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Better-Than-Chance Classification for Signal Detection– Supplementary

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1. Large Sample

The results, reported in Figure 1, are qualitatively similar to the high-dim–small-sample of Figure **??**.

2. Departure From Sphericity

3. Departure From Shift Alternatives

3.1 *Logistic Regression*

3.2 *Mixture Class*

Golland and Fischl [2003] and Golland et al. [2005] study accuracy-tests using simulation, neuroimaging data, genetic data, and analytically. The finite Vapnik–Chervonenkis dimension requirement [Golland et al., 2005, Sec 4.3] implies a the problem is low dimensional and prevents the permutation p-value from (asymptotically) concentrating near 1. They find that the power increases with the size of the test set. This is seen in Fig.4 of Golland et al. [2005], where the size of the test-set, K, governs the discretization. We attribute this to the reduced discretization of the accuracy statistic.

When discussing the power of the resubstitution accuracy, Golland et al. [2005] simulate power by sampling from a Gaussian mixture family of models, and not from a location family as our

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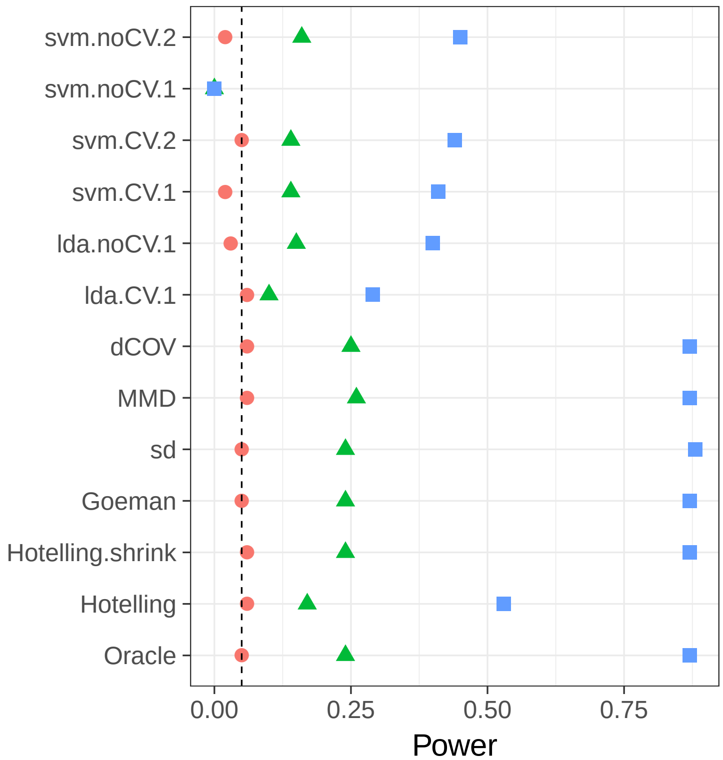


Fig. 1: The same as Figure ?? with $n = 4,000; p = 2,300$.

own simulations. Under their model (with some abuse of notation)

$$\begin{aligned} x_1 &\sim \pi\mathcal{N}\left(\mu_1, I\right) + (1-\pi)\mathcal{N}\left(\mu_2, I\right), \\ x_0 &\sim (1-\pi)\mathcal{N}\left(\mu_1, I\right) + \pi\mathcal{N}\left(\mu_2, I\right). \end{aligned}$$

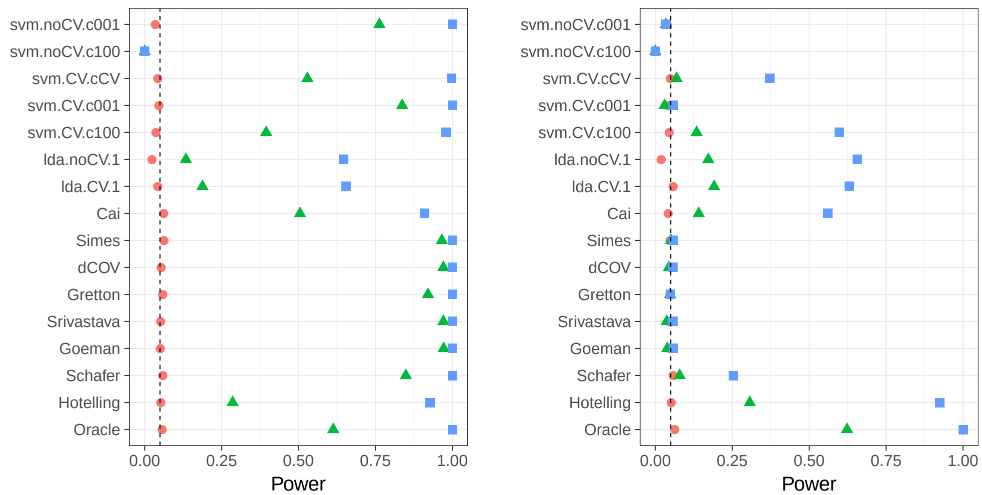
Varying π interpolates between the null distribution ($\pi = 0.5$) and a location shift model ($\pi = 0$). We now perform the same simulation as Golland et al. [2005], but in the same dimensionality of our previous simulations. We re-parameterize so that $\pi = 0$ corresponds to the null model:

$$\begin{aligned} x_1 &\sim (1/2-\pi)\mathcal{N}\left(\mu_1, I\right) + (1/2+\pi)\mathcal{N}\left(\mu_2, I\right), \\ x_0 &\sim (1/2+\pi)\mathcal{N}\left(\mu_1, I\right) + (1/2-\pi)\mathcal{N}\left(\mu_2, I\right). \end{aligned} \tag{3.1}$$

From Figure 4, we see that for the mixture class of Golland et al. [2005] locations tests are still preferred over accuracy-tests.

4. Departure from Homoskedasticity and Scalar Invariance

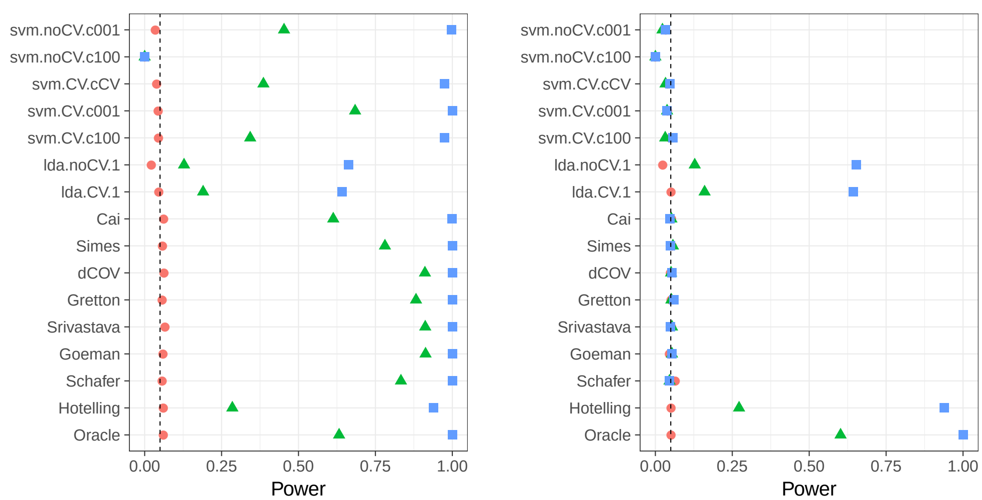
Our previous simulations assume variables have unit variance. Practitioners are already accustomed to z-score features before learning a regularized predictor (e.g. ridge regression) so this is not an unrealistic setup. Implicit z-scoring is sometime an integral part of a test statistic. This is known as *scalar invariance*. The *Srivastava* statistic, for instance, is scalar invariant. It can be



(a) Signal in direction of highest variance PC of Σ.

(b) Signal in direction of lowest lowest variance PC of Σ.

Fig. 2: Long-memory Brownian motion correlation: $\Sigma = D^{-1}RD^{-1}$ where D is diagonal with $D_{jj} = \sqrt{R_{jj}}$, and $R_{k,l} = \min\{k, l\}$.



(a) Signal in direction of highest variance PC of Σ.

(b) Signal in direction of lowest variance PC of Σ.

Fig. 3: Arbitrary Correlation. $\Sigma = D^{-1}RD^{-1}$ where D is diagonal with $D_{jj} = \sqrt{R_{jj}}$, and $R = A'A$ where A is a Gaussian $p \times p$ random matrix with independent $\mathcal{N}(0, 1)$ entries.

(roughly) thought of as the l_2 norm of the p-vector of coordinate-wise t-statistics. The *Goeman* statistic, for instance, is not scalar invariant. It can be (roughly) thought of as the l_2 norm of the p-vector of variable-wise mean differences. Under heteroskedasticity, the *Goeman* statistic will give less importance to signal in the high-variance directions than signal in the low-variance

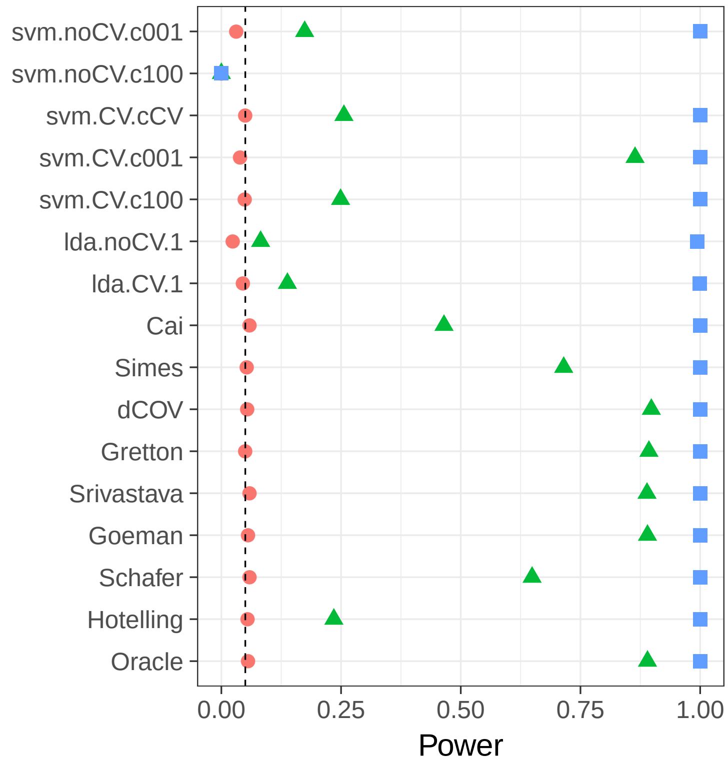


Fig. 4: **Mixture Alternatives.** $\mathbf{x}_i$ is distributed as in Eq.(3.1). μ is a p-vector with $3/\sqrt{p}$ in all coordinates. The effect, π, is color and shape coded and varies over 0 (red circle), 1/4 (green triangle) and 1/2 (blue square).

directions. *Srivastava* will give all coordinates the same importance.

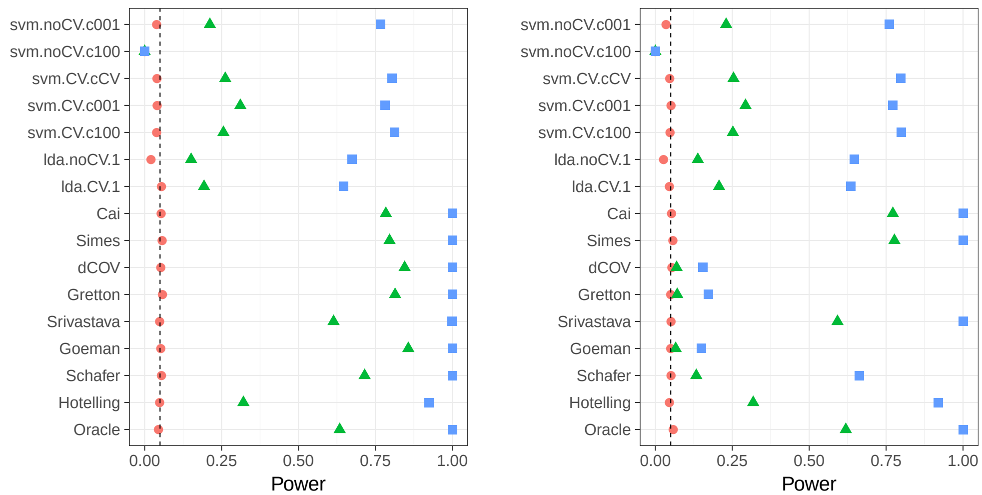
In Figure 5a we can see the difference between the scalar-invariant *Srivastava* and *Goeman* statistics. We also see that two-group tests dominate accuracy-tests also in the heteroskedastic case.

4.1 *Tie Breaking*

As already stated in the introduction, the accuracy statistic is highly discrete. Especially the resubstitution accuracy-tests. Discrete test statistics lose power by not exhausting the permissible false positive rate. A common remedy is a *randomized test*, in which the rejection of the null is decided at random in a manner that exhausts the false positive rate. Formally, denoting by $\mathcal{T}$ the observed test statistic, by $\mathcal{T}_\pi$, its value after under permutation π, and by $\mathbb{P}\{A\}$ the proportion of permutations satisfying A then the randomized version of our tests imply that if the permutation p-value, $\mathbb{P}\{\mathcal{T}_\pi \geqslant \mathcal{T}\}$, is greater than α then we reject the null with probability

$$max\left\{\frac{\alpha - \mathbb{P}\{\mathcal{T}_\pi > \mathcal{T}\}}{\mathbb{P}\{\mathcal{T}_\pi = \mathcal{T}\}}, 0\right\}.$$

Figure 6 reports the same analysis as in Figure **??**, after allowing for random tie breaking. It demonstrates that the power disadvantage of accuracy-tests, cannot be remedied by random tie



(a) μ in the high variance PC of Σ.

(b) μ in the low variance PC of Σ.

Fig. 5: Heteroskedasticity: Σ is diagonal with $\Sigma_{jj} = j$.

breaking.

5. Sparse Alternatives

In our set of simulations we discussed "dense" alternatives, in the sense that all coordinates carry signal. Dense alternatives are motivated by neuroimaging where most brain locations in a regions carry signal. In a genetic application, a "sparse" alternative may be more plausible. Figure 7 reports power when μ is sparse. As usual, two-group tests dominate accuracy-tests, only this time, the winners are not the T^2 type statistics, but rather, the tests for sparse shifts (*Cai*, *Simes*).

6. Fixed SNR

For a fair comparison between simulations, in particular between those with different Σ, we needed to fix the difficulty of the problem. We fix the Kullback–Leibler Divergence between distributions of sample means. Abusing notation, we fix $KL[\bar{x}_1, \bar{x}_0] = c^2 p$, which is the same as fixing $\|\mu\|^2_\Theta$, with the exception of the large sample (**??**) and the heavytailed analysis (**??**).

Our choice implies that the Euclidean norm of $\mu := \mathbb{E}(x_1) - \mathbb{E}(x_0)$ varies with Σ, with the sample size, and with the direction of the signal. An initial intuition may suggest that detecting signal in the low variance PCs is easier than in the high variance PCs. This is true when fixing $\|\mu\|_2$, but not when fixing $\|\mu\|_\Theta$.

For completeness, Figure 8 reports the power analysis under $AR(1)$ correlations, but with $\|\mu\|_2$ fixed. We compare the power of a shift in the direction of some high variance PC (Figure 8a), versus a shift in the direction of a low variance PC (Figure 8b). The intuition that it is easier to detect signal in the low variance directions is confirmed.

Other authors have also observed the need for fixing the SNR for a fair comparison between tests. In Ramdas et al. [2015], authors prefer to use sparse alternatives. With sparse alternatives,

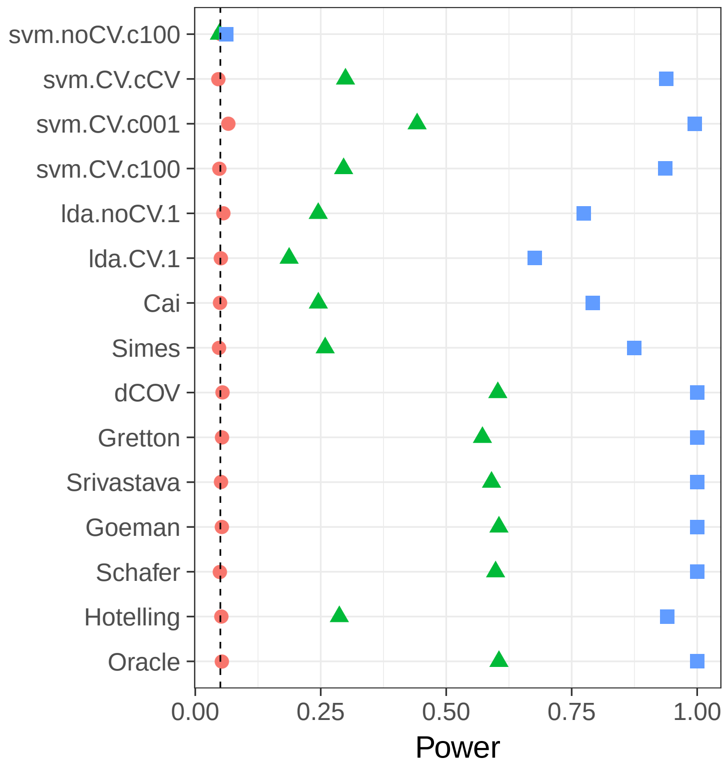


Fig. 6: The same as Figure **??**, with random tie breaking.

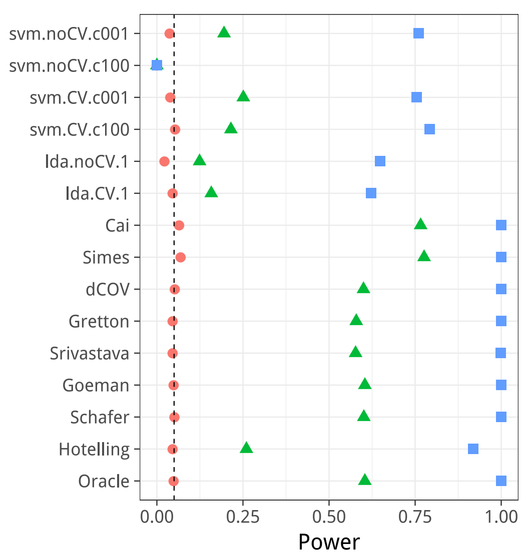
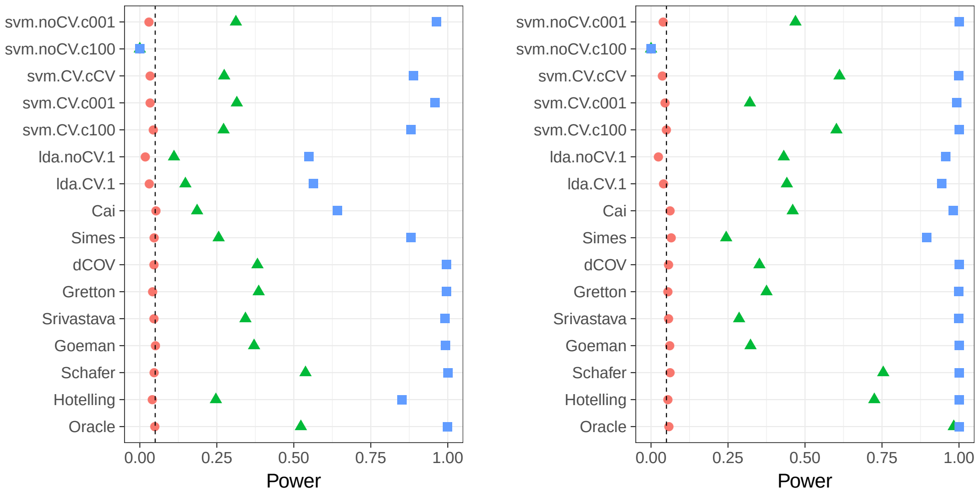


Fig. 7: Sparse μ.



(a) μ in PC7 of Σ. **(b)** μ in PC15 of Σ.

Fig. 8: Short memory, AR(1) correlation. $\|\mu\|_2$ fixed.

the difficulty of the problem is governed by the sparsity of the signal and not only the dimension of the data. In Chen et al. [2010], authors fix $\|\mu\|_2^2/\|\Sigma\|_{Frob}^2$ where $\|\Sigma\|_{Frob}^2 = \mathrm{Tr}(\Sigma'\Sigma)$ is the Frobenius matrix norm. Clearly, $\|\mu\|_2^2/\|\Sigma\|_{Frob}^2$ is invariant to the direction of the signal with respect to the noise. For this reason, we prefer fixing $\|\mu\|_\Theta$.

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