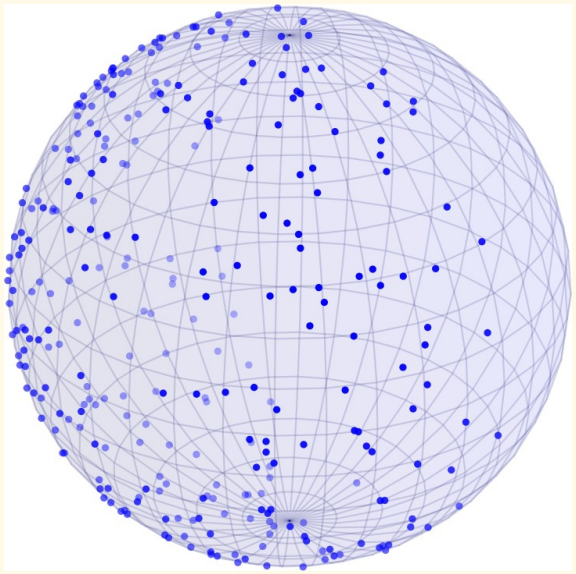
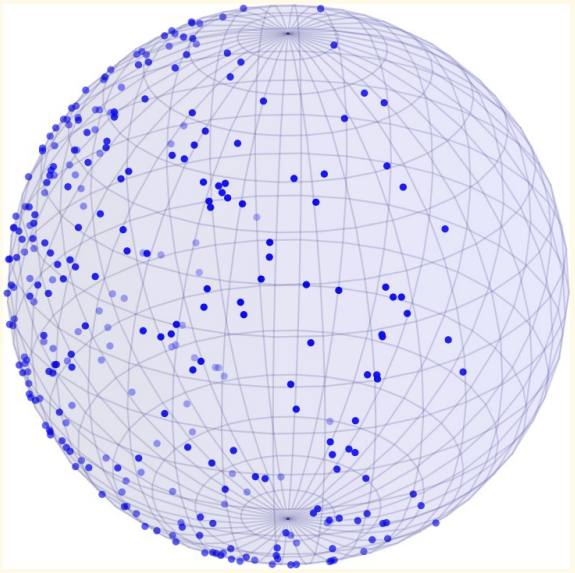
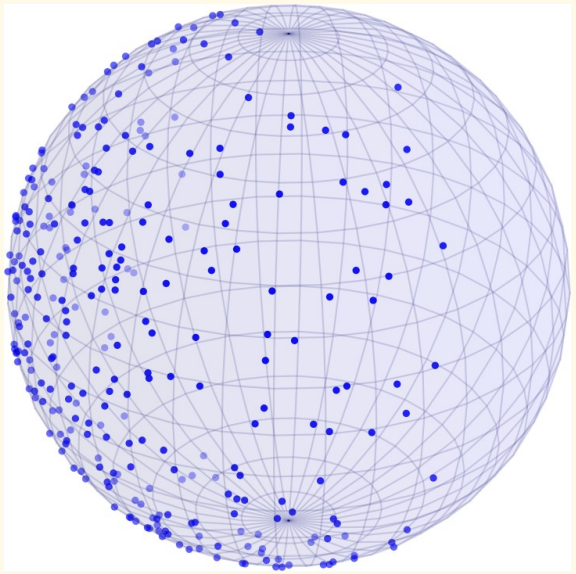
Means for n = 100



Small point mass



Medium point mass



Large point mass

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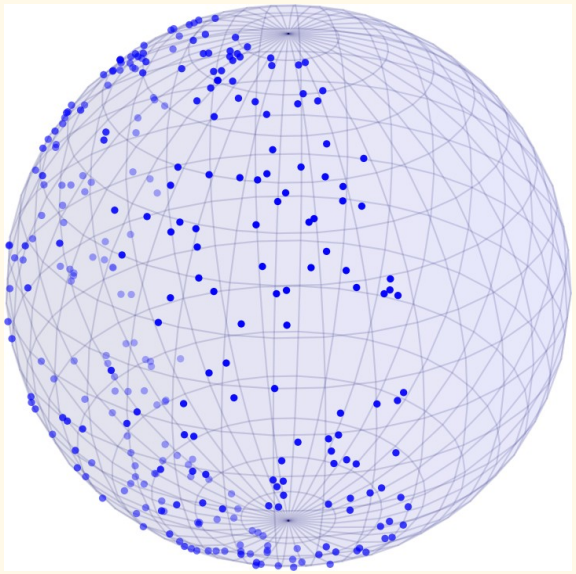
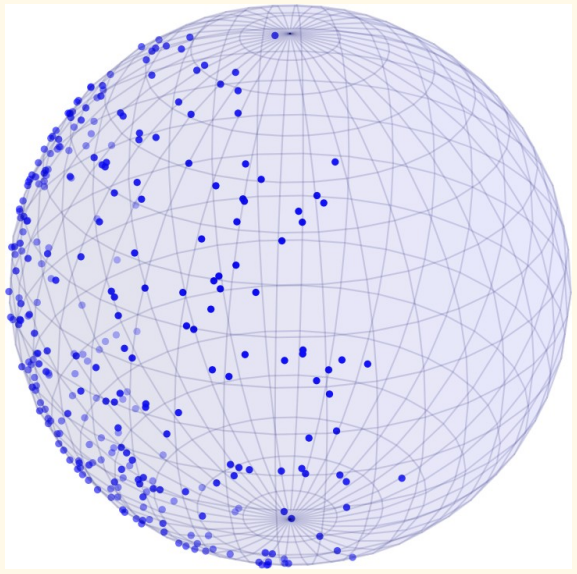
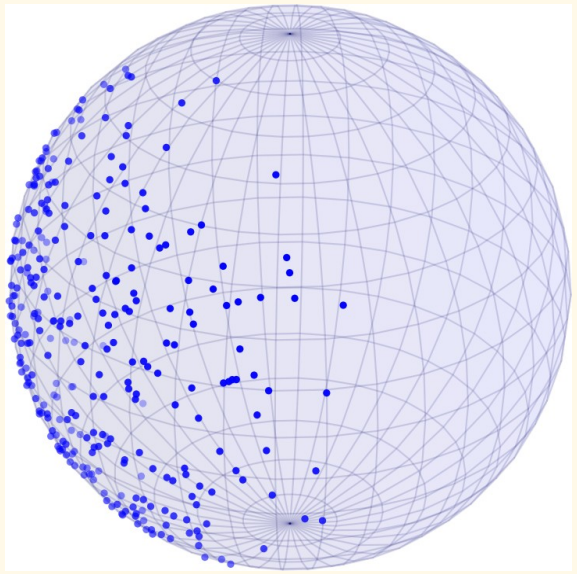
Means for n = 1,000



Small point mass



Medium point mass



Large point mass

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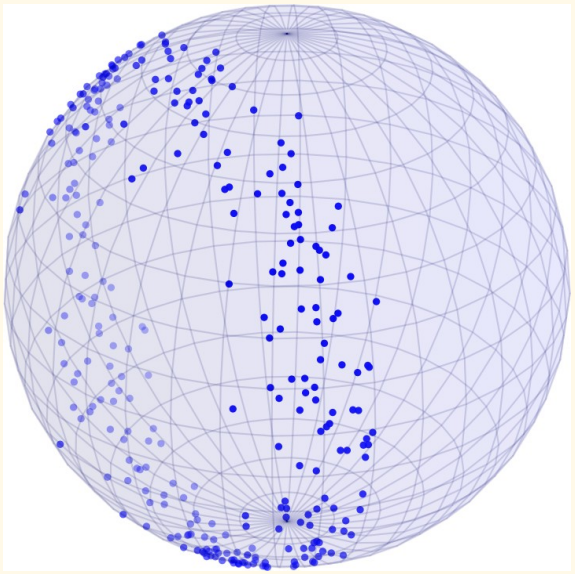
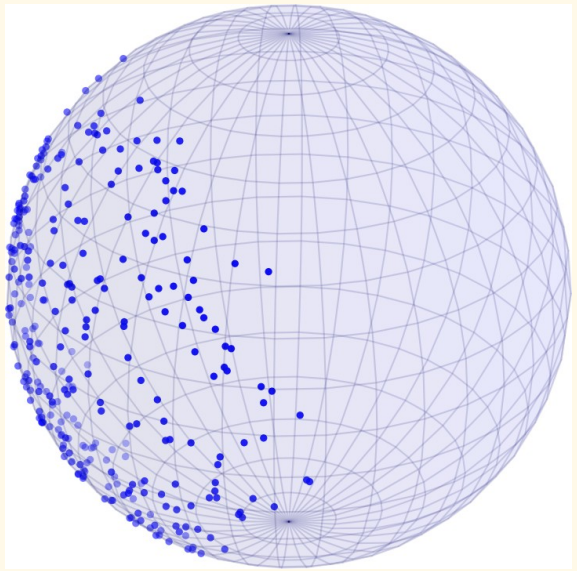
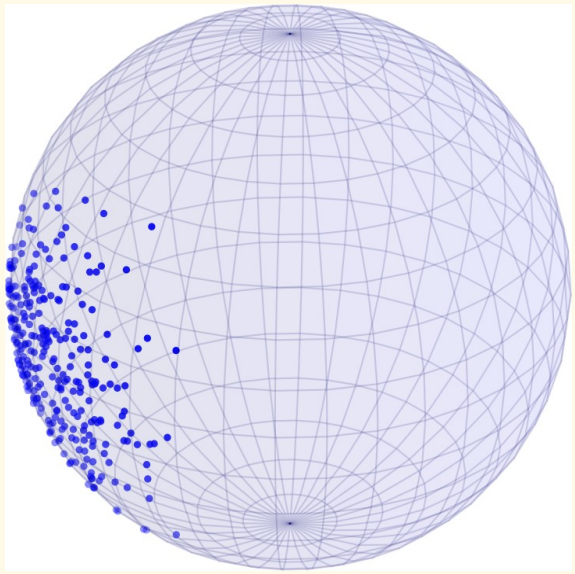
Means for n = 10,000



Small point mass



Medium point mass



Large point mass

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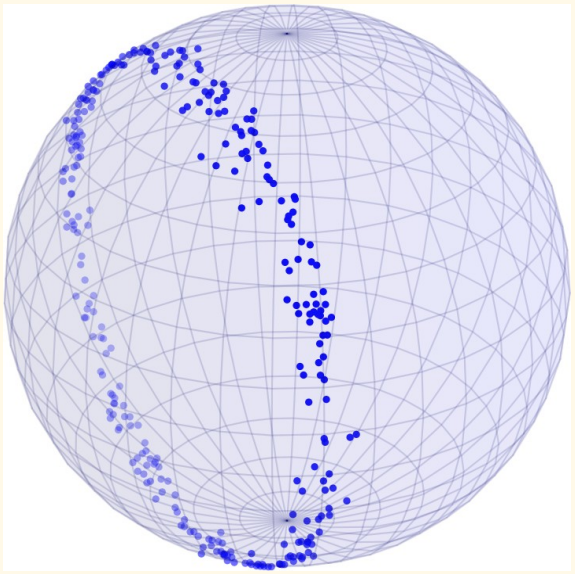
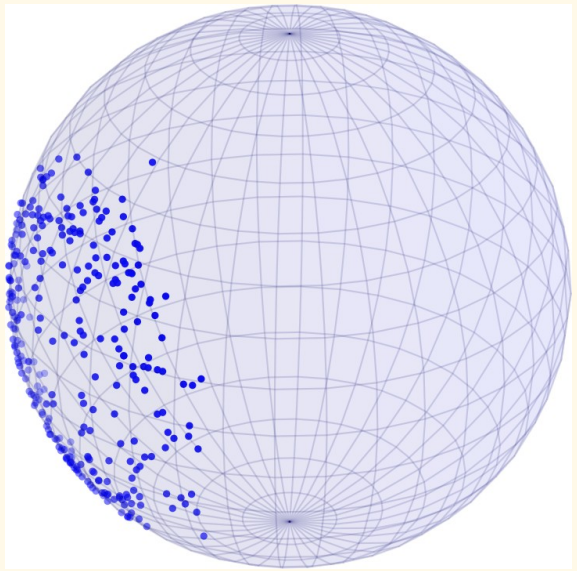
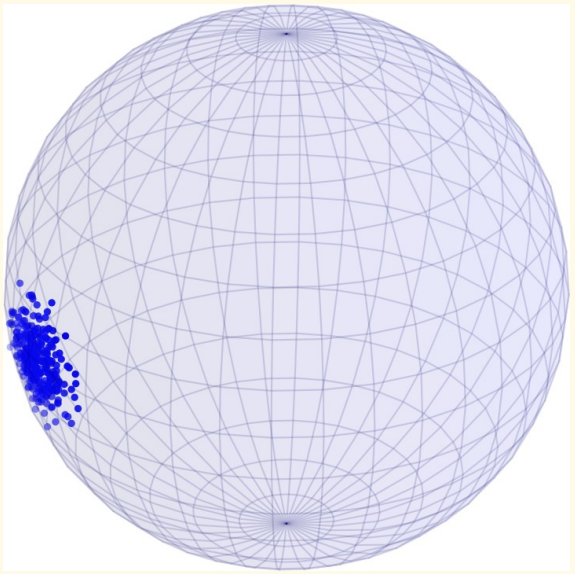
Means for n = 100,000



Small point mass



Medium point mass



Large point mass

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Observations

- For *small point mass*, the *mean is not unique*, but on a circle around the north pole.
- For *large point mass*, the *mean is unique* on the north pole.
- For *medium point mass*, the mean is unique on the north pole, but *convergence is very slow*!

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A Generalized CLT

Assume

1) μ_0 is unique.

2) The population Fréchet function has an expansion

$$F_0(x) - F_0(\mu_0) = \sum_{j=1}^{d} a_j \left| x_j \right|^r + O\left(x^{r+1}\right)$$

Then $\sqrt{n}\left(\mu_n - \mu_0\right)_j \left|\left(\mu_n - \mu_0\right)_j\right|^{r-2}$ approaches a Gaussian distribution centered at 0 for $n \to \infty$.

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What does this mean?

- If the Fréchet function is not a quadratic function at its minimum μ_0, the standard CLT does not hold.
- If the order of the Fréchet function is r, $\left(\mu_n - \mu_0\right)^{r-1}$ converges to 0 as $\frac{1}{\sqrt{n}} = n^{-1/2}$.
- This means that $\mu_n - \mu_0$ converges to 0 as $n^{-1/(2r-2)}$.
- *Larger data sets do not help so much!*

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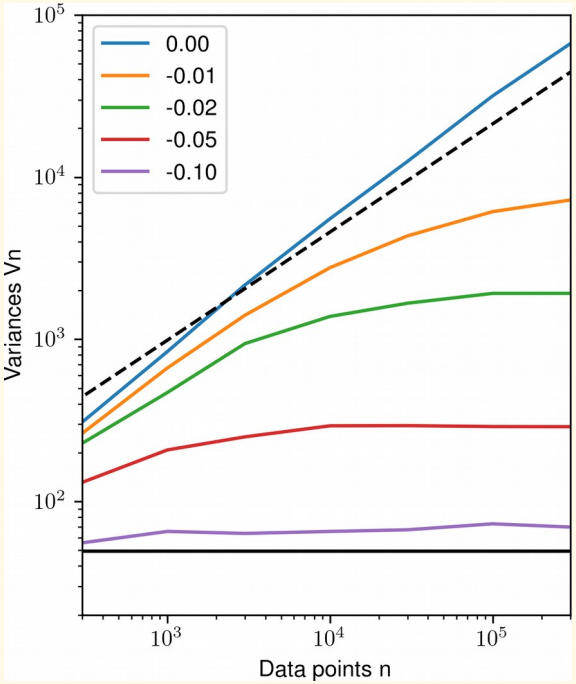
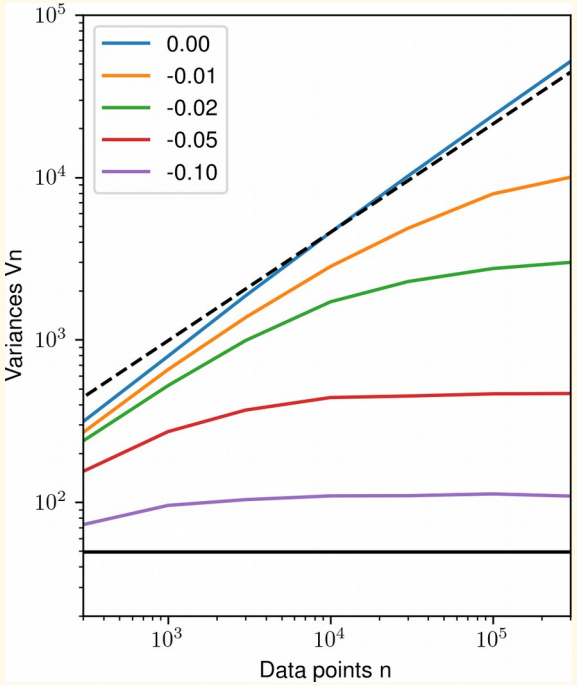
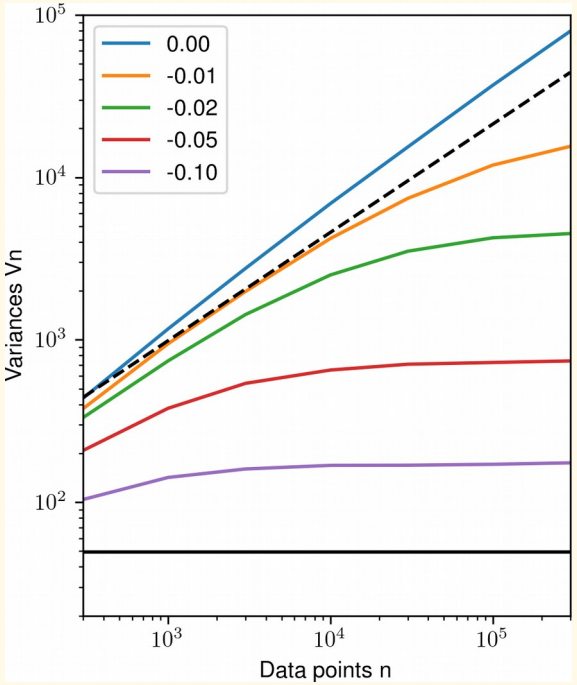
Only One Pathological Example?







d=2 d=10 d=100

Distributions with larger point mass also *need very large data sets* for normal convergence! *Worse for higher dimension*!

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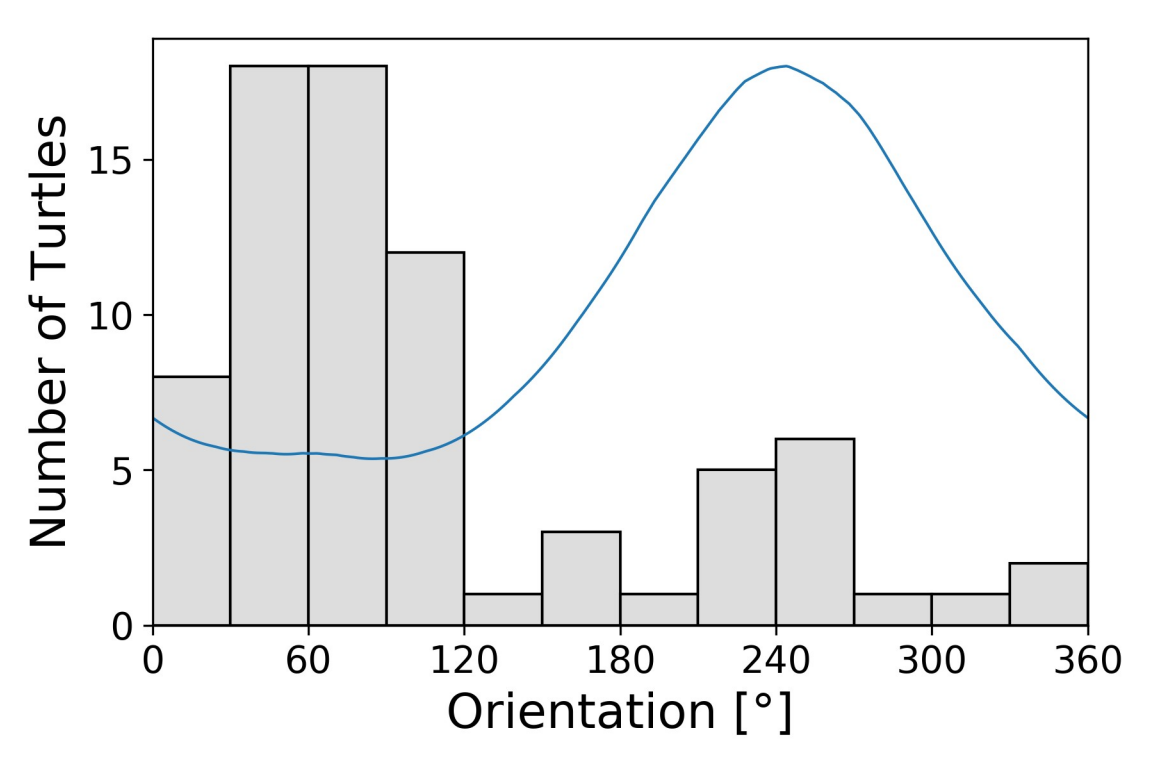
A Real World™ Example



Movement direction of female turtles after laying eggs on the beach.

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How to Check Convergence Rate?

- Consider a data set $x_1, x_2, \ldots, x_n$.
- Draw $y_1, y_2, \ldots, y_m$ with replacement from the data and calculate the mean $\mu_m^* = \operatorname{argmin}_{\mu \in M} \frac{1}{m} \sum_{k=1}^{m} d(y_k, \mu)^2$.
- Do this B times to get $\mu_m^{*1}, \mu_m^{*2}, \ldots, \mu_m^{*B}$. This is called *m-out-of-n bootstrap with B replicates*.
- Then calculate $V_m^* = \frac{1}{B}\left(d(\mu_m^{*1}, \mu_n)^2 + d(\mu_m^{*2}, \mu_n)^2 + \ldots + d(\mu_m^{*B}, \mu_n)^2\right)$.

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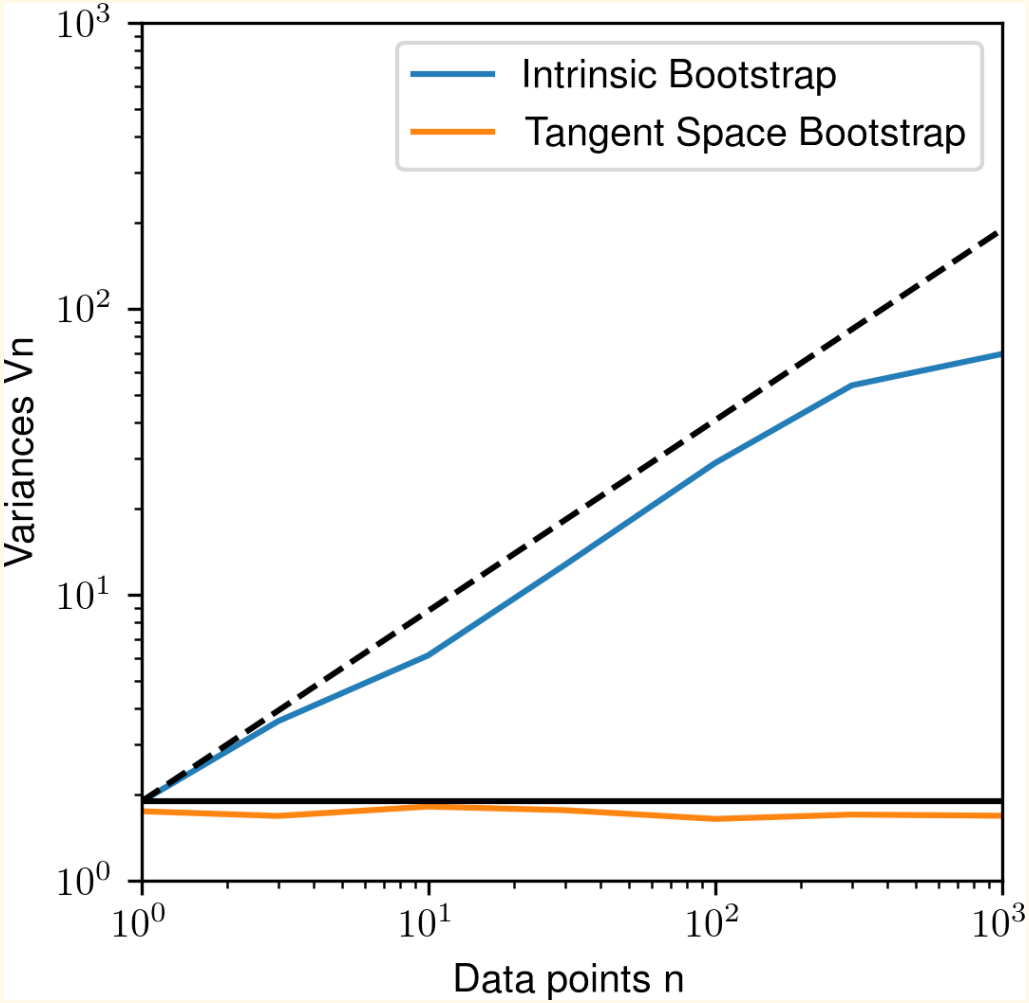
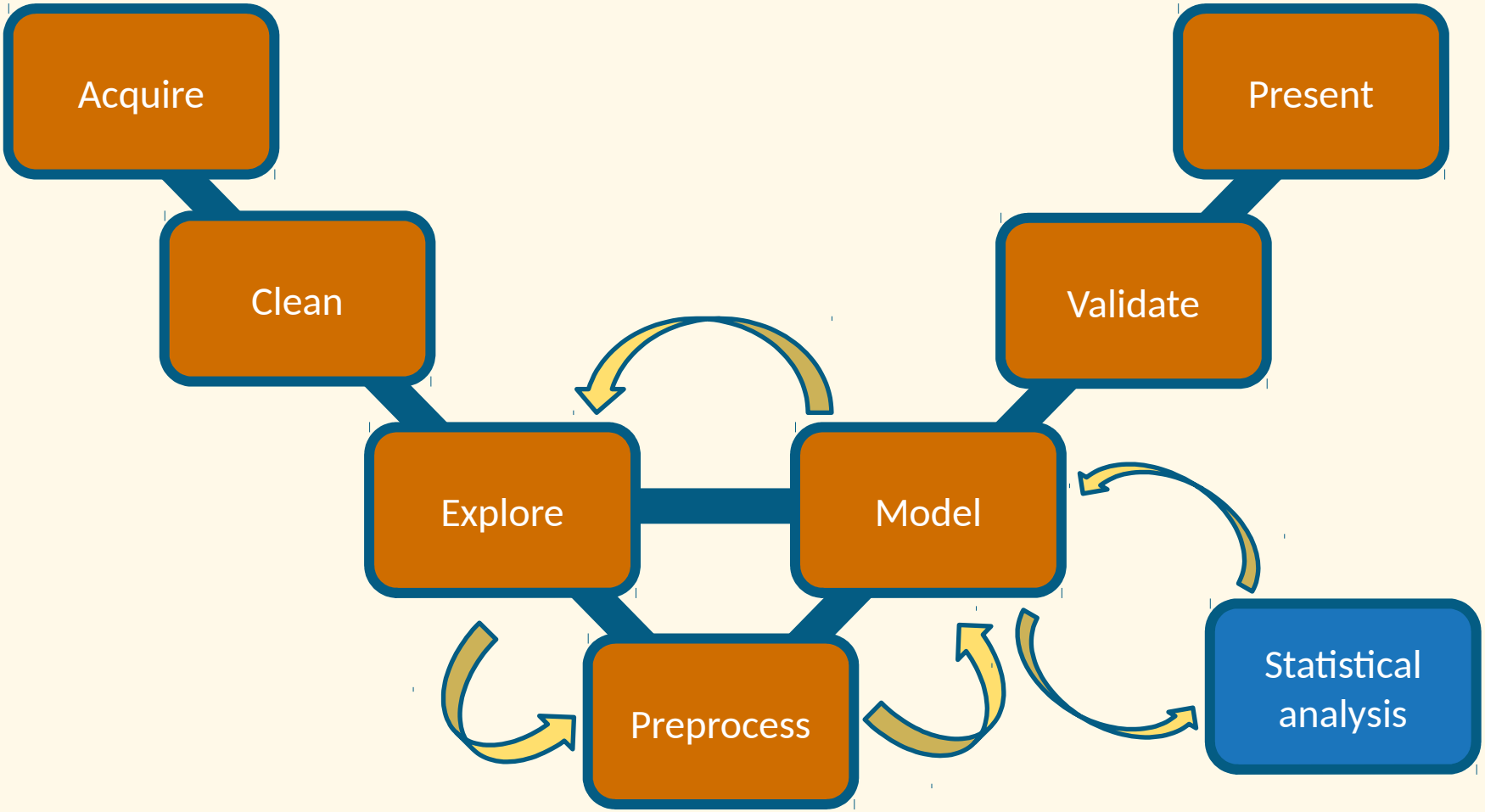
Slow Rate of Convergence



How to avoid ruining the V?



Here's the Upshot

- Terrible things lurk in the shadows: *Overfitting*, *Curse of Dimensionality*, *slow Asymptotics*.
- Statistics knows many of these abominations.
- Statistics can *identify* and *quantify problems*.
- Statistics has learned some *coping strategies*.
- Statistics has the tools to *interpret wreckages*.

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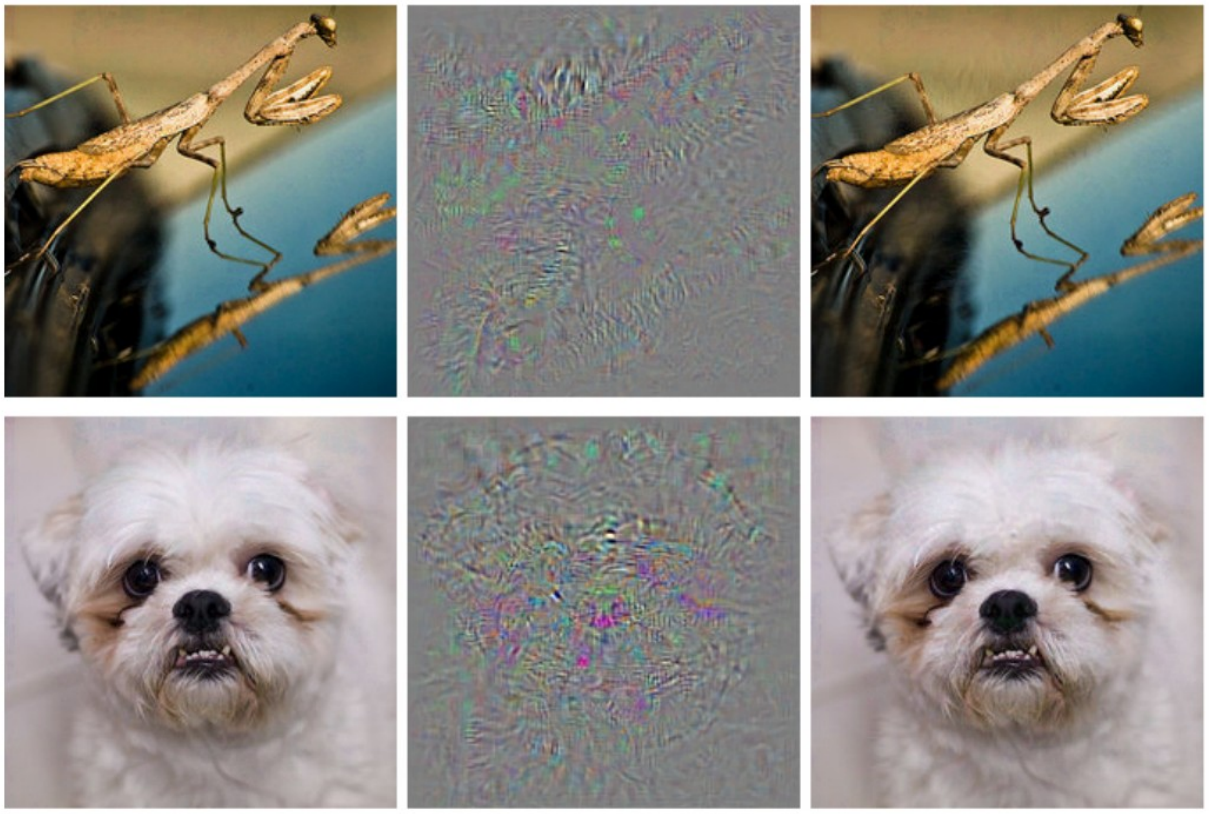
Neural Network without Statistics

Mantis



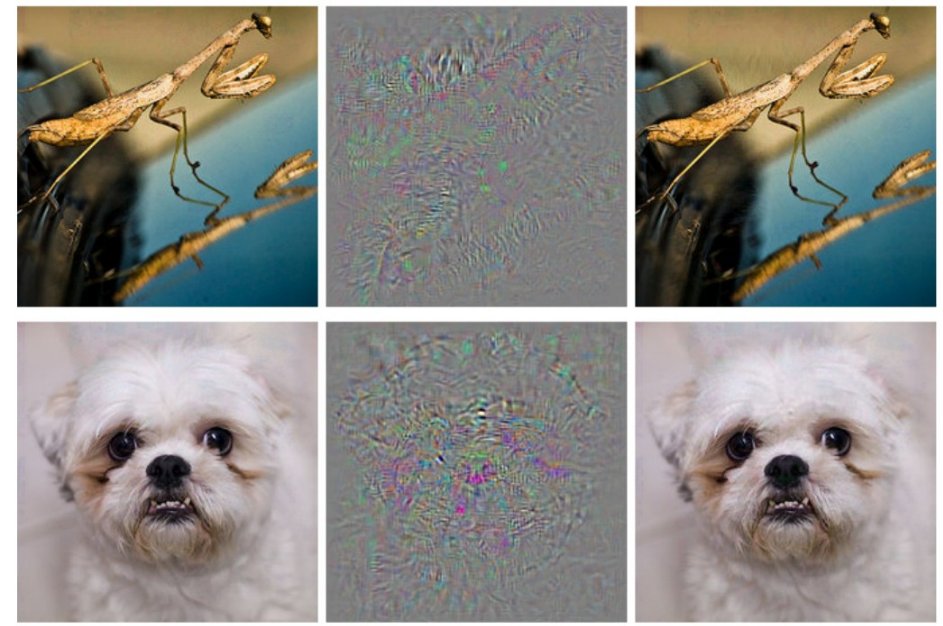
Ostrich

Dog

Ostrich

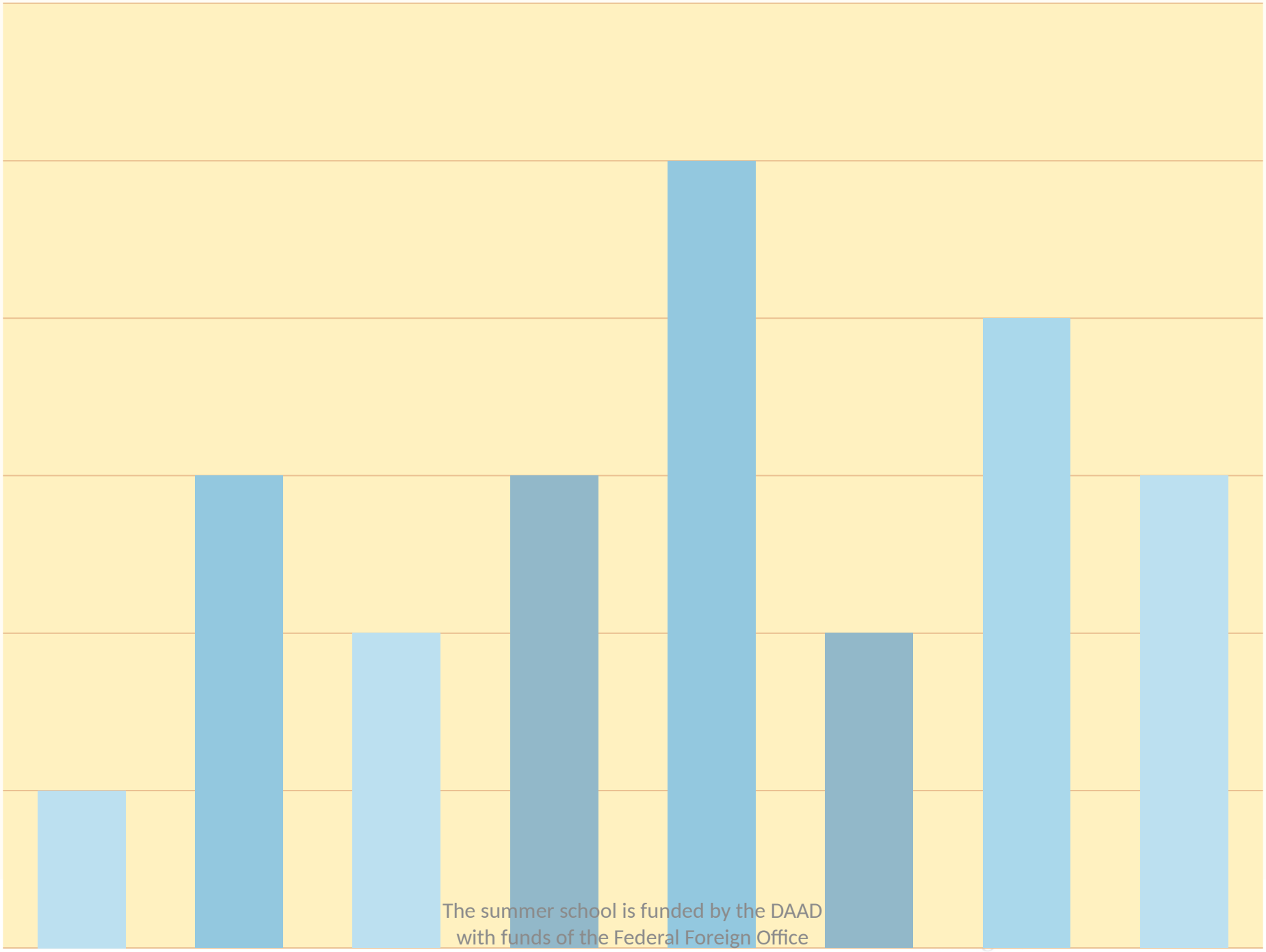
Image: C. Szegedy, W. Zaremba, I. Sutskever, J. Bruna, D. Erhan, I. Goodfellow, and R. Fergus, “Intriguing properties of neural networks,” arXiv preprint arXiv:1312.6199, 2013.

Neural Network on Statistics



"With the high dimension and the overfitting, I suppose it could be a mantis, a dog, an ostrich or a submarine. That's assuming that the CLT holds for these data."

Image: C. Szegedy, W. Zaremba, I. Sutskever, J. Bruna, D. Erhan, I. Goodfellow, and R. Fergus, "Intriguing properties of neural networks," arXiv preprint arXiv:1312.6199, 2013.



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