High-Dimensional Asymptotics of Prediction: Ridge Regression*

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1 Introduction

- a new way to analyze and understand ridge regression in high dimensions
  - focus on out-of-sample prediction
  - in a linear regression model with dense random effects
- main result: formula for the asymptotic predictive risk
- consequences:
  - an exact inverse relationship between prediction error and estimation error (perhaps surprising?)
  - a thorough study of the "regimes of learning problem", similar in spirit to Liang and Srebro (2010) (answer some of their conjectures)
- main tool: asymptotic random matrix theory

2 Basics and Notation

- The *spectral distribution* of a symmetric matrix A is the cumulative distribution function of its eigenvalues: $F_A(x) = p^{-1} \sum_{i=1}^{p} \mathrm{I}(\lambda_i(A) \leq x)$.
- High-dimensional asymptotics
  - $n, p \to \infty$ where $p/n \to \gamma$ for some aspect ratio $0 < \gamma < \infty$
  - $n \times p$ data matrix $X = Z\Sigma^{1/2}$ for some $n \times p$ matrix Z with i.i.d. mean 0, variance 1 entries, and $p \times p$ covariance matrix Σ
  - the spectral distribution F_Σ of Σ converges weakly to a limit H, called the population spectral distribution (PSD).
- Examples:
  1. $\Sigma = I_p$ for all p.
  2. autoregressive AR(1) model with $\Sigma_{ij} = \rho^{|i-j|}$, or more generally ARMA time series models.
- the sample covariance matrix is $\widehat{\Sigma} = n^{-1} X^\top X$

The following is a basic result in the field of random matrix theory.

Theorem (Marchenko and Pastur (1967); Silverstein (1995))**.** *The spectral distribution $F_{\widehat{\Sigma}}$ of the sample covariance matrix $\widehat{\Sigma}$ converges weakly, with probability 1, to a limiting distribution F—the empirical spectral distribution (ESD)—supported on* $[0, \infty)$.

*based on part of a paper with Stefan Wager, available at http://arxiv.org/abs/1507.03003

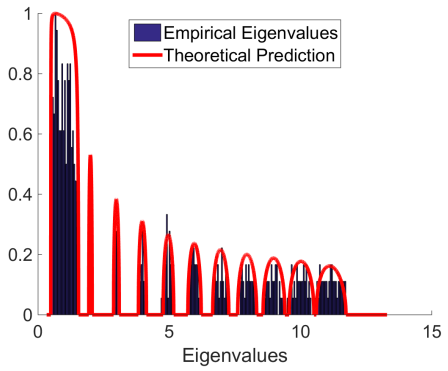

Figure 1: The density of the limit ESD, when the PSD is an equal mixture of two components: (1) a mixture of ten point masses at 2,3, . . . , 11, with weights forming an arithmetic progression with step $r = 0.005$ as follows: $0.0275, 0.0325, \ldots, 0.0725$; and (2) a uniform distribution - or a 'boxcar' - on $[0.5, 1.5]$, with mixture weight $1/2$. $\gamma = 0.01$.

Example: Figure 1. The PSD is a mixture of point masses, while the ESD is a mixture of "bumps" centered around those point masses. Note that the ESD is different from the PSD – it is more spead out. This implies for instance that plug-in estimators of functionals of the parameter Σ or H will be in general be biased.

Closed form expressions exist only for $H = \delta_1$, in which case the ESD has the density:

$$f(x;\gamma) = \frac{\sqrt{(\gamma_+ - x)(x - \gamma_-)}}{2\pi\gamma x} I(x \in [\gamma_-, \gamma_+]), \tag{1}$$

More generally, the limiting empirical spectral distribution is determined uniquely by a fixed point equation for its *Stieltjes transform*, which is defined for any distribution G supported on $[0, \infty)$ as

$$m_G(z) = \int_{l=0}^{\infty} \frac{dG(l)}{l - z}, \quad z \in \mathbb{C} \setminus \mathbb{R}^+.$$

The Stieltjes transform of a probability distribution G contains all information about G. If G has a density g, the inversion formula for Stieltjes transforms is

$$g(x) = \frac{1}{\pi} \lim_{\varepsilon \to 0^+} \text{Imag}\{m_G(x + i\varepsilon)\}. \tag{2}$$

Note that a Stieltjes transform is analytic in the upper half $\mathbb{C}^+$ of the complex plane. With these definitions, an equivalent statement to the Marchenko-Pastur theorem is the following: The Stieltjes transform of the spectral measure of $\widehat{\Sigma}$ satisfies

$$m_{\widehat{\Sigma}}(z) = \frac{1}{p} \text{tr}\left(\left(\widehat{\Sigma} - z\, I_{p\times p}\right)^{-1}\right) \text{ converges to } m(z) \tag{3}$$

with probability one, for any $z \in \mathbb{C} \setminus \mathbb{R}^+$; here, we wrote $m(z) := m_F(z)$. In addition to $m(z)$, we also define the companion Stieltjes transform $v(z)$, which is the Stieltjes transform of the limiting spectral distribution of the matrix $\underline{\widehat{\Sigma}} = n^{-1} X X^\top$. This is related to $m(z)$ by

$$\gamma\,(m(z) + 1/z) = v(z) + 1/z \quad \text{for all} \quad z \in \mathbb{C} \setminus \mathbb{R}^+. \tag{4}$$

Silverstein and Choi (1995) show that $v(z)$ is the unique solution with positive imaginary part of the Silverstein equation:

$$-\frac{1}{v(z)} = z - \gamma \int \frac{t\, dH(t)}{1 + tv(z)}, \; z \in \mathbb{C}^+. \tag{5}$$

This equation can be solved by a fixed-point algorithm to compute $v(z)$ for all $z \in \mathbb{C}^+$.

Our goal will be to express the quantities of interest (estimation error, prediction error of ridge rergesson etc), in terms of the "irreducible quantities" m, v; and then interpret the results for insight.

For this, it will be useful to have expressions for more complicated trace functionals involving both Σ, and $\widehat{\Sigma}$, such as the following formula from (Ledoit and Péché, 2011):

$$\frac{1}{p}\operatorname{tr}\left(\Sigma\left(\widehat{\Sigma}+\lambda I_{p\times p}\right)^{-1}\right)\to_{a.s.}\frac{1}{\gamma}\left(\frac{1}{\lambda\, v(-\lambda)}-1\right)\quad\text{as } n,\, p\to\infty; \tag{6}$$

3 Main Result

Setup:

- Observation model: n independent observations $y_i = x_i \cdot w + \varepsilon_i$ from a p-dimensional linear model. ε_i are independent random variables with mean 0 and variance 1.
- Estimate w by ridge regression: $\hat{w}_\lambda = (X^\top X + \lambda\, n\, I_{p\times p})^{-1} X^\top Y$.
- Expected predictive risk $r_\lambda(X) = \mathbb{E}\left[(y-\hat{y}_\lambda)^2 \,\middle|\, X\right]$, where $(x,\, y)$ is a new test example and $\hat{y}_\lambda = \hat{w}_\lambda \cdot x$.

Under these conditions, with Gaussian w, ε, $\lambda_p^* = \gamma_p \alpha^2$ is the Bayes-optimal regularization parameter, where $\gamma_p = p/n$.

Assumptions:

- Random weights: w is random with $\mathbb{E}[w] = 0$, $\operatorname{Var}[w] = p^{-1}\alpha^2 I_{p\times p}$;
  - note: $\alpha^2 = \mathbb{E}[\|w\|_2^2]$ is the expected signal strength.
- High-dimensional asymptotics: as above + some additional moment conditions.

By elementary calculations, the finite sample risk $r_{\lambda_p^*}(X)$ has a simple expression

$$r_{\lambda_p^*}(X) = 1 + \frac{\gamma_p}{p}\operatorname{tr}\left(\Sigma\left(\widehat{\Sigma}+\frac{\gamma_p}{\alpha^2}I_{p\times p}\right)^{-1}\right).$$

Theorem 3.1. *The finite sample predictive risk converges almost surely to an asymptotic limit given by:*

$$r_{\lambda_p^*}(X)\to_{a.s.} R^*(H,\alpha^2,\gamma) := \frac{1}{\lambda^* v(-\lambda^*)}. \tag{7}$$

When $\Sigma = I_{p\times p}$, we have an explicit expression for the Stieltjes transform (e.g., Bai and Silverstein, 2010, p. 52), valid for $\lambda > 0$:

$$m_I(-\lambda;\gamma) = \frac{-(1-\gamma+\lambda)+\sqrt{(1-\gamma+\lambda)^2+4\gamma\lambda}}{2\gamma\lambda}.$$

This also leads to a closed form expression for the risk.

$$R^*(\alpha^2,\gamma) = \frac{1}{2}\left[1+\frac{\gamma-1}{\gamma}\alpha^2+\sqrt{\left(1-\frac{\gamma-1}{\gamma}\alpha^2\right)^2+4\alpha^2}\right]. \tag{8}$$

Example: To verify finite-sample accuracy, we perform a simulation with the `BinaryTree` and `Exponential` models. The results in Figure 2 show that the formulas given in Theorem 3.1 appear to be accurate, even in small sized problems.

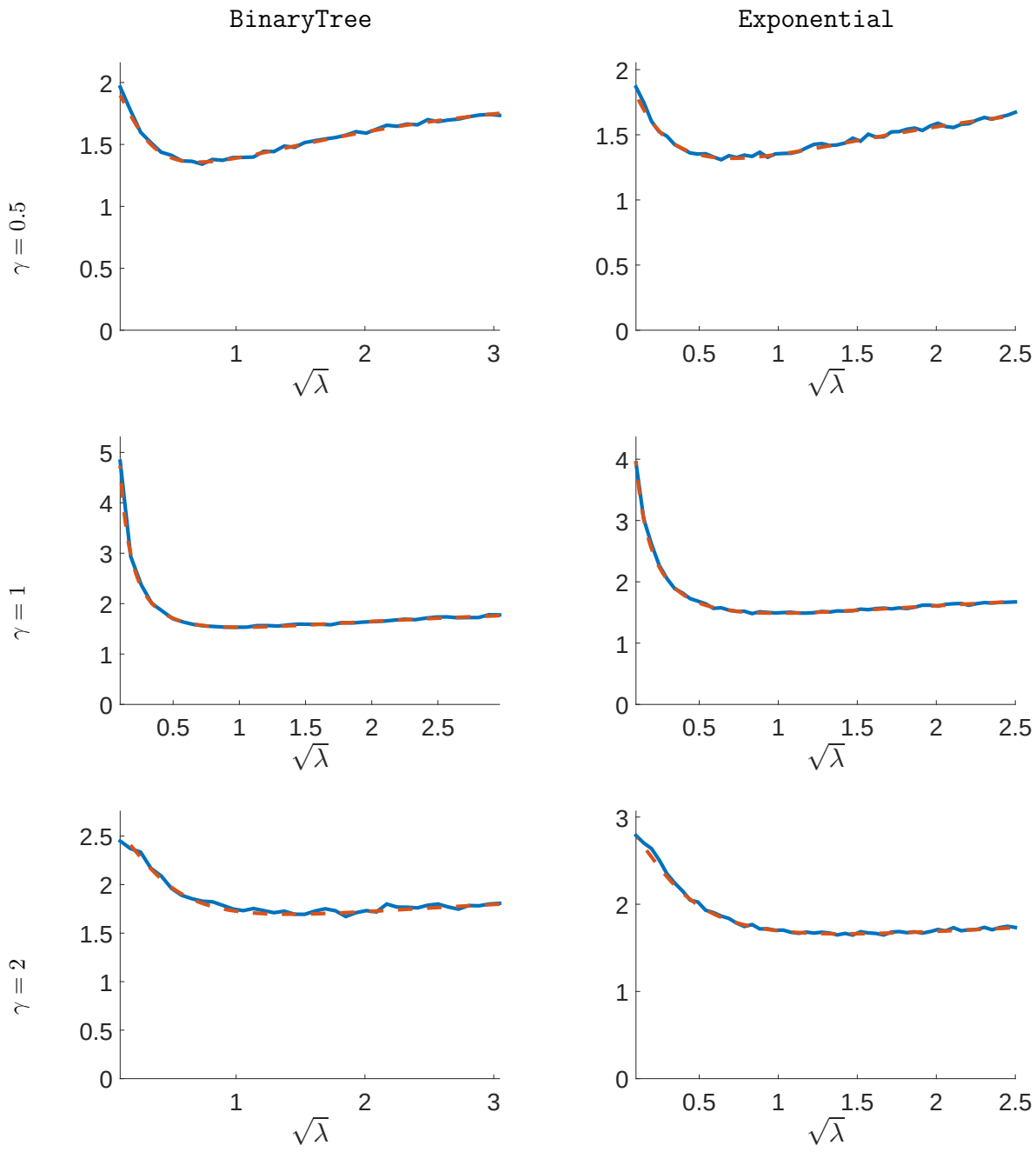

Figure 2: Prediction error of ridge regression in the `BinaryTree` and `Exponential` model. The theoretical formula (red, dashed) is overlaid with the results from simulations (blue, solid). The signals are drawn from $w \sim \mathcal{N}\left(0, p^{-1} I_{p\times p}\right)$. For `BinaryTree`, we train on $n = \gamma^{-1} p$ samples, where $p = 2^4$; for `Exponential` on $n = 20$. We take 100 instances of random training data sets, and for each we test on 500 samples. We report the average test error over all 50,000 test cases.

3.1 An Inaccuracy Principle for Ridge Regression

Our results reveal an intriguing inverse relationship between the prediction and estimation errors of ridge regression.

- mean-squared estimation error $R_{E,n}(\lambda) = \mathbb{E}\left[\|\hat{w}_\lambda - w^*\|^2\right]$
- can show
$$R_{E,n}(\lambda_p^*) = \frac{\gamma_p}{p} \operatorname{tr}\left(\left(\widehat{\Sigma} + \lambda_p^* I_{p\times p}\right)^{-1}\right) \tag{9}$$
- optimally tuned ridge regression satisfies, under the conditions of Theorem 3.1,
$$R_{E,n}(\lambda^*) \to_{a.s.} R_E := \gamma\, m\left(-\lambda^*\right) \text{ for } \lambda^* = \gamma\alpha^{-2},$$
where $m(\cdot)$ is the Stieltjes transform of the limiting empirical spectral distribution (see, e.g., Tulino and Verdú, 2004, Chapter 3). So, by (4)

Corollary 3.2. *Under the conditions of Theorem 3.1, the asymptotic predictive and estimation risks of optimally-tuned ridge regression are inversely related, by the equation*
$$1 - \frac{1}{R_P} = \gamma\left(1 - \frac{R_E}{\alpha^2}\right).$$

- Both sides are non-negative: R_P cannot fall below the intrinsic noise level $\operatorname{Var}\left[Y \,\middle|\, X\right] = 1$, while $R_E \le \limsup R_{E,n}(\lambda^*) \le \limsup R_{E,n}(0) = \alpha^2$.
- Not both prediction and estimation can be easy.
- Intuitively, when the features are highly correlated and v is correspondingly large, prediction is easy because y lies close to the "small" column space of the feature matrix X, but estimation of w is hard due to multi-collinearity. [1]

3.2 Regimes of Learning

- How does the prediction error or ridge regression depend on α^2?
- Called the "regimes of learning" problem in Liang and Srebro (2010). Conjecture:
  - for small α^2 dimension-independent Rademacher bounds
  - for large α^2 the error rate should strongly depend on γ.
- use Theorem 3.1 to examine the two limiting behaviors of the risk, for weak and strong signals.
- weak-signal limit:
  - 0th order: $\lim_{\alpha^2\to 0} R^*(H, \alpha^2, \gamma) = 1$, reflecting that for a small signal, we predict a near-zero outcome due to a large regularization.
  - 1st order: $\lim_{\alpha^2\to 0}(R^*(H, \alpha^2, \gamma) - 1)/\alpha^2 = \mathbb{E}_H T$, where $\mathbb{E}_H T$ is the large-sample limit of the normalized traces $p^{-1}\operatorname{tr}\Sigma$.
    - the difficulty of the prediction is determined to first order by the average eigenvalue, or equivalently by the average variance of the features, and does not depend on the size of the ratio $\gamma = p/n$. This is in line with the conjectures in Liang and Srebro (2010).

Strong-signal limit: depends the aspect ratio γ, and experiences a phase transition at $\gamma = 1$.

[1] A similar heuristic was given by Liang and Srebro (2010), without theoretical justification.

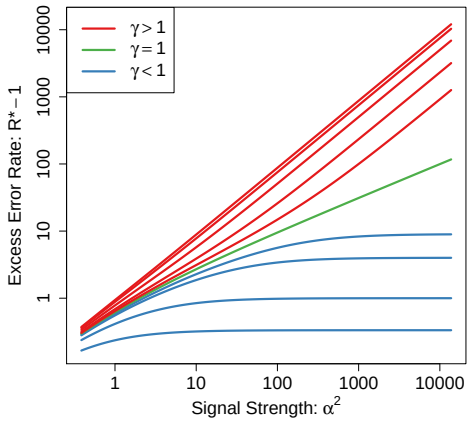

Figure 3: Phase transition for predictive risk of ridge regression with identity covariance $\Sigma = I$. Error rates are plotted for $\gamma = 0.25$, 0.5, 0.8, 0.9, 1, 1.1, 1.3, 2, 4, and 8.

- When $\gamma < 1$, the predictive risk converges to

$$\lim_{\alpha^2 \to \infty} R^*(H, \alpha^2, \gamma) = \frac{1}{1-\gamma} \tag{10}$$

  regardless of Σ. This quantity is known to be the n, $p \to \infty$, $p/n \to \gamma$ limit of the risk of ordinary least squares (OLS). Thus when $p < n$ and we have a very strong signal, ridge regression cannot outperform OLS, although of course it can do much better with a small α.

- When $\gamma > 1$, the risk $R^*(H, \alpha^2, \gamma)$ can grow unboundedly large with α. Moreover, we can verify that

$$\lim_{\alpha^2 \to \infty} \alpha^{-2} R^*(H, \alpha^2, \gamma) = \frac{1}{\gamma\, v(0)} \geq 0. \tag{11}$$

  Thus, the limiting error rate depends on the covariance matrix through $v(0)$. In general there is no closed-form expression for $v(0)$, which is instead characterized as the unique $c > 0$ for which

$$\frac{1}{\gamma} = \int_{t=0}^{\infty} \frac{tc}{1+tc}\, dH(t).$$

  In the special case $\Sigma = I$, however, the limiting expression simplifies to $1/(\gamma v(0)) = (\gamma - 1)/\gamma$. In other words, when $p > n$, optimally tuned ridge regression can capture a constant fraction of the signal, and its test-set fraction of explained variance tends to γ^{-1}.

- Finally, in the threshold case $\gamma = 1$, the risk $R^*(H, \alpha^2, \gamma)$ scales with α:

$$\lim_{\alpha^2 \to \infty} \alpha^{-1} R^*(H, \alpha^2, \gamma) = \frac{1}{\sqrt{\mathbb{E}_H\left[T^{-1}\right]}}, \tag{12}$$

  where $\mathbb{E}_H\left[T^{-1}\right]$ is the large-sample limit of $p^{-1} \operatorname{tr}\left(\Sigma^{-1}\right)$. Thus, the absolute risk R^* diverges to infinity, but the normalized error $\alpha^{-2} R^*(H, \alpha^2, \gamma)$ goes to 0. This appears to be a rather unusual risk profile.

- In summary, we find that for general covariance Σ, the strong-signal risk $R^*(\alpha^2, \gamma)$ scales as $\Theta(1)$ if $\gamma < 1$, as $\Theta(\alpha)$ if $\gamma = 1$, and as $\Theta(\alpha^2)$ if $\gamma > 1$. See Figure 3.

This leads a complete and exact answer the regimes of learning question posed by Liang and Srebro (2010) in the case of ridge regression. The results (11) and (12) not only show that the scalings found by Liang and Srebro (2010) with $\Sigma = I$ hold for arbitrary Σ, but make explicit how the slopes depend on the limiting population spectral distribution.

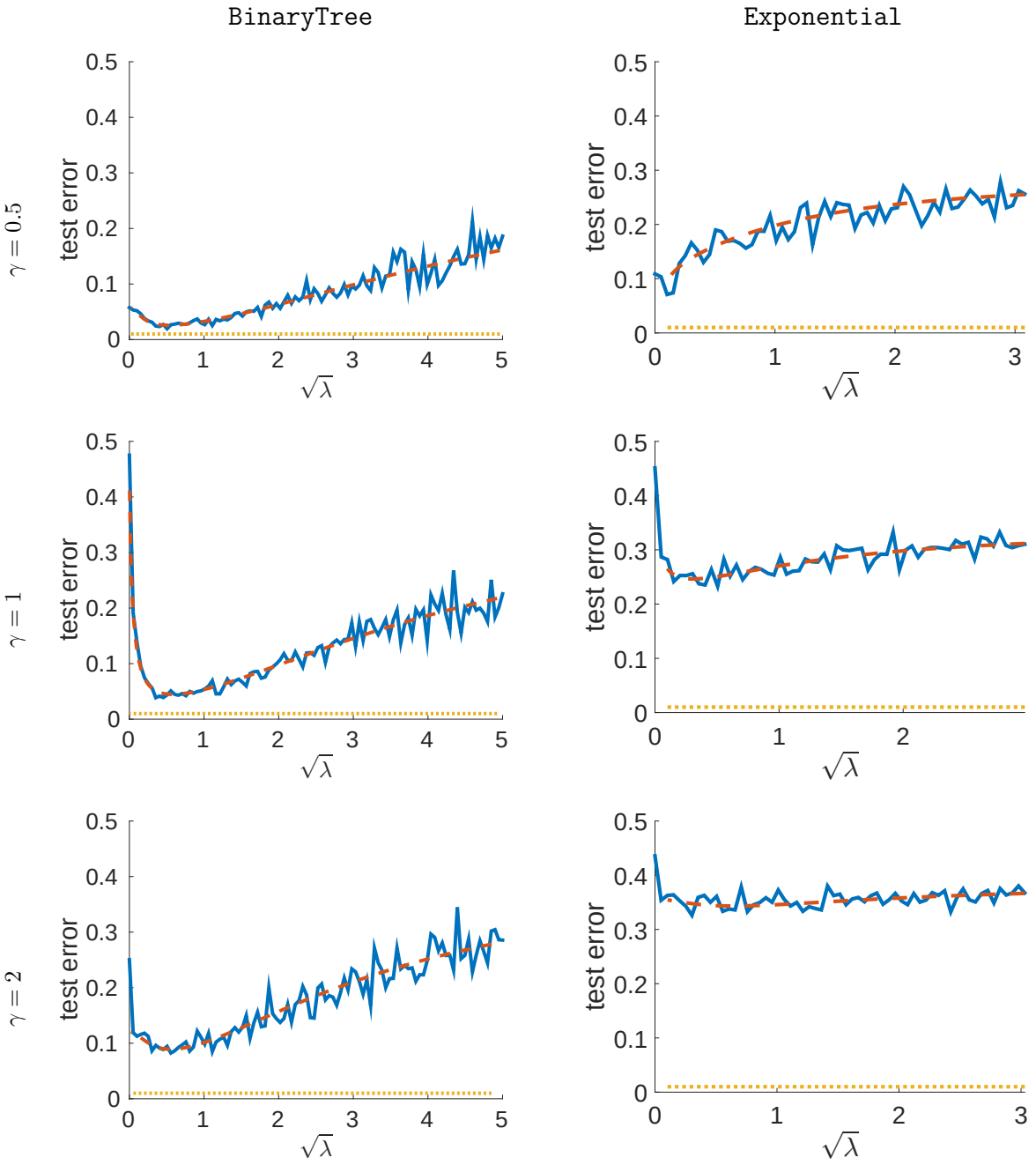

Figure 4: Classification error of RDA in the `BinaryTree` and `Exponential` models. The theoretical formula (red, dashed) is overlaid with the results from simulations (blue, solid); we also display the oracle error (yellow, dotted). The class means are drawn from $\mu_{\pm 1} \sim \mathcal{N}\left(0,\, \alpha^2\, p^{-1} I_{p\times p}\right)$, where α is calibrated such that the oracle classifier always has an error rate of 1%. For `BinaryTree`, we train on $n = \gamma^{-1} p$ samples, where $p = 1024$; for `Exponential`, we use $n = 500$ samples. We test the trained model on 10,000 new samples, and report the average classification error. Our asymptotically-motivated theoretical formulas appear to be accurate here, even though we only have a moderate problem size. The parameter λ, defined in Section **??**, quantifies the strength of the regularization.

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