

Learning in high dimension: some insights from statistical physics

after Florent Krzakala's second lecture in les Houches:

<https://florentkrzakala.com/files/leshouches2020/courses/florent>

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Statistical Machine Learning

Classification in statistical learning



Input space $\mathcal{X} = [0, 1]^{27 \times 27}$, label set $\mathcal{Y} = \{0, \dots, 9\}$

Sample $S_n = (X_1, Y_1), \dots, (X_n, Y_n)$ (MNIST: 70000 images + labels)

Rule (or *hypothesis*) $f : \mathcal{X} \rightarrow \mathcal{Y}$

Classification algorithm $\mathcal{A}_n : \begin{matrix} (\mathcal{X} \times \mathcal{Y})^n & \rightarrow & \mathcal{Y}^\mathcal{X} \\ S_n & \mapsto & \hat{f}_n \end{matrix}$

Statistical Learning

Assumption: the data was and will be generated by a random mechanism:

$$S_n = (X_1, Y_1), \dots, (X_n, Y_n) \stackrel{iid}{\sim} P \quad \text{probability law on } \mathcal{X} \times \mathcal{Y}$$

Prediction $\hat{Y}_i = f(X_i)$ induces a loss $\ell(\hat{Y}_i, Y_i)$ ex: $\ell(\hat{Y}_i, Y_i) = \mathbb{1}\{\hat{Y}_i \neq Y_i\}$

Oracle: rule f minimizing $L(f) = \mathbb{E}_P[\ell(f(X), Y)]$ Minimizer = Bayes risk

Look for rules in hypotheses class $\mathcal{F} \subset \mathcal{Y}^{\mathcal{X}}$

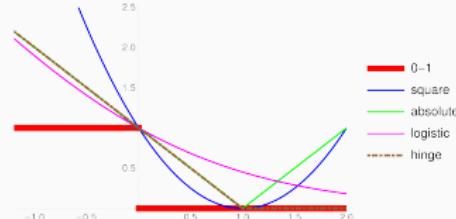
For computational reasons (continuous optimisation is a lot easier than combinatorial optimization), one often considers relaxations:

- \mathcal{Y} is taken to be convex Ex: $\{-1, 1\} \subset \mathbb{R}$, $\{0, \dots, 9\} \hookrightarrow \mathbb{R}^{10}$
- $\mathcal{F} = \{f_{\theta} : \theta \in \Theta \subset \mathbb{R}^p\}$ and consider $\text{sign}(f_{\theta}(X_i))$ as the prediction
- $\ell(\cdot, Y_i)$ = a smooth, convex function

$$\text{Ex: } \ell(\hat{Y}_i, Y_i) = (\hat{Y}_i - Y_i)^2 \text{ or } \log_2(1 + \exp(-\hat{Y}_i \times Y_i))$$

Examples:

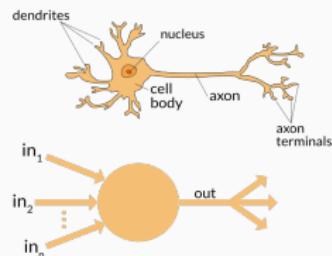
- linear classification $f_{\theta}(x) = x \cdot \theta$, $\theta \in \mathbb{R}^d$ ex: image filters
- neural networks $f_{\theta} = \sigma_D \circ T_D \circ \dots \circ \sigma_1 \circ T_1$



Feedforward Neural Networks: Mimicking Brains?

Neuron: $x \mapsto \sigma(\langle w, x \rangle + b)$ with

- parameter $w \in \mathbb{R}^p, b \in \mathbb{R}$
- (non-linear) activation function $\sigma : \mathbb{R} \rightarrow \mathbb{R}$
typically $\sigma(x) = \frac{1}{1+\exp(-x)}$ or $\sigma(x) = \max(x, 0)$ called ReLU

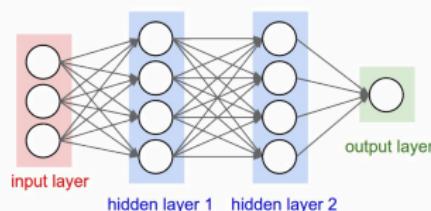


Layer: $x \mapsto \sigma(Mx + \mathbf{b})$ with

- parameter $M \in M_{q,p}(\mathbb{R}), \mathbf{b} \in \mathbb{R}^q$
- component-wise activation function $\sigma = \sigma^{\otimes q}$

Network: composition of layers $f_\theta = \sigma_D \circ T_D \circ \dots \circ \sigma_1 \circ T_1$ with

- architecture $A = (D, (p_1, \dots, p_{D-1}))$
- $x_0 = x, x_d = \sigma_d(T_d x_{d-1}) \in \mathbb{R}^{p_d}$
- $T_d x = M_d x + \mathbf{b}_d$
- parameter $\theta = (M_1, \mathbf{b}_1, \dots, \dots, M_D, \mathbf{b}_D)$
 $\theta \in \Theta_A = \prod_{d=1}^D \mathcal{M}_{p_{d-1}, p_d}(\mathbb{R}) \times \mathbb{R}^{p_d}$
- depth D (\triangle st. nb layers), width $\max_{1 \leq d \leq D} p_d$



Empirical Risk Minimization

Goal: find θ minimizing $L(\theta) = \mathbb{E}_P[\ell(f_\theta(X), Y)]$

But the learnt rule $\hat{f}_n = f_{\hat{\theta}_n}$ depends only on the sample S_n

PAC learning: for every $\epsilon, \delta > 0$, find the *sample size* $n(\epsilon, \delta)$ such that whatever the law P , if $n \geq n(\delta, \epsilon)$ then with probability at least $1 - \delta$ one has $L(\hat{\theta}_n) < \min_{\theta \in \Theta} L(\theta) + \epsilon$

Idea: Empirical Risk Minimization (ERM):

$$\hat{\theta}_n = \arg \min_{\theta \in \Theta} L_n(\theta) := \frac{1}{n} \sum_{i=1}^n \ell(f_\theta(X_i), Y_i)$$

PAC learning theory (pessimistic): uniform law of large numbers

$$\mathbb{P} \left(\forall \theta \in \Theta, \quad |L_n(\theta) - L(\theta)| \leq c \sqrt{\frac{\dim \Theta + \log \frac{1}{\delta}}{n}} \right) \geq 1 - \delta$$

Bias-variance tradeoff

The classical PAC theory does not work unless $n \gg \dim \Theta$

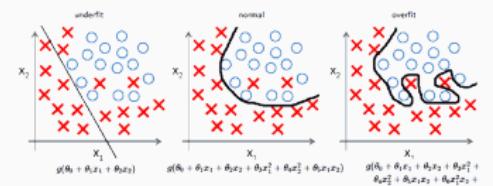
Consider different models $(\Theta_d)_{d \geq 1}$ Example: images at different resolutions

Decomposition of the (quadratic) risk

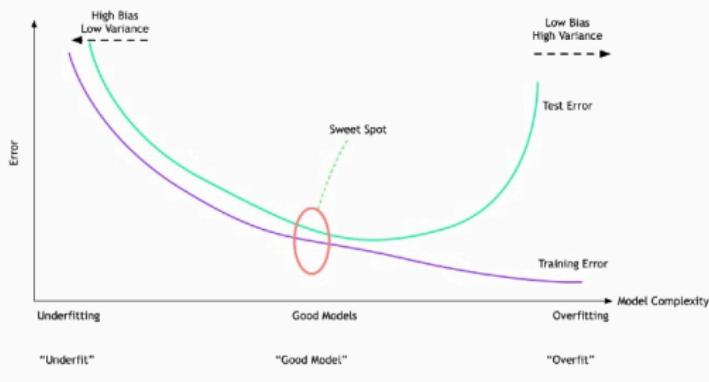
$$\mathbb{E}[L(\hat{\theta}_n)] = b_d^2 + v_d$$

- Bias: $b_d = \min_{\theta \in \Theta_d} L(\theta)$ decreases with d
- Variance term: $v_d = \frac{\dim \Theta_d}{n}$ increases with d

\implies best choice = bias-variance balance



think: polynomial regression



src: <https://miro.medium.com>

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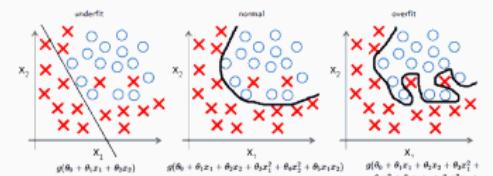
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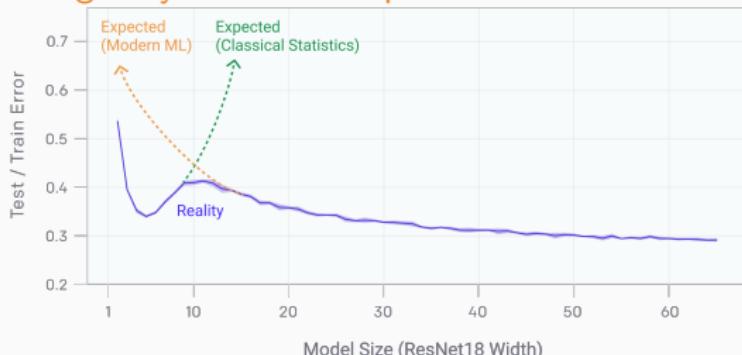
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think: polynomial regression

This statement is challenged by numerical experiments on neural networks



src: <https://miro.medium.com>

Linear Models

Linear models

$$\hat{Y} = X \cdot \theta, \theta \in \mathbb{R}^d$$

Matrix notation: $\mathbf{X} = \begin{pmatrix} X_1 \\ \vdots \\ X_n \end{pmatrix} \in M_{n,d}(\mathbb{R}), Y = \begin{pmatrix} Y_1 \\ \vdots \\ Y_n \end{pmatrix} \in \mathbb{R}^n$

L^2 loss $\ell(\hat{Y}_i, Y_i) = (\hat{Y}_i - Y_i)^2$ solution: Ordinary Least Square (OLS)

$\hat{\theta}_n \in \arg \min_{\theta \in \mathbb{R}^d} \|Y - X\theta\|_2^2$ satisfies the normal equations $XX^T\theta = X^T Y$

If $\text{rank}(X^T X) = d$ (requires $n \geq d$)

there is a unique solution

$$\hat{\theta}_n = (X^T X)^{-1} X^T Y$$

Classical statistics theory

Otherwise, many solutions

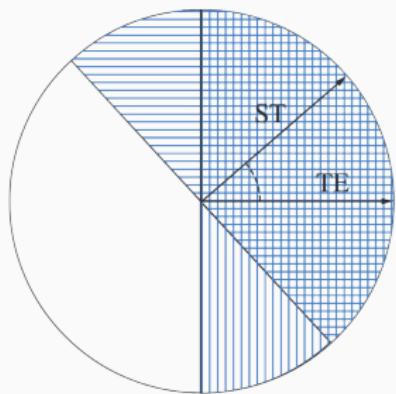
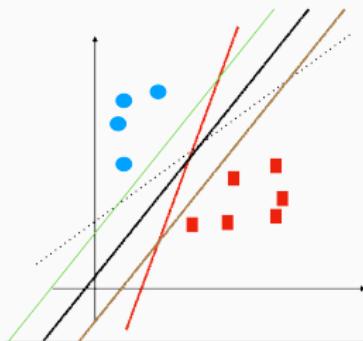
Popular: least-norm solution

$$\hat{\theta}_n = X^T (X X^T)^{-1} Y$$

Statistically spurious

Physics model: the teacher-student framework

- The model is true: $Y_i = \text{sign}(X_i \cdot \theta^*)$
- $X_i \sim \mathcal{N}(0, I_d)$ cf images?
- $\theta^* \sim \mathcal{N}(0, I_d)$ cf Bayesian approach?
- High-dimensional limit as $n, d \rightarrow \infty$ with $\alpha = n/d$ fixed



- volume of students with generalization error ϵ : $v(\epsilon) \propto \epsilon^{d \times \text{entropy}(\epsilon)}$

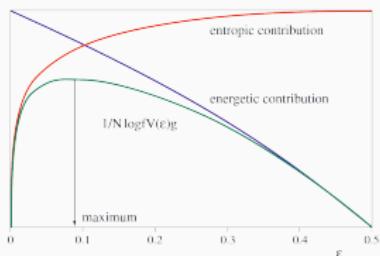
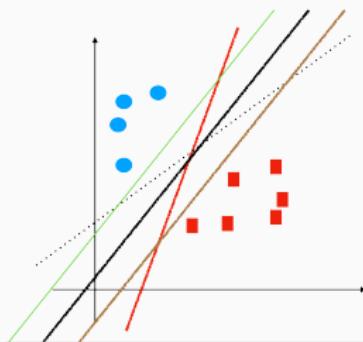
- probability that a student with generalization error ϵ makes no mistake:
 $p(\epsilon) \propto \epsilon^{n \times \text{energy}(\epsilon)}$
⇒ average generalization error of ERM:

$$\int v(\epsilon)p(\epsilon)d\epsilon \approx \arg \max_{\epsilon} \text{entropy}(\epsilon) + \alpha \text{energy}(\epsilon)$$

in the limit when $\alpha = n/d$ fixed

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- High-dimensional limit as $n, d \rightarrow \infty$ with $\alpha = n/d$ fixed



src: *Learning to generalize*, Opper'01

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Statistical physics analysis

⇒ "spin glasses", physics analysis in the 1990's (Opper & Kinzel, etc.)
rigorous proofs recently (Florent Krzakala, Lenka Zdeborova, etc.):
can compute

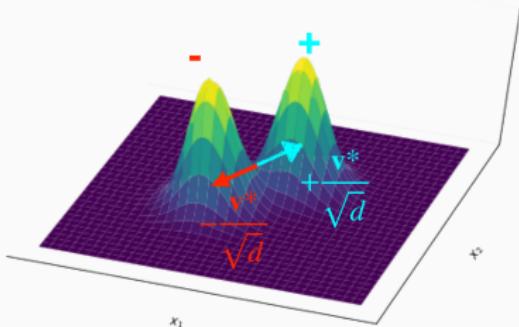
- the "Bayes risk" $\mathbb{E}[L(\theta)|S_n] =$ mean risk of ERM
- the risk of the minimal-norm ERM

in the limit, as a function of α .

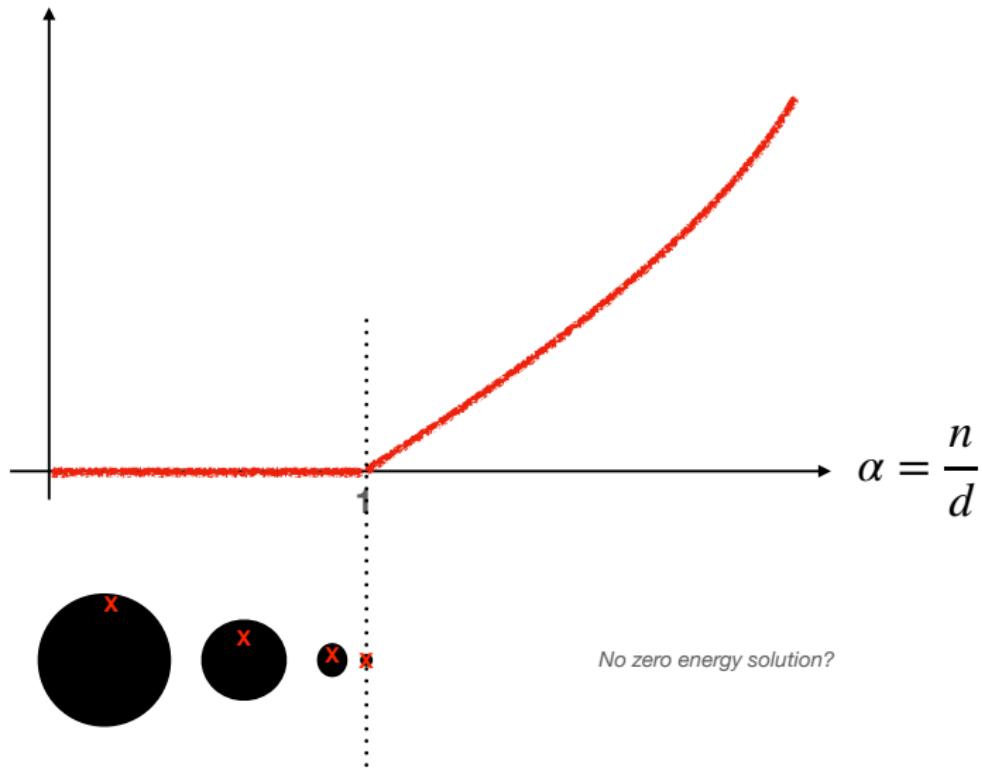
Other model discussed: Gaussian Mixture

$$x_i \sim \mathcal{N} \left(\frac{Y_i v^*}{\sqrt{d}}, \Delta \right)$$

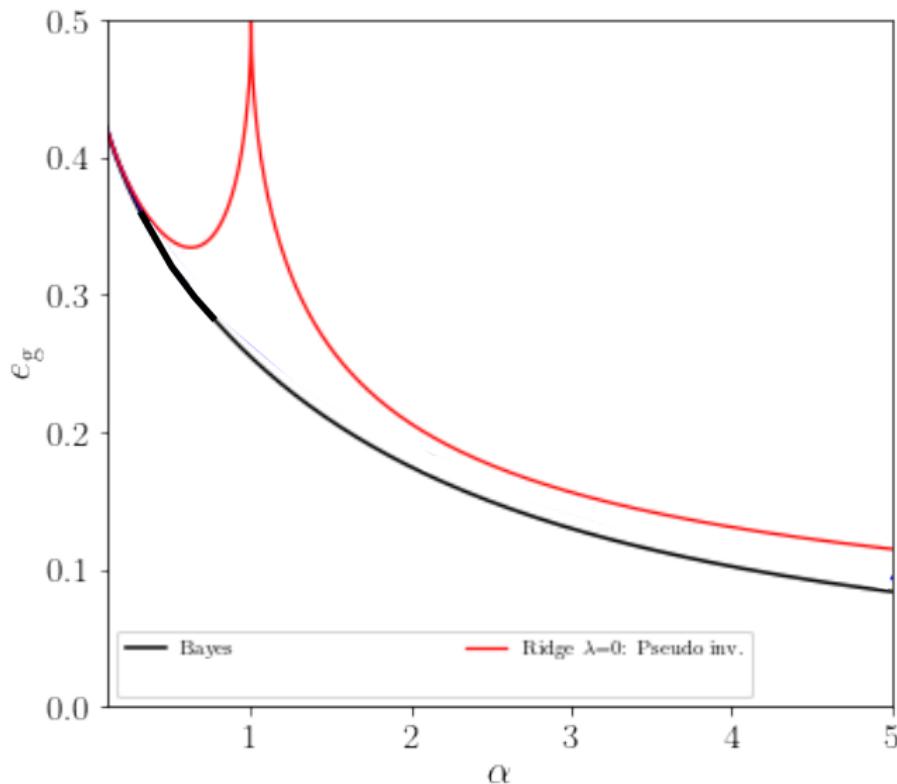
Similar results



Least norm solution



Least norm solution: “double descent”



Gradient Descent

Iterative optimization of θ :

$$\theta^t = \theta^{t-1} - \eta_t \nabla_{\theta} L_n(\theta^{t-1})$$

Here $f_{\theta}(x) = x \cdot \theta \implies$

$$\nabla_{\theta} L_n(\theta^{t-1}) = \frac{1}{n} \sum_{i=1}^n \partial_1 \ell(f_{\theta}(X_i), Y_i) X_i \in \text{span}(X_1, \dots, X_n)$$

Representer theorem

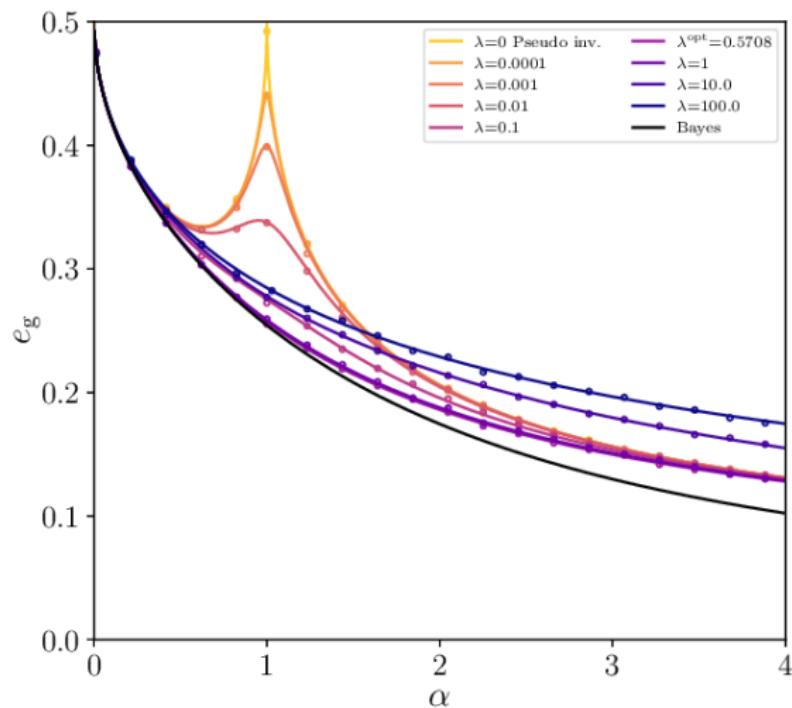
$$\min_{\theta \in \mathbb{R}^d} L_n(\theta) = \min_{\theta \in \text{span}(X_1, \dots, X_n)} L_n(\theta)$$

In fact, if $\theta = \theta_X + \theta_{X^\perp}$, then $L_n(\theta) = \frac{1}{n} \sum_{i=1}^n \ell(X_i \cdot \theta, Y_i) = L_n(\theta_X)$

\implies if $\theta_{X^\perp}^0 = 0$ gradient descent finds the solution with minimal norm

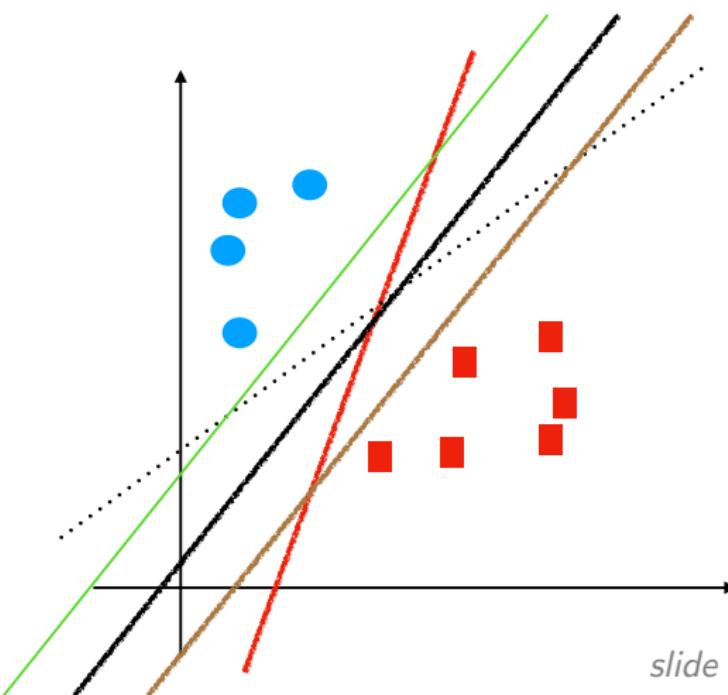
\implies other approach: minimize *ridge loss* $L_n^{\lambda}(\theta) = L_n(\theta) + \lambda \|\theta\|^2$

Ridge loss

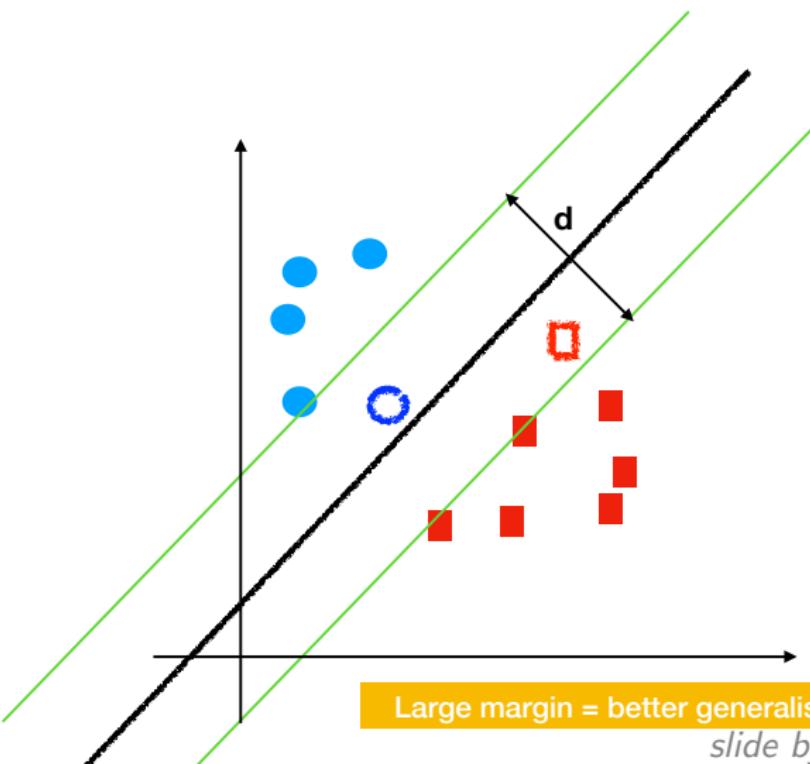


Pushing the boundaries

Which frontier should we choose?



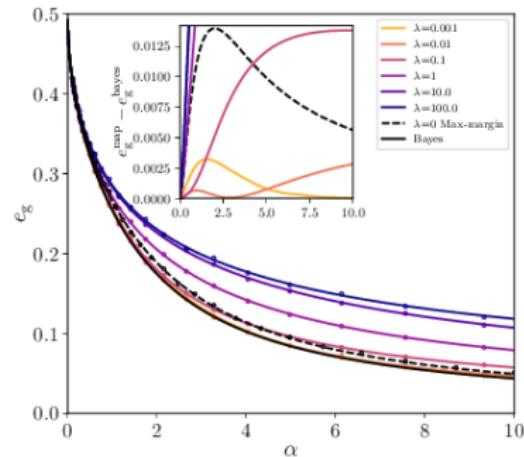
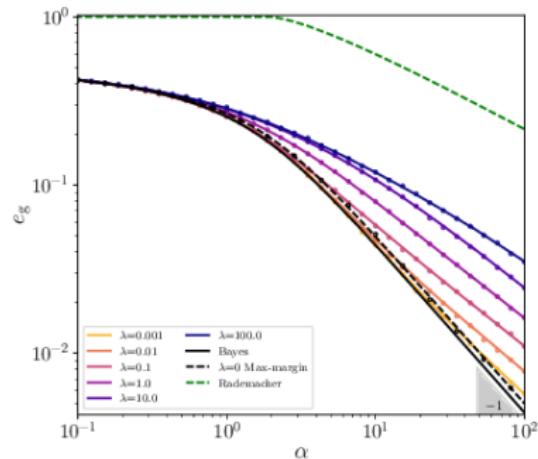
Pushing the boundaries



Large margin = better generalisation properties!

slide by Florent Krzakala

Chasing the Bayes optimal result



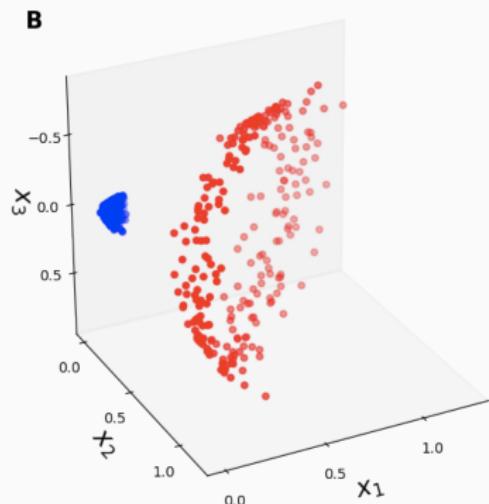
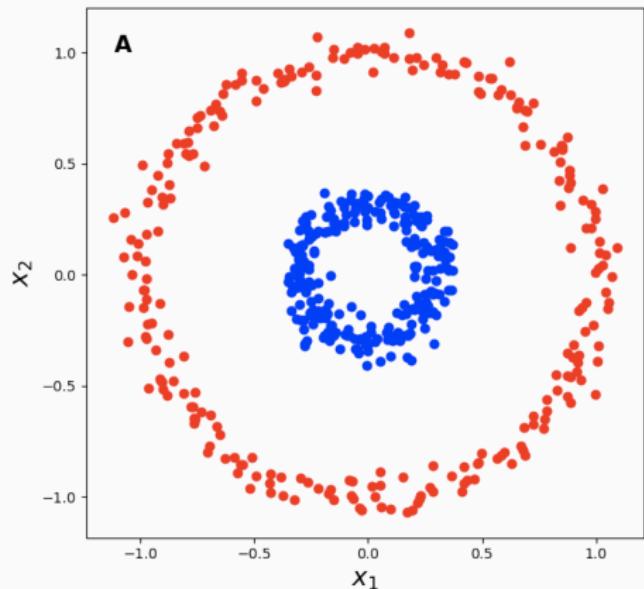
Regularized logistic losses (almost) achieve Bayes optimal results!

Beyond Linear Models

Lifting the data: feature map

Find a better representation of the data that makes it linearly separable

$$X_i \mapsto \Phi(X_i)$$



$$\Phi(x_1, x_2) = (x_1^2, x_2^2, \sqrt{2}x_1x_2)$$

src: <http://gregorygundersen.com/>

Template matching

Representer theorem: can search for

$$\hat{\theta}_n = \sum_{i=1}^n \beta_i X_i$$

The resulting prediction is hardly more than comparison with data:

$$f_{\hat{\theta}_n}(x) = \sum_{i=1}^n \beta_i X_i \cdot x$$

(cf nearest neighbor method)

⇒ can consider more general similarity functions than scalar product:

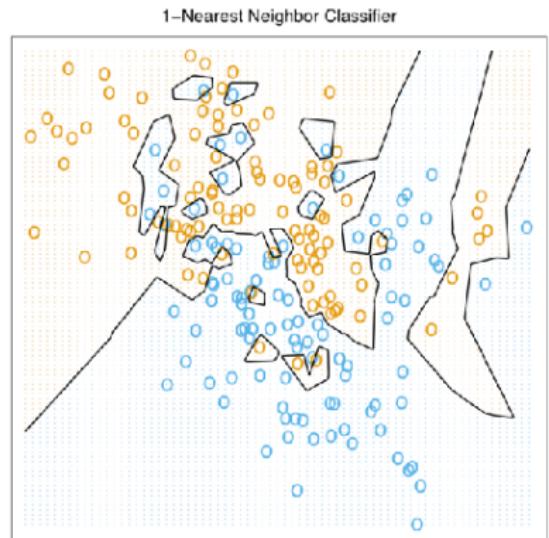
$$f_{\theta}(x) = \sum_{i=1}^n \beta_i K(X_i, x)$$

where K is a carefully chosen *kernel*

Ex: Gaussian Kernel

$$K(\mathbf{X}_i, \mathbf{X}_j) = e^{-\beta \|\mathbf{X}_i - \mathbf{X}_j\|_2^2}$$

As $\beta \rightarrow \infty$ converges to 1NN methods

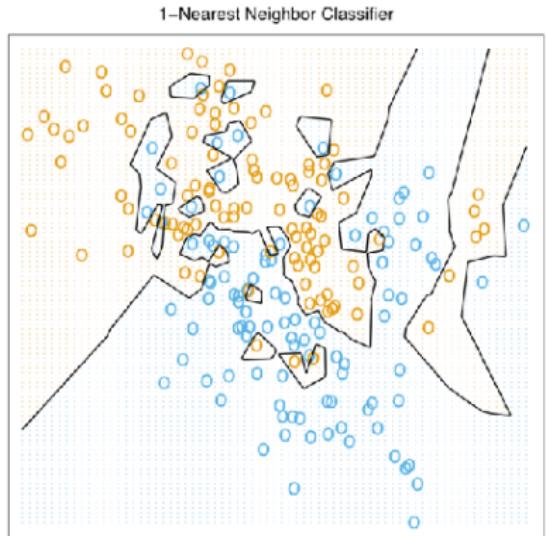
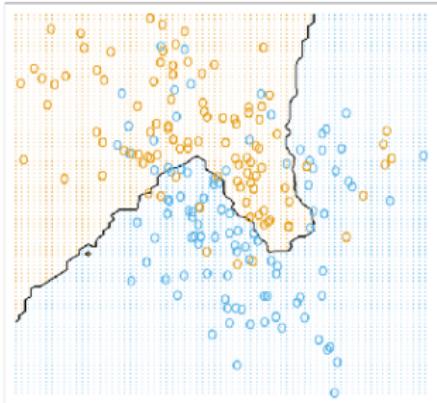


Warning: β = inverse temperature \neq the one of previous slide

Ex: Gaussian Kernel

$$K(\mathbf{X}_i, \mathbf{X}_j) = e^{-\beta \|\mathbf{X}_i - \mathbf{X}_j\|_2^2}$$

For lower values, interpolate
between neighbours



Warning: β = inverse temperature \neq the one of previous slide

Mercer's Theorem & the feature map

If $K(s,t)$ is symmetric and positive-definite, then there is an orthonormal basis $\{e_i\}$ of $L^2[a, b]$ consisting of « eigenfunctions » such that the corresponding sequence of eigenvalues $\{\lambda_i\}$ is nonnegative.

$$K(s, t) = \sum_{j=1}^{\infty} \lambda_j e_j(s) e_j(t)$$

All symmetric positive-definite Kernels can be seen as a projection
in an infinite dimensional space

Original space
(data space)
dimension d

Feature map
 $\Phi = g(X)$

Features space
(After projection)
dimension D (possibly infinite)

X_i

$$K(\mathbf{X}_i, \mathbf{X}_j) = \Phi_i \cdot \Phi_j$$

$$\Phi_i = \begin{pmatrix} \sqrt{\lambda_1} e_1(X_i) \\ \sqrt{\lambda_2} e_2(X_i) \\ \sqrt{\lambda_3} e_4(X_i) \\ \vdots \\ \sqrt{\lambda_D} e_D(X_i) \end{pmatrix}$$

Example: Gaussian Kernel, 1D

$$K(\mathbf{X}_i, \mathbf{X}_j) = e^{-\frac{1}{2\sigma^2} \|\mathbf{X}_i - \mathbf{X}_j\|_2^2}$$

$$\begin{aligned} e^{\frac{-1}{2\sigma^2} (x_i - x_j)^2} &= e^{\frac{-x_i^2 - x_j^2}{2\sigma^2}} \left(1 + \frac{2x_i x_j}{1!} + \frac{(2x_i x_j)^2}{2!} + \dots \right) \\ &= e^{\frac{-x_i^2 - x_j^2}{2\sigma^2}} \left(1 \cdot 1 + \sqrt{\frac{2}{1!}} x_i \cdot \sqrt{\frac{2}{1!}} x_j + \sqrt{\frac{(2)^2}{2!}} (x_i)^2 \cdot \sqrt{\frac{(2)^2}{2!}} (x_j)^2 + \dots \right) \\ &= \phi(x_i)^T \phi(x_j) \end{aligned} \tag{1.25}$$

$$\text{where, } \phi(x) = e^{\frac{-x^2}{2\sigma^2}} \left(1, \sqrt{\frac{2}{1!}} x, \sqrt{\frac{2^2}{2!}} x^2, \dots \right)$$

Infinite dimensional feature (polynomial) map!

Kernel methods

$$\mathcal{R} = \frac{1}{n} \sum_{i=1}^n \mathcal{L}(y_i, f_\beta(\mathbf{X}_i))$$

$$f_\beta(\mathbf{X}) = \sum_{j=1}^n \beta_j K(\mathbf{X}_j, \mathbf{X}) \quad \beta \in \mathbb{R}^n$$

Gradient descent

$$\beta^t = \beta^{t-1} - \eta \nabla_\beta \mathcal{R}$$

Gradient flow

$$\dot{\beta}^t = - \nabla_\beta \mathcal{R}$$

$$\mathcal{R} = \frac{1}{n} \sum_{i=1}^n \mathcal{L}(y_i, f_\theta(\Phi_i))$$

Feature map $\Phi = g(X)$

$$f_\theta(\Phi) = \theta \cdot \Phi \quad \theta \in \mathbb{R}^{D=\infty}$$

Gradient descent

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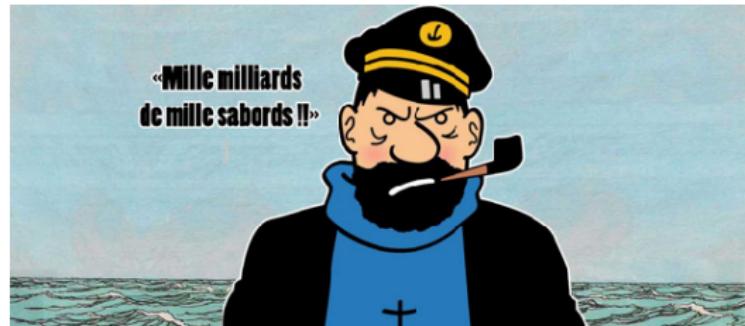
Gradient flow

$$\dot{\theta}^t = - \nabla_\theta \mathcal{R}$$

$$K(X_i, X_j) = \Phi_i \cdot \Phi_j$$

$$\mathbf{K} = \begin{pmatrix} K(X^1, X^1) & K(X^1, X^2) & \dots & K(X^1, X^N) \\ K(X^2, X^1) & K(X^2, X^2) & \dots & K(X^2, X^N) \\ \dots & \dots & \dots & \dots \\ K(X^N, X^1) & K(X^N, X^2) & \dots & K(X^N, X^N) \end{pmatrix}$$

Say you have one million examples....



Kernel methods

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Kernel methods

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Gradient flow

$$\dot{\theta}^t = - \nabla_\theta \mathcal{R}$$

Feature map $\Phi = g(X)$

$$\theta \in \mathbb{R}^{D=\infty}$$

Idea 1: truncate the expansion
of the feature map
(e.g. polynomial features)

Idea 2: approximate the
feature map by sampling

Random Fourier Features [Recht-Rahimi '07]

Take $F_1, \dots, F_D \stackrel{iid}{\sim} Q$ Fourier coefficients in \mathbb{R}^d and choose feature map

$$\Phi(x) = \frac{1}{\sqrt{D}} \begin{pmatrix} e^{i F_1 \cdot x} \\ \vdots \\ e^{i F_D \cdot x} \end{pmatrix}$$

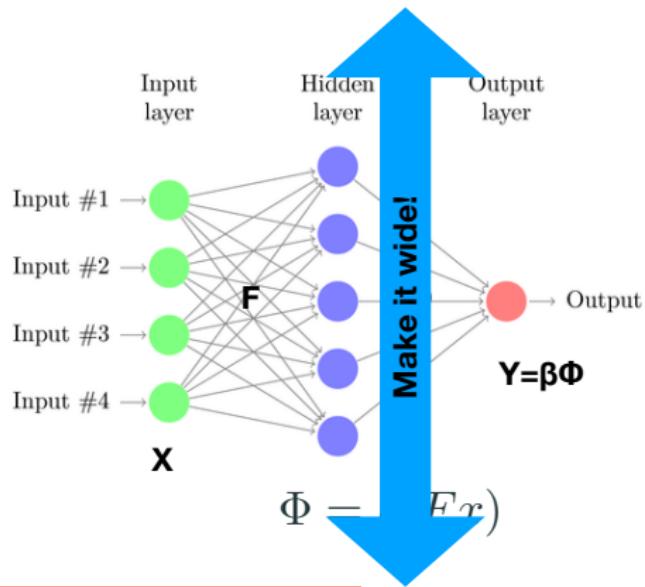
Then

$$K(X_j, X_k) = \Phi(X_j) \cdot \Phi(X_k) = \frac{1}{D} \sum_{\ell=1}^D e^{i F_\ell \cdot (X_j - X_k)} \xrightarrow{D \rightarrow \infty} \int e^{i f \cdot (X_j - X_k)} dQ(f)$$

→ if dQ/df = Fourier transform of κ , then $K(X_j, X_k) \approx \kappa(X_j - X_k)$

Kernel	$\kappa(\Delta)$	$dQ(f)$
Gaussian	$e^{-\ \Delta\ ^2/2}$	$(2\pi)^{-d/2} e^{-\ f\ ^2/2}$
Laplacian	$e^{-\ \Delta\ _1}$	$\prod_k \frac{1}{\pi(1+f_k^2)}$
Cauchy	$\prod_k \frac{2}{1+\Delta_k^2}$	$e^{-\ f\ _1}$

Equivalent representation: A WIIIIIIIDE random 2-layer neural network



Fix the « weights » in the first layer randomly...
... and to learn only the weights in the second layer

Infinitely wide neural net with random weights converges to kernel methods
(Neal '96, Williams 98, Recht-Rahimi '07)

Deep connection with genuine neural networks in the “Lazy regime”

[Jacot, Gabriel, Hongler '18; Chizat, Bach '19; Geiger et al. '19] by Florent Krzakala

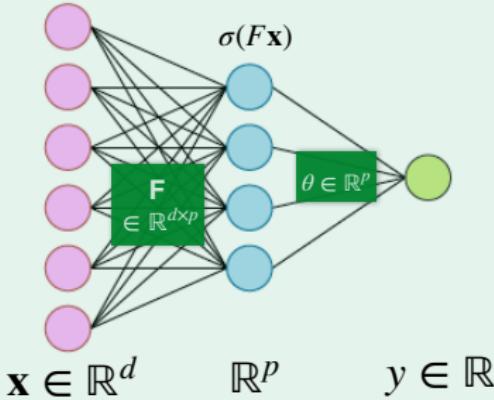
Random feature model...

Dataset:

- n vector $\mathbf{x}_i \in \mathbb{R}^d$, drawn randomly from $\mathcal{N}(0, \mathbf{1}_d)$
- n labels y_i given by a function $y_i^0 = f^0(\mathbf{x} \cdot \theta^*)$

Architecture:

Two-layers neural network with fixed first layer \mathbf{F}



Cost function:

$$\mathcal{L} = \frac{1}{n} \sum_{i=1}^n \ell(y_i, y_i^0) + \lambda \|\theta\|_2^2$$

$\ell(\cdot) =$

- Logistic loss
- Hinge loss
- Square loss
- ...



What is the training error & the generalisation error in the high dimensional limit ($d, p, n \rightarrow \infty$)?

... and its solution

[Loureiro, Gerace, FK, Mézard, Zdeborova, '20]

Definitions:

Consider the unique fixed point of the following system of equations

$$\begin{cases} \hat{V}_s = \frac{\alpha}{\gamma} \kappa_1^2 \mathbb{E}_{\xi, y} \left[\mathcal{Z}(y, \omega_0) \frac{\partial_\omega \eta(y, \omega_1)}{V} \right], \\ \hat{q}_s = \frac{\alpha}{\gamma} \kappa_1^2 \mathbb{E}_{\xi, y} \left[\mathcal{Z}(y, \omega_0) \frac{(\eta(y, \omega_1) - \omega_1)^2}{V^2} \right], \\ \hat{m}_s = \frac{\alpha}{\gamma} \kappa_1 \mathbb{E}_{\xi, y} \left[\partial_\omega \mathcal{Z}(y, \omega_0) \frac{(\eta(y, \omega_1) - \omega_1)}{V} \right], \\ \hat{V}_w = \alpha \kappa_\star^2 \mathbb{E}_{\xi, y} \left[\mathcal{Z}(y, \omega_0) \frac{\partial_\omega \eta(y, \omega_1)}{V} \right], \\ \hat{q}_w = \alpha \kappa_\star^2 \mathbb{E}_{\xi, y} \left[\mathcal{Z}(y, \omega_0) \frac{(\eta(y, \omega_1) - \omega_1)^2}{V^2} \right], \end{cases} \quad \begin{cases} V_s = \frac{1}{\hat{V}_s} \left(1 - z g_\mu(-z) \right), \\ q_s = \frac{\hat{m}_s^2 + \hat{q}_s}{\hat{V}_s} \left[1 - 2zg_\mu(-z) + z^2 g'_\mu(-z) \right] \\ \quad - \frac{\hat{q}_w}{(\lambda + \hat{V}_w)\hat{V}_s} \left[-zg_\mu(-z) + z^2 g'_\mu(-z) \right], \\ m_s = \frac{\hat{m}_s}{\hat{V}_s} \left(1 - z g_\mu(-z) \right), \\ V_w = \frac{\gamma}{\lambda + \hat{V}_w} \left[\frac{1}{\gamma} - 1 + zg_\mu(-z) \right], \\ q_w = \gamma \frac{\hat{q}_w}{(\lambda + \hat{V}_w)^2} \left[\frac{1}{\gamma} - 1 + z^2 g'_\mu(-z) \right], \\ \quad + \frac{\hat{m}_s^2 + \hat{q}_s}{(\lambda + \hat{V}_w)\hat{V}_s} \left[-zg_\mu(-z) + z^2 g'_\mu(-z) \right], \end{cases} \quad \begin{cases} \eta(y, \omega) = \operatorname{argmin}_{x \in \mathbb{R}} \left[\frac{(x - \omega)^2}{2V} + \ell(y, x) \right] \\ \mathcal{Z}(y, \omega) = \int \frac{dx}{\sqrt{2\pi V^0}} e^{-\frac{1}{2V^0}(x - \omega)^2} \delta(y - f^0(x)) \end{cases}$$

where $V = \kappa_1^2 V_s + \kappa_\star^2 V_w$, $V^0 = \rho - \frac{M^2}{Q}$, $Q = \kappa_1^2 q_s + \kappa_\star^2 q_w$, $M = \kappa_1 m_s$, $\omega_0 = M/\sqrt{Q\xi}$, $\omega_1 = \sqrt{Q}\xi$ and g_μ is the Stieltjes transform of FF^T

$$\kappa_0 = \mathbb{E}[\sigma(z)], \kappa_1 \equiv \mathbb{E}[z\sigma(z)], \kappa_\star \equiv \mathbb{E}[\sigma(z)^2] - \kappa_0^2 - \kappa_1^2 \text{ and } \vec{z}^\mu \sim \mathcal{N}(\vec{0}, \mathbf{I}_p)$$

Then in the high-dimensional limit:

$$\epsilon_{gen} = \mathbb{E}_{\lambda, \nu} \left[(f^0(\nu) - \hat{f}(\lambda))^2 \right]$$

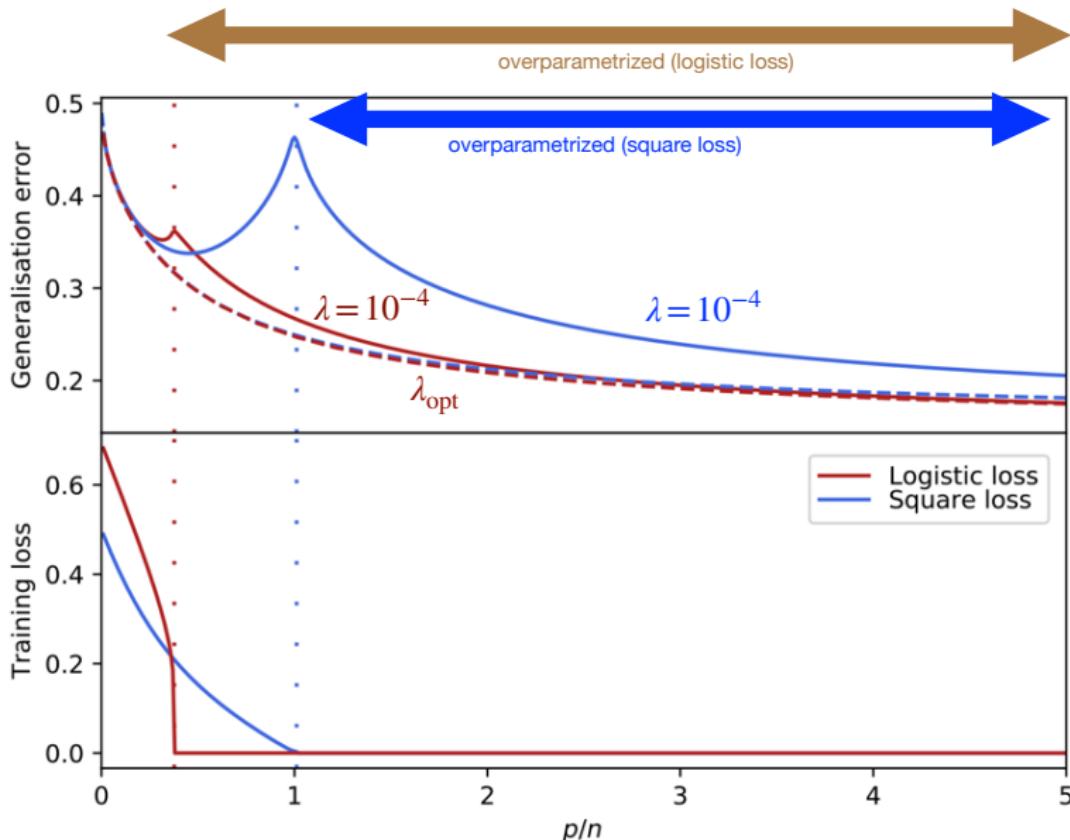
$$\text{with } (\nu, \lambda) \sim \mathcal{N} \left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \rho & M^\star \\ M^\star & Q^\star \end{pmatrix} \right)$$

$$\mathcal{L}_{\text{training}} = \frac{\lambda}{2\alpha} q_w^\star + \mathbb{E}_{\xi, y} \left[\mathcal{Z}(y, \omega_0^\star) \ell(y, \eta(y, \omega_1^\star)) \right]$$

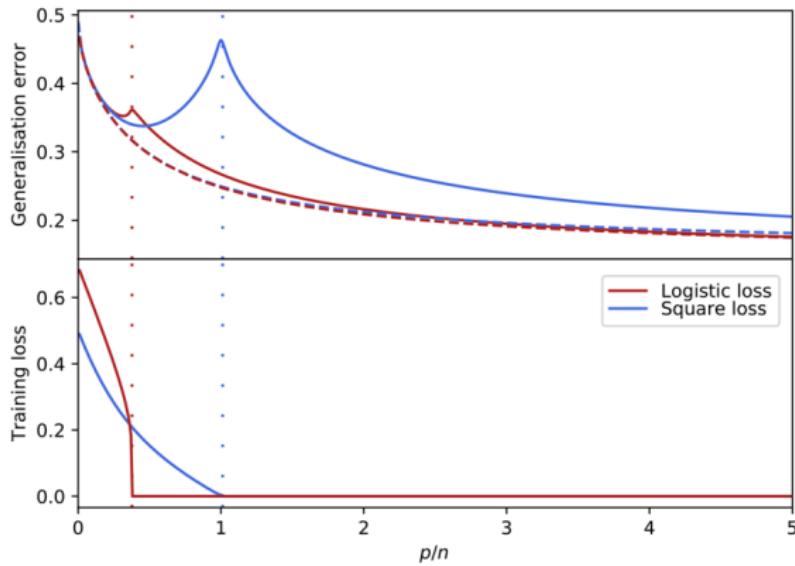
$$\text{with } \omega_0^\star = M^\star / \sqrt{Q^\star \xi}, \omega_1^\star = \sqrt{Q^\star \xi}$$

Agrees with [Louart , Liao , Couillet'18 & Mei-Montanari '19] who solved a particular case using random matrix theory: linear function f^0 , $\ell(x, y) = \|x - y\|_2^2$ & Gaussian band weights F

A classification task



A classification task



Implicit regularisation of gradient descent

[Rosset, Zhy, Hastie, '04]

[Neyshabur, Tomyoka, Srebro, '15]

As $\lambda \rightarrow 0$, in the overparametrized regime,
Logistic converges to max-margin, ℓ_2 converges to least norm

slide by Florent Krzakala